

# Combinatorial and Algebraic Properties of Nonnegative Matrices

Thesis by  
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(and whoever they might dedicate it to,

ad infinitum)

## ABSTRACT

We study the combinatorial and algebraic properties of Nonnegative Matrices. Our results are divided into three different categories.

1. We show the first quantitative generalization of the 100 year-old Perron-Frobenius theorem, a fundamental theorem which has been used within diverse areas of mathematics. The Perron-Frobenius theorem shows that any irreducible nonnegative matrix  $R$  will have a largest positive eigenvalue  $r$ , and every other eigenvalue  $\lambda$  is such that  $\operatorname{Re}\lambda < r$  and  $|\lambda| \leq r$ . We capture the notion of irreducibility through the widely studied notion of edge expansion  $\phi$  of  $R$  which intuitively measures how well-connected the underlying digraph of  $R$  is, and show a quantitative relation between the spectral gap  $\Delta = 1 - \operatorname{Re}\lambda/r$  (where  $\lambda \neq r$  has the largest real part) of  $R$  to the edge expansion  $\phi$  as follows.

$$\frac{1}{15} \cdot \frac{\Delta(R)}{n} \leq \phi(R) \leq \sqrt{2 \cdot \Delta(R)}.$$

This also provides a more general result than the Cheeger-Buser inequalities since it applies to any nonnegative matrix.

2. We study constructions of specific nonsymmetric matrices (or nonreversible Markov Chains) that have small edge expansion but large spectral gap, taking us in a direction more novel and unexplored than studying symmetric matrices with constant edge expansion that have been extensively studied. We first analyze some known but less studied Markov Chains, and then provide a novel construction of a nonreversible chain for which

$$\phi(R) \leq \frac{\Delta(R)}{\sqrt{n}},$$

obtaining a bound exponentially better than known bounds. We also present a candidate construction of matrices for which

$$\phi(R) \leq 2 \frac{\Delta(R)}{n},$$

which is the most beautiful contribution of this thesis. We believe these matrices have properties remarkable enough to deserve study in their own right.

3. We connect the edge expansion and spectral gap to other combinatorial properties of nonsymmetric matrices. The most well-studied property is mixing time, and we provide elementary proofs of the relation between mixing time and the edge



expansion, and also other bounds relating the mixing time of a nonreversible chain to the spectral gap and to its additive symmetrization. Further, we provide a unified view of the notion of capacity and normalized capacity, and show the monotonicity of capacity of nonreversible chains amongst other results for nonsymmetric matrices. We finally discuss and prove interesting lemmas about different notions of expansion and show the first results for tensor walks or nonnegative tensors.

## PUBLISHED CONTENT AND CONTRIBUTIONS

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*Chapter 1*

## INTRODUCTION

That the sun will not rise tomorrow is no less intelligible a proposition, and implies no more contradiction than the affirmation, that it will rise.

~ David Hume, *An Enquiry Concerning Human Understanding*

**1.1 On chance and its evolution**

A primary idea in the history of human thought is that of chance, and is further made indispensable due to the functionality accorded by its *measurability*. This measurability of chance is distinct from its *meaning* – the latter being its different interpretations, and amongst the two notable ones are the Bayesian perspective – purely for rational decision making – and the Frequentist perspective – a much stronger and less justified statement about the nature of sequences of events – and there are multiple other interpretations none of which are satisfactory or comprehensive enough to provide a rigorous and justified universal meaning of chance. From a sufficiently critical perspective, we find a certain form of conditioned non-determinism to be a more fundamental and universal concept for understanding observed events than chance. However, although deep and arguably more primary and important than everything that we will write further on, our concern in this thesis will not be the meaning of chance (and not even its measurability), but primarily its *evolution*.

To proceed further, we assume we have a possibility of  $n$  states, where  $n$  may be finite or infinite ( $\aleph_0$ ,  $\aleph_1$ , or more) such that there is an associated chance  $p$  over the collection of states. Note that the different states could correspond to states of any system or universe in general. Let the chance  $p$  evolve to  $p'$  at a different point in

time (we have an implicit notion of *distinct* events which produces an implicit notion of time or steps for us). To understand the evolution of chance more mathematically, we shall assume that  $p' = Ap$ , and the operator  $A$  which takes  $p$  to  $p'$  will be our primary object of study.

## 1.2 Markov Chains and the Perron-Frobenius theorem

It is possible to consider a large number of properties of  $A$  (and  $p$ ), but to understand the operator  $A$  in a mathematically meaningful manner, we make various simplifying assumptions about  $A$  and  $p$ . Our first assumption is that we will consider only a finite state space in this thesis, always referred to by  $n$ . We will assume that  $A$  is *independent of  $p$*  and *finite-dimensional*. Thus  $A$  could be represented as a finite collection of constants. Throughout the thesis (except the final section on tensors), we further assume that  $A$  is *linear*, and thus can be expressed as an  $n \times n$  matrix. At this point, the study becomes restricted to general linear operators, and we make the final assumption that  $A$  is *entry-wise nonnegative*, to say something stronger about  $A$  than general linear operators.

Such an  $A$  is referred to as a Markov chain, first studied by Andrey Markov in 1906, motivated by a disagreement with Pavel Nekrasov who had claimed that independence was necessary for the weak law of large numbers to hold [Mar06; Sen96]. Markov chains have an illustrious history and have been thoroughly studied over the past 100 years, and have been applied to diverse areas within mathematics.

Arguably the most fundamental theorem about Markov chains is the Perron-Frobenius theorem. For simplicity, assume that  $A$  is entry-wise positive. Then Perron's theorem [Per07] says that there is a positive number  $r$  which is an eigenvalue of  $A$ , all other eigenvalues  $\lambda \neq r$  of  $A$  are such that  $|\lambda| < r$ , and the corresponding left and right eigenvectors corresponding to  $r$  are entry-wise positive. This theorem was extended to all irreducible  $A$  by Frobenius [Fro12], where  $A$  is irreducible if the underlying graph with non-negative edge weights  $A_{i,j}$  is strongly-connected, i.e. there is a directed path of non-zero weights between every pair of vertices. In the irreducible case, there is one specific difference – for all other eigenvalues  $\lambda \neq r$  of  $A$ , it is the case that  $|\lambda| \leq r$  and  $\text{Re}\lambda < r$ . The resulting theorem is referred to as the Perron-Frobenius theorem.

The Perron-Frobenius theorem is fundamental to many areas within mathematics, and has been extensively used in a large number of applications (see [Mac00], [BP94] for instance), such as Markov Chains [LPW09] (traditionally, Markov chains have been

nonnegative row stochastic matrices in order to preserve the probability simplex); theory of Dynamical Systems [KH97]; a large number of results in economics such as Okishio’s theorem [Bow81], Hawkins–Simon condition [HS49], Leontief Input/Output Economic Model [Leo86], and Walrasian Stability of Competitive Markets [TA85]; Leslie population age distribution model in Demography [Les45; Les48]; DeGroot learning process in social networks [DeG74; Fre56; Har59]; PageRank and internet search engines [Pag+99; LM11]; Thurston’s classification of surface diffeomorphisms in Low-Dimensional Topology [Thu88]; Kermack–McKendrick threshold in Epidemiology [KM91; KM32; KM33]; Statistical Mechanics (specifically partition functions) [Tol79]; the Stein–Rosenberg theorem and Seidel versus the Jacobi iterative methods for solving linear equations in Matrix Iterative Analysis [Var62]; and see the comprehensive [BP94] for more.

However, already at this juncture, there is an interesting question that will be the main focus of the first part of this thesis. The Perron–Frobenius theorem provides a *qualitative* result about the irreducibility and eigenvalues of the matrix, i.e., it says that if  $A$  is irreducible, then every eigenvalue  $\lambda$  of  $A$  except  $r$  is such that  $\operatorname{Re}\lambda < r$ . Our main question is – What is the *quantitative* version of this result? Assume that  $\lambda$  is some eigenvalue except  $r$  such that it has the maximum real part. Then specifically, we can ask,

**Question 1.** Is there a quantitative relation between some measure of irreducibility of  $A$  and the gap  $r - \operatorname{Re}\lambda$ ?

This question will be our first primary consideration. In fact, this question has been completely answered in the case that  $A$  is symmetric. The result holds even for reversible  $A$  where  $A$  is reversible if  $D_u A D_v = D_v A^T D_u$ , but syntactically (and intuitively) both reversibility and symmetricity are exactly the same (see Lemma 3.0.3). To understand the symmetric version of this question, we will require some more definitions.

### 1.3 The Cheeger–Buser Inequalities

We start by defining the spectral gap and edge expansion of symmetric matrices  $A$ . For the sake of simplicity of exposition, assume that  $A$  is irreducible and the largest eigenvalue of  $A$  is 1, and the corresponding positive eigenvector is  $w$ . The first notion is that of the *spectral gap*, which is again simple to define for symmetric matrices. Since  $A$  is symmetric, let the real eigenvalues of  $A$  be  $1 \geq \lambda_2(A) \geq \dots \geq \lambda_n(A)$ .

Define the spectral gap of  $A$  as

$$\Delta(A) = 1 - \lambda_2(A).$$

The second notion is the edge expansion (or expansion) of  $A$  to quantify the notion of irreducibility of  $A$ , which is defined as

$$\phi(A) = \min_{S \subset [n]: \sum_{i \in S} w_i^2 \leq \frac{1}{2} \sum_i w_i^2} \frac{\sum_{i \in S, j \in \bar{S}} A_{i,j} w_i w_j}{\sum_{i \in S, j} A_{i,j} w_i w_j}.$$

It might appear notationally cumbersome, but it is intuitively simple to understand by looking at the equivalent definition for a symmetric doubly stochastic matrix  $A$ , in which case  $w$  is just the all ones vector. In that case, we would have

$$\phi(A) = \min_{S: |S| \leq n/2} \frac{\sum_{i \in S, j \in \bar{S}} A_{i,j}}{|S|}.$$

Thus, given a set  $S$ , the edge expansion of the set is exactly the total average weight of edges that leaves the set  $S$ , i.e. goes from  $S$  to  $\bar{S}$ . Intuitively, that is still the case for general  $A$ , except that the edges are re-weighted by the eigenvector  $w$  (the reasons for which will become clear later). This notion of edge expansion is a simple and sufficiently general quantitative notion of the irreducibility of  $A$ . Note that if  $\phi(A) = 0$ , then there is some set  $S$  such that the total mass of edges leaving the set is 0, implying that there is no way to reach a vertex in  $\bar{S}$  from the set  $S$ , implying that the matrix is disconnected and thus has 0 irreducibility or is reducible. Similarly, if  $\phi(A) \approx 0$ , it means that there are two *almost* disconnected sets in  $A$  and thus  $A$  is badly connected or has high reducibility. Similarly, if  $\phi(A) \geq c$  (where  $c$  any constant independent of the size of  $A$ ), it implies that for every set  $S$ , there is a constant fraction of the mass of edges leaving  $S$ . This means that a random walk starting at a uniformly random vertex in any set  $S$  is very likely to *leave*  $S$ , and it will not be restrained to  $S$ , implying that  $A$  is very well-connected, or has high irreducibility. Thus the edge expansion  $\phi$  captures the notion of irreducibility neatly. Further, we remark that given  $A$ , it is NP-hard to decide if the edge expansion of  $A$  is greater than some given input number [GJS74].

Given these two definitions, we are ready to answer Question 1 for symmetric matrices by relating  $\phi(A)$  with  $\Delta(A)$ . The upper bound on  $\phi(A)$  in terms of  $\Delta(A)$  was obtained by Cheeger [Che70], albeit over Riemannian manifolds, and it was translated to symmetric matrices by [AM85; SJ89; Dod84; Nil91]. The lower bound on  $\phi(A)$  in terms of  $\Delta(A)$  was obtained by Buser [Bus82] for Riemannian manifolds,



and the translation to symmetric matrices is a direct consequence of the variational characterization of eigenvalues for symmetric matrices. Together, the following bounds are referred to as the Cheeger-Buser inequalities:

$$\frac{1}{2}\Delta(A) \leq \phi(A) \leq \sqrt{2 \cdot \Delta(A)}. \quad (1.3.1)$$

The bounds are tight, the lower bound exactly holding for the hypercube, and the upper bound for the undirected cycle up to constants. Note that this helps us understand the connectivity or irreducibility of  $A$  in terms of the spectral gap, exactly as we had hoped, and provides a quantitative version of the Perron-Frobenius theorem for symmetric (or reversible) matrices. The Cheeger-Buser inequalities have been used in many different results in clustering and expander graph construction amongst others [TM06; ARV09; HLW06; ST96], and higher-order Cheeger inequalities have also been shown relatively recently [LOT14].

The general problem for any nonnegative matrix (not necessarily symmetric/reversible) remains open, and that will indeed lead to our main result.

#### 1.4 Quantitative generalization of the Perron-Frobenius theorem

We first redefine the edge expansion and spectral gap of a general irreducible nonnegative matrix  $R$ , that is not necessarily symmetric. We will use  $R$  for matrices whose left and right eigenvectors for the largest eigenvalue are not the same and  $A$  otherwise. Again for the sake of simplicity of exposition, assume that  $R$  has largest eigenvalue 1, and let the eigenvalues of  $R$  (roots of the equation  $\det(\lambda I - R) = 0$ ) be arranged so that  $1 \geq \operatorname{Re}\lambda_2(R) \geq \dots \geq \operatorname{Re}\lambda_n(A)$ . Then define the spectral gap of  $R$  as

$$\Delta(R) = 1 - \operatorname{Re}\lambda_2(R).$$

Unlike the eigenvalues which are basis-independent, the edge expansion depends on the explicit entries of the matrix (for it to be meaningful in terms of probability), and we will assume thus that  $R$  is nonnegative, and also irreducible (for purely technical reasons), and the positive (from the Perron-Frobenius theorem) left and right eigenvectors for eigenvalue 1 of  $R$  are  $u$  and  $v$  respectively. Then define the edge expansion of  $R$  as

$$\phi(R) = \min_{S \subset [n]: \sum_{i \in S} u_i v_i \leq \frac{1}{2} \sum_i u_i v_i} \frac{\sum_{i \in S, j \in \bar{S}} R_{i,j} u_i v_j}{\sum_{i \in S, j \in [n]} R_{i,j} u_i v_j}.$$

We extend these definitions to reducible  $R$ , by taking limit infimums within a ball of irreducible matrices around  $R$ , and the formal definition of  $\phi(R)$  is given in 2.0.3

and 2.0.4, and that of  $\Delta(R)$  is given in 2.0.2 and 2.0.6. With these definitions, we can present the main theorem of this thesis here.

**Theorem 1.4.1.** *Let  $R$  be an  $n \times n$  nonnegative matrix, with edge expansion  $\phi(R)$  defined as 2.0.4 and 2.0.6, and the spectral gap  $\Delta(R)$  defined as 2.0.2 and 2.0.6.*

*Then*

$$\frac{1}{15} \cdot \frac{\Delta(R)}{n} \leq \phi(R) \leq \sqrt{2 \cdot \Delta(R)}.$$

We remark that this exactly helps to answer Question 1, and provides a generalization of the Perron-Frobenius theorem. It is more general than the Cheeger-Buser inequalities since it holds for all nonnegative matrices but is not a generalization of it since the lower bound becomes weaker for the case of symmetric matrices.

We make some comments about Theorem 1.4.1. The first is that the upper bound is exactly same as in the case of symmetric matrices. The upper bound was shown for doubly stochastic matrices  $A$  by Fiedler, and it is straightforward to extend it to all  $R$ . In fact, given the Cheeger inequality, it is simple to use the inequality for showing the upper bound on  $\phi(R)$  in Theorem 1.4.1. However, unlike the symmetric case, obtaining a lower bound on  $\phi(R)$  or the equivalent of the Buser inequality is much more difficult. The primary source of the difficulty is that there is no Courant-Fisher variational characterization of eigenvalues for nonsymmetric matrices. In fact, this characterization for symmetric matrices is at the heart of most theorems in spectral theory about symmetric matrices, and the latter are completely understood by it. However, different ideas are required to deal with the nonsymmetric case.

The lower bound on  $\phi(R)$  in Theorem 1.4.1 is proven using a sequence of lemmas each of which is independently usable in different contexts. The main idea is to show that  $\phi(R^k) \leq k \cdot \phi(R)$  (for all integers  $k$ ), and use the Schur decomposition of  $R$  to relate  $\phi(R^k)$  to the spectral gap of  $R$ . A detailed exposition on this is given in Section 3.7 before the theorem is proved. The main difference in Theorem 1.4.1 from the Cheeger-Buser inequalities is the factor of  $n$ , which makes the bound extremely weak. However, the strength of the lower bound on  $\phi(R)$  in the theorem is in the factors that are *not* present.

The first straightforward thing to note is that the dependence on  $n$  is linear and not exponential. This is crucial, since our initial attempts to prove this result was by using tools from perturbation theory – since  $\phi(R)$  can be understood as a perturbation to a matrix of disconnected components. It is possible to understand the change in the coefficients of the characteristic polynomial from the change in the matrix, and

further relate it to the change in the spectral gap. However, this brings in factors exponentially depending on  $n$ . Another direction is to use results similar to Baur-Fike [BF60] (see Lemma 3.6.1), but it is very limited since it holds only for diagonalizable  $R$ , and depends on the eigenvector condition number. The eigenvector condition number is  $\mathcal{K}(R) = \|V\|_2 \|V^{-1}\|_2$  where  $V$  is an invertible matrix that transforms  $R$  to its Jordan decomposition  $R = VJV^{-1}$ . Since the eigenvector condition number can be enormous even for small matrices, the dependence on  $\mathcal{K}(R)$  makes the Baur-Fike result much weaker than what we seek. There is an extension of Baur-Fike to non-diagonalizable matrices by Saad [Saa11], but it has an exponential dependence on  $n$  and a dependence on  $\mathcal{K}(R)$ . Note, however, that our result in Theorem 1.4.1 does not depend on  $\mathcal{K}(R)$ . We also reprove Baur-Fike using Schur decomposition, which removes  $\mathcal{K}(R)$ , but instead has a dependence on  $\exp(n)$  and  $\sigma(R) = \|R\|_2$  – the largest singular value of  $R$  (See Lemma 3.6.3). There are two other factors that could appear in our proof of Theorem 1.4.1, and were indeed present in the initial version of our proofs but were sequentially removed in subsequent iterations – the largest singular value  $\sigma(R)$  of  $R$ , and the eigenvalue condition number  $\kappa(R) = \min_i u_i \cdot v_i$  where  $u$  and  $v$  are the positive eigenvectors corresponding to the largest eigenvalue 1 of  $R$ , and normalized so that  $\sum_i u_i v_i = 1$ . The removal of  $\sigma$  is possible by a neat trick (Lemma 3.0.3), but the removal of  $\kappa(R)$  is nontrivial. In fact, in the published version of our result [MS19], we have a weaker bound of

$$\frac{1}{15} \cdot \frac{\Delta(R)}{n + \ln\left(\frac{1}{\kappa(R)}\right)} \leq \phi(R).$$

In the attempt to construct matrices showing the necessity of  $\kappa(R)$  in the lower bound, it turned out that for all possible extremes of matrices,  $\kappa(R)$  was indeed unnecessary. This made us reconsider all the lemmas in our proof, and indeed, it was possible to rewrite them to remove the dependence on  $\kappa(R)$  entirely and arrive at Theorem 1.4.1.

We would also like to comment on the regime where the lower bound on  $\phi(R)$  in Theorem 1.4.1 is useful. Due to the factor of  $n$ , the bound is most meaningful when  $\phi(R) \ll 1/n$ . As such, the utility of the bound is perhaps in treating it as a perturbation result, where tiny perturbations – say  $O(1/n^2)$  or  $O(1/n \log n)$  or  $O(1/n \log^2(n))$  – closely affect the spectral gap, and the gap between the eigenvalues and the positive eigenvalue in the perturbed matrix can be bounded by the resulting perturbation expressed in  $\phi$  (see Section ??).

Thus, the lack of dependence on  $\exp(n)$  (since we do not use perturbation theory),  $\mathcal{K}(R)$  (since we do not use the Jordan decomposition but the Schur decomposition),

$\sigma(R)$  (since we transform  $R$  to an  $A$  that preserves the eigenvalues and edge expansion and has equal maximum singular and eigenvalues), and  $\kappa(R)$  (since we ensure all the intermediate lemmas are tight and crucially that the right eigenvector  $v$  for eigenvalue 1 is in the kernel of  $I - R$ ) is where the primary importance of the lower bound on  $\phi(R)$  lies, since it helps to answer the first question and exactly quantify the Perron-Frobenius theorem. It means  $\Delta(R)$  is proportional to  $\phi(R)$  up to the scaling factor of  $n$ . However, since there is no dependence on  $n$  in the symmetric case (inequalities 1.3.1), it raises the second main question – is the dependence on  $n$  in Theorem 1.4.1 necessary, or is it more an artefact of our proof method? More specifically,

**Question 2.** Are there matrices  $R$  for which  $\phi(R) \approx \frac{\Delta(R)}{n}$ ?

### 1.5 Constructions of nonreversible matrices

Answering Question 2 takes us in novel and sparsely explored areas. To answer it in the strictest sense, we will now seek doubly stochastic matrices that achieve the bound required in Question 2. The main reason is that they have the uniform vector as both the left and right eigenvector for eigenvalue 1, and it would seem possible on the outset – since the left and right eigenvector is the same and has no variance, that at least for doubly stochastic matrices, the lower bound on  $\phi$  in Theorem 1.4.1 is possibly much weak. We need to study the edge expansion of irreversible or non-symmetric matrices carefully.

The edge expansion of symmetric matrices has been amply studied, and the matrices with constant edge expansion are called (combinatorial) expanders. These matrices have remarkable properties, making them a fundamental building block within combinatorics, and matrices with constant edge expansion and few non zero entries (edges) are complicated (in construction or proof) and have a rich history, since they have “magical” properties and help to construct seemingly impossible objects or algorithms (see [HLW06]). Question 2 however is irrelevant in the symmetric case since the edge expansion and spectral gap are tightly related, and we seek a gap of a factor of  $n$  between the two quantities.

The first steps in this direction were already taken in the work of Maria Klawe [Kla81; Kla84] who showed that certain affine-linear constructions of matrices have inverse polylog( $n$ ) edge expansion (see construction 4.3.1). It was observed by Umesh Vazirani [Vaz17], that it is possible to orient the edges in the construction of Klawe to obtain doubly stochastic matrices with constant spectral gap but expansion that

was  $1/\text{polylog}(n)$ ! This is quite remarkable, since it shows that there are doubly stochastic matrices with

$$\phi(A_{KV}) \approx \frac{\Delta(A_{KV})}{(\log n)^c}$$

for some constant  $c$ . In fact, there are many other affine-linear constructions, all achieving similar bounds. A construction to note in particular is that of de Bruijn matrices described and analyzed in detail in Section 4.4. For these matrices, it turns out that

$$\phi(A_{dB}) \approx \frac{\Delta(A_{KV})}{\log n}.$$

These are beautiful matrices, and their properties are listed in Lemma 4.4.3. These constructions indicate that a dependence on some function of  $n$  cannot be avoided. However, Question 2 can be rephrased as follows.

**Question 3.** Are there doubly stochastic matrices  $A$  with

$$\frac{\phi(A)}{\Delta(A)} \in o\left(\frac{1}{\log n}\right)$$

or is it the case that for all doubly stochastic matrices, for some constant  $c$ ,

$$c \cdot \frac{\Delta(A)}{\log(n)} \leq \phi(A)?$$

This is the primary question for consideration, since if it is true that the edge expansion is at least the spectral gap by  $\log(n)$ , it would mean that our lower bound on  $\phi(R)$  in Theorem 1.4.1 is exponentially far from the truth (at least for doubly stochastic matrices), and newer techniques would be required for a stronger bound. Further, it would also mean that the spectral gap provides a good estimate of the edge expansion which in itself is difficult to compute since the  $\log(n)$  factors are essentially negligible in most applications. However, we show the following striking construction.

**Theorem 1.5.1.** *There is a family of doubly stochastic matrices  $A_n$ , called Rootn matrices, such that for every  $n$ ,*

$$\phi(A_n) \leq \frac{\Delta(A_n)}{\sqrt{n}}.$$

This construction of Rootn matrices is presented in Section 4.8 and arrived at, presented, and discussed in detail in Sections 4.5, 4.6, 4.7, 4.8. This construction

is exponentially better than known constructions, and shows that the factor of  $n$  in Theorem 1.4.1 is indeed closer to the truth. The construction for Rootn matrices is arrived at by carefully fixing the eigenvalues in the triangular matrix in the schur decomposition to create a constant spectral gap, and choosing a unitary such that the resulting matrix is doubly stochastic and has minimum edge expansion .

As such, the final question that remains is the gap between  $\sqrt{n}$  and  $n$ . To resolve this problem, we take a direction different from the one that was used to construct Rootn matrices. Observing Rootn matrices, we learn a possible structure of the matrix to fix the edge expansion , and then set the entries in the matrix very carefully to maximize the spectral gap, as discussed in Section 4.9. This leads us to the most beautiful contribution of this thesis – Chet Matrices – that help to show the following.

**Theorem 1.5.2.** *There is a family of matrices  $C_n$  for which  $\sum_i C_n(i, j) = 1$  and  $\sum_j C_n(i, j) = 1$  for all  $i, j$ , called Chet matrices, such that for every  $n$ , if  $\phi(C_n)$  is defined as for doubly stochastic matrices (see 2.0.3), then*

$$\phi(C_n) \leq 2 \cdot \frac{\Delta(C_n)}{n}.$$

The construction is presented in Section 4.10. However, there is something in the construction that is still unknown. We are unable to show that Chet Matrices are nonnegative for all  $n$ . It seems to be the case for  $n$  up till 500 that we tested numerically (see Appendix A.4), but we do not have a proof for all  $n$ . In spite of this, these matrices have many remarkable properties listed in Section 4.11, and proving their nonnegativity is one of the main open problems of this thesis. To show their nonnegativity, we phrase a sequence of Trace conjectures in Section 4.12, which if true would (almost) imply the nonnegativity of Chet Matrices. We believe these conjectures are interesting in their own right.

The results so far give a complete answer to the first question we had asked initially, since we have tight bounds and (almost) matching constructions. We now proceed to other combinatorial properties and relate them to the edge expansion and spectral gap.

## 1.6 Relations with other combinatorial properties

### Mixing Time

The most widely studied property of Markov chains that is indispensable to algorithms is mixing time. To simplify exposition, consider an irreducible doubly stochastic

matrix  $A$  such that it is  $\frac{1}{2}$ -lazy, i.e., for every  $i$ , we have that  $A_{i,i} \geq \frac{1}{2}$ , which is required purely for a technical reason (ergodicity), and any other constant would also be sufficient. This condition ensures that except the eigenvalue 1, all other eigenvalues  $\lambda$  of  $A$  are such that  $|\lambda| < 1$ . Thus, if we write the Jordan decomposition of  $A = VJV^{-1}$ , it is clear that for large enough  $t$ ,  $A^t \approx \frac{1}{n} \mathbf{1} \cdot \mathbf{1}^T$  (where  $\mathbf{1}$  is the all ones vector), since all other eigenvalues in  $A$  will become close to zero and only the space corresponding to eigenvalue 1 remains. Note that this also means, that if we start with some probability distribution  $p$ , for large enough  $t$ ,  $A^t p \approx_\epsilon \frac{1}{n} \mathbf{1}$  (in say,  $\ell_1$  norm). The smallest such  $t$  which works for *any* starting  $p$  is referred to as the mixing time of  $A$  or  $\tau_\epsilon$ . Note that similarly, we can formally define the mixing time for any irreducible and  $\frac{1}{2}$ -lazy nonnegative matrix  $R$  with largest eigenvalue 1 and corresponding left and right eigenvectors  $u$  and  $v$ , such that  $\langle u, v \rangle = 1$ . This will be the smallest  $t$  such that  $R^t \approx_\epsilon v \cdot u^T$ .

There is extensive literature on mixing time, different methods to bound it and different tools that can be used for specific types of chains. Our aim will mostly be to obtain general bounds on the mixing time, and relate it to other combinatorial and algebraic quantities.

The mixing time of symmetric (or reversible)  $A$  is comprehensively studied and sufficiently well understood (see [AF02; LPW09; MT06]). Due to the spectral decomposition of  $A$ , the mixing time  $\tau_\epsilon$  for a reversible chain is bounded as

$$c_1 \cdot \frac{1}{\Delta(A)} \leq \tau_\epsilon(A) \leq c_2 \cdot \frac{\ln\left(\frac{n}{\epsilon \cdot \kappa(A)}\right)}{\Delta(A)}$$

for some constants  $c_1$  and  $c_2$ . Thus, the mixing time is approximately the inverse of the spectral gap, up to the factor of  $\log(n)$  and the eigenvalue condition number  $\kappa(A)$ . The factor  $\kappa(A)$  will in fact appear in all bounds related to the mixing time, and it is easy to see that it cannot be removed by taking even a  $3 \times 3$  matrix which is very close to being reducible.

Regarding general chains that are not necessarily symmetric, again many different results are known for specific chains, and the most general is the result of Mihail [Mih89], which directly relates the mixing time to edge expansion (Mihail shows it for row stochastic  $R$ , but it directly extends to all  $R$  by syntactic changes).

$$\tau_\epsilon(R) \leq c \cdot \frac{\ln\left(\frac{n}{\epsilon \cdot \kappa(R)}\right)}{\phi^2(R)}.$$

This shows that the mixing time is inversely proportional to the edge expansion of  $R$ . Our first result is essentially a one-line proof of the above result, that can be derived from one of our main lemmas relating the mixing time of a matrix  $A$  (derived from  $R$ ) which has identical left and right eigenvector  $w$  for eigenvalue 1 to the second singular value of  $A$ . We also show a lower bound on  $\tau_\epsilon(R)$  in terms of  $\phi(R)$ , which is also known (see [LPW09]), but we write the bound for general  $\epsilon$ .

We also relate the mixing time to the spectral gap in the irreversible case, and get the following theorem.

**Theorem 1.6.1.** *Let  $\tau_\epsilon(R)$  be the mixing time of an irreducible  $\frac{1}{2}$ -lazy nonnegative matrix  $R$ . Then*

$$\tau_\epsilon(R) \leq c \cdot \frac{n + \ln\left(\frac{1}{\epsilon \cdot \kappa(R)}\right)}{\Delta(R)},$$

*and our constructions of Rootn and Chet Matrices in Sections 4.8 and 4.10 show that the factor of  $n$  is again necessary.*

The interesting thing in the result 1.6.1 is that  $n$  is additive and not multiplicative in the numerator. The next thing we study is the relation between the mixing time of  $A$  (irreducible, nonnegative,  $\frac{1}{2}$ -lazy with left and right eigenvector  $w$  for eigenvalue 1) and the mixing time of  $\tilde{A} = \frac{1}{2}(A + A^T)$ , and show two-sided and tight bounds between them. We also relate the mixing time of  $A$  to that of  $\exp(t \cdot (I - A))$ .

We mostly present simple/elementary proofs of many known bounds on Mixing time, and present some new results in Section 5.1. Our main contribution is to show how all the (optimal) bounds are achievable using only a few key tools and lemmas, and it also helps us obtain many bounds in a form that we have not come across.

### Capacity and Normalized Capacity

The next quantity we explore has been studied extensively for symmetric matrices in different communities under different names at different points of time, which we refer to as *capacity*. The term and the problem arise from the study of harmonic functions and the Dirichlet problem. Again to present a simplified definition, assume we have an irreducible nonnegative matrix  $A$  with largest eigenvalue 1 and the corresponding left and right eigenvector  $w$ . Let the Laplacian of  $A$  be  $L = I - A$ , let  $U$  be some subset of the vertices, and let  $a \in \mathbb{R}^{|U|}$  be some real vector over  $U$ . We want to find a vector  $q \in \mathbb{R}^n$  such that  $q_i = a_i$  for  $i \in U$ , i.e.  $q$  is same as  $a$  on  $U$ , and  $(Lq)_i = 0$  for  $i \in \bar{U}$ . Since  $A$  is irreducible, it is not difficult to see that there is a



unique vector  $q$  satisfying the equations. Given such a  $q$ , the capacity is defined as follows.

$$\text{cap}_A(U, \bar{a}) = \langle q, Lq \rangle.$$

The vector  $\bar{a}$  is such that  $\bar{a}_i = a_i/w_i$ . This gives us the capacity of the vector  $\bar{a}$  on the set  $U$  for the matrix  $A$  (It is not the capacity of  $a$  due to a technical condition). Our definition is completely general, and special cases of capacity for symmetric matrices have been studied (see [DS84]) by interpreting the graph as an electrical network, with the edge weights  $A_{i,j} = A_{j,i}$  denoting the conductance of the edge  $\{i, j\}$ . Further, if  $a \in \{0, 1\}^{|U|}$ , the  $U$  can be written as  $U = S \cup T$  with  $a$  being 1 on  $S$  and 0 on  $T$ , and the resulting capacity can be referred to as  $\text{cap}(S, T)$ . For symmetric matrices, the vector  $q$  is exactly the voltages at each vertex when the vertices in  $S$  are put at voltage 1 and the vertices in  $T$  are put at voltage 0. Further, if the entire graph is modified such that there is one vertex  $s$  for  $S$  and  $t$  for  $T$ , and one edge between them, then the effective resistance between  $s$  and  $t$  or the sets  $S$  and  $T$  in the original graph is exactly

$$\frac{1}{\text{cap}_{S,T}(A)}.$$

In fact, it is possible to create many different results and algorithms through the usage of capacity for symmetric matrices, and there have been many results in this direction, see for instance [DS84; SS11; Lyo83; Cha+96; Tet91].

Our aim is to study capacity in its full generality for nonsymmetric matrices. We show many basic results some of which are folklore for symmetric matrices, but our main result is the following, discussed and shown in Section 5.11.

**Theorem 1.6.2.** *Let  $A_\alpha = \alpha A + (1 - \alpha)A^T$ , then for every  $U$  and  $a$ , if  $0 \leq \beta \leq \alpha \leq \frac{1}{2}$ , then*

$$\text{cap}_{U,a}(A_\alpha) \leq \text{cap}_{U,a}(A_\beta).$$

We remark a few things again about this result. The first is that the result is simple if we compare a nonsymmetric matrix to a symmetric matrix, i.e. it is simple to show that for  $\tilde{A} = \frac{1}{2}(A + A^T)$ ,

$$\text{cap}_{U,\bar{a}}(\tilde{A}) \leq \text{cap}_{U,\bar{a}}(A).$$

This is in fact a direct consequence of Dirichlet's theorem, which itself is a consequence of the Cauchy-Schwarz inequality. The remarkable thing in Theorem 1.6.2 is that it helps to compare the capacity of two *nonsymmetric* matrices, and thus the general tools of symmetric matrices – specifically the Cauchy-Schwarz inequality –

cannot be used. The proof is relatively long and intricate, but we find it striking that capacity monotonically increases as  $\alpha$  decreases and goes from  $\frac{1}{2}$  to 0. Other related results can also be found in Section 5.11.

### A different notion of expansion and Tensor walks

In the last section, we take the first steps towards a new definition of expansion inspired by the recent studies of expansion in high-dimensional expanders [Baf+20], and we show a neat lemma similar to the standard notion of edge expansion for it in Section 5.14 which we believe could be useful in the study of high dimensional objects. The second and final thing we study are tensor walks. Due to the meteoric rise in interest in both machine learning and quantum information, tensors have become a fundamental tool in both the areas. However, the results related to them are extremely specific to the application, and the task of showing general results is in its infancy. This is mostly due to the behavior of tensors that is different from matrices in almost every aspect. To highlight this, consider a 3-tensor  $T$  indexed as  $T_{i,j,k}$ , with  $i, j, k \in [n]$ . Given probability vectors  $p_t \in \mathbb{R}_{\geq 0}^n$ , we can define one step of the walk as

$$p_t(i) = \sum_{j,k} T_{i,j,k} p_{t-1}(j) p_{t-2}(k).$$

To ensure  $p_t$  is also a probability distribution, we can enforce that for any  $j, k$ ,  $\sum_i T_{i,j,k} = 1$ . Note that one step of the walk is no longer a linear operation, but it is a very meaningful walk, and there are an enormous number of areas where such walks naturally appear. The same definition can be extended to any  $k$ -tensor. The surprising thing is that even a 3-tensor could have an *exponential* (in  $n$ ) number of eigenvalues (defined appropriately). There are even multiple variants of the Perron-Frobenius theorem for nonnegative tensors (see [CPZ08; FGH13] for instance), however, even many basic questions remain unanswered. The first question is, do positive tensors have a unique fixed point? In fact, surprisingly, this turns out to be false, and an example was shown in [CZ13]. Our primary result here is to delineate a condition for which it is sufficient for the walk to have a unique fixed point. We say a  $k$ -tensor is stochastic over index  $i$ , if for every fixing of the other indices  $l_1, l_2, \dots, l_{k-1}$ ,

$$\sum_{i=1}^n T_{l_1, l_2, i, l_3, \dots, l_{k-1}} = 1.$$

We say  $T$  is 2-line stochastic if it is stochastic over the output index  $i$  and any input index. Our main theorem is the following.

**Theorem 1.6.3.** *Let  $T$  be a  $k$ -tensor in  $n$  dimensions with positive entries, and let  $T$  be 2-line stochastic. Then  $T$  has a unique positive fixed point.*

This result can be found in Section 5.15. It raises an extremely important question: how fast does the walk converge to the fixed point? We leave this question for future considerations.

The thesis is organized as follows. We first give the Preliminary definitions in Section 2, proceed to prove our Theorem 1.4.1 in Section 3, show theorems 1.5.1 in Section 4.8 and 1.5.2 in Section 4.10, and theorems 1.6.1, 1.6.2 and 1.6.3 in Sections 5.1, 5.11 and 5.15 respectively. We conclude with some summarizing final thoughts in Section 5.15.

*Chapter 2*

PRELIMINARIES – SPECTRAL GAP, EDGE EXPANSION, AND  
THE PERRON-FROBENIUS THEOREM

As for the rest of my readers, they will accept such portions as apply to them. I trust that none will stretch the seams in putting on the coat, for it may do good service to him whom it fits.

~ Henry David Thoreau, *Walden*

We will consider nonnegative matrices throughout this thesis using  $R$  or  $A$ , also referred to as chains or graphs. For any nonnegative matrix  $R \in \mathbb{R}_{\geq 0}^{n \times n}$ , there is an implicit underlying graph on  $n$  vertices with the edge  $(i, j)$  having weight  $R_{j,i}$ , and we assume there is no edge if  $R_{j,i} = 0$ . Note that the subscripts are reversed since we assume right multiplication by a vector, although this will not matter anywhere in this thesis except for internal consistency in lemmas and proofs.

Given a matrix  $R$ , we say that  $R$  is *strongly connected* or *irreducible*, if there is a path from  $s$  to  $t$  for every pair  $(s, t)$  of vertices in the underlying digraph on edges with positive weight, i.e. for every  $(s, t)$  there exists  $k > 0$  such that  $R^k(s, t) > 0$ . We say  $R$  is *weakly connected*, if there is a pair of vertices  $(s, t)$  such that there is a path from  $s$  to  $t$  but no path from  $t$  to  $s$  in the underlying digraph (on edges with positive weight).

We start by stating the Perron-Frobenius theorem. The theorem was shown for positive matrices  $R$  by Perron in [Per07], and for irreducible matrices  $R$  by Frobenius in [Fro12]. In the last hundred years, the theorem has been used extensively in many different areas of mathematics as discussed in the Introduction, and has become a fundamental tool within spectral theory and dynamical systems.

**Theorem 2.0.1.** (Perron-Frobenius theorem [Per07; Fro12]) *Let  $R \in \mathbb{R}^{n \times n}$  be a nonnegative matrix. Then the following hold for  $R$ .*

1.  *$R$  has some nonnegative eigenvalue  $r$ , such that all other eigenvalues have magnitude at most  $r$ , and  $R$  has nonnegative left and right eigenvectors  $u$  and  $v$  for  $r$ .*
2. *If  $R$  has some positive left and right eigenvectors  $u$  and  $v$  for some eigenvalue  $\lambda$ , then  $\lambda = r$ .*
3. *If  $R$  is irreducible, then the eigenvalue  $r$  is positive and simple (unique),  $u$  and  $v$  are positive and unique, and all other eigenvalues  $\lambda$  are such that  $|\lambda| \leq r$ , and  $\operatorname{Re}\lambda < r$ .*

Many nice proofs of the theorem can be found in different lecture notes. We will state all our results for irreducible matrices, and they will extend for general matrices by using limit infimums. By the Perron-Frobenius (Theorem 2.0.1, part 3), an irreducible nonnegative matrix  $R$  will have a simple positive eigenvalue  $r$  such that all eigenvalues have magnitude strictly less than  $r$ , and it will be called the *trivial* or *stochastic* or PF eigenvalue of  $R$ , and all other eigenvalues of  $R$  will be called *nontrivial*. The left and right eigenvectors corresponding to  $r$  will be called the *trivial* or *PF left eigenvector* (generally referred to as  $u$ ) and *trivial* or *PF right eigenvector* (generally referred to as  $v$ ). This leads us to the following definition.

**Definition 2.0.2.** (*Spectral gap of irreducible nonnegative matrices*) *Let  $R$  be an  $n \times n$  irreducible nonnegative matrix. Let the eigenvalues  $\lambda_1$  to  $\lambda_n$  of  $R$  be arranged so that  $\lambda_1 > \operatorname{Re}\lambda_2 \geq \operatorname{Re}\lambda_3 \geq \dots \geq \operatorname{Re}\lambda_n$ , where due to the Perron-Frobenius Theorem 2.0.1,  $\lambda_1$  is real and positive and  $\operatorname{Re}\lambda_2 < \lambda_1$ . Define the spectral gap of  $R$  as*

$$\Delta(R) = 1 - \frac{\operatorname{Re}\lambda_2(R)}{\lambda_1(R)}.$$

◇

Note that  $0 \leq \Delta(R) \leq 2$  from the Perron-Frobenius theorem, since  $|\lambda_i(R)| < \lambda_1(R)$ . We remind the reader that the eigenvalues of  $R$  are simply the roots of the characteristic polynomial, i.e. of the equation  $\det(\lambda I - R) = 0$ . We will also consider singular values of nonnegative matrices  $A$  with identical positive left and right eigenvector  $w$  for PF eigenvalue 1, and denote them as  $1 = \sigma_1(A) \geq \sigma_2(A) \geq \dots \geq \sigma_n(A) \geq 0$  (see Lemma 3.0.3 for proof of  $\sigma_1(A) = 1$ ). We denote  $(i, j)$ 'th entry of  $M \in \mathbb{C}^{n \times n}$

by  $M_{i,j}$ , or if  $M$  already as a subscript, then as  $M_t(i, j)$  as will be clear from context. We denote the conjugate-transpose of  $M$  as  $M^*$  and the transpose of  $M$  as  $M^T$ . Any  $M \in \mathbb{C}^{n \times n}$  has a *Schur decomposition* (see, e.g., [Lax07])  $M = UTU^*$  where  $T$  is an upper triangular matrix whose diagonal entries are the eigenvalues of  $M$ , and  $U$  is a unitary matrix ( $UU^* = U^*U = I$ ). When we write “vector” we mean by default a column vector. For a vector  $v$ , we again write or  $v_i$  to denote its  $i$ 'th entry or  $v_t(i)$  in case a subscript is already present. For any two vectors  $x, y \in \mathbb{C}^n$ , we use the standard *inner product*  $\langle x, y \rangle = \sum_{i=1}^n x_i^* \cdot y_i$  defining the norm  $\|x\|_2 = \sqrt{\langle x, x \rangle}$ . We write  $u \perp v$  to indicate that  $\langle u, v \rangle = 0$ . Note that  $\langle x, My \rangle = \langle M^*x, y \rangle$ . We denote the operator norm of  $M$  by  $\|M\|_2 = \max_{u: \|u\|_2=1} \|Mu\|_2$ , and recall that the operator norm is at most the Frobenius norm, i.e.,  $\|M\|_2 \leq \|M\|_F := \sqrt{\sum_{i,j} |M_{i,j}|^2}$ . We write  $D_u$  for the diagonal matrix whose diagonal contains the vector  $u$ . We will use the phrase “positive” to mean entry-wise positive, and the phrase “expansion” to mean edge expansion. We note the Birkhoff-von Neumann theorem, which states that every doubly stochastic matrix  $A$  can be written as  $A = \sum \alpha_i P_i$ , where  $P_i$  are permutation matrices and the  $\alpha_i \geq 0$  and  $\sum \alpha_i = 1$ .

Recall the Courant-Fischer variational characterization of eigenvalues for symmetric real matrices, applied to the second eigenvalue:

$$\max_{u \perp v_1} \frac{\langle u, Mu \rangle}{\langle u, u \rangle} = \lambda_2(M),$$

where  $v_1$  is the eigenvector for the largest eigenvalue of  $M$ . We will use the symbol  $J$  for the all 1's matrix divided by  $n$ , i.e.,  $J = \frac{1}{n} \mathbf{1} \cdot \mathbf{1}^T$ . We will denote the standard basis vectors as  $e_1, \dots, e_n$ . We denote the all 1's vector by  $\mathbf{1}$ , and we say that any subset  $S \subseteq [n]$  is a *cut*, denote its complement by  $\bar{S}$ , and denote the *characteristic vector of a cut* as  $\mathbf{1}_S$ , where  $\mathbf{1}_S(i) = 1$  if  $i \in S$  and 0 otherwise. We first present the definition of edge expansion for doubly stochastic matrices.

**Definition 2.0.3.** (*Edge expansion of doubly stochastic matrices*) For a doubly stochastic matrix  $A$ , the *edge expansion of the cut  $S$*  is defined as

$$\phi_S(A) := \frac{\langle \mathbf{1}_S, A\mathbf{1}_{\bar{S}} \rangle}{\langle \mathbf{1}_S, A\mathbf{1} \rangle}$$

and the *edge expansion of  $A$*  is defined as

$$\phi(A) = \min_{S, |S| \leq n/2} \phi_S(A) = \min_{S, |S| \leq n/2} \frac{\sum_{i \in S, j \in \bar{S}} A_{i,j}}{|S|}.$$

◇

We wish to extend these notions to general nonnegative matrices  $R$ . Since eigenvalues and singular values of real matrices remain unchanged whether we consider  $R$  or  $R^T$ , the same should hold of a meaningful definition of edge expansion. However, note that Definition 2.0.3 has this independence only if the matrix is Eulerian, i.e.,  $R\mathbf{1} = R^T\mathbf{1}$ . Thus, to define edge expansion for general matrices, we transform  $R$  using its left and right eigenvectors  $u$  and  $v$  to obtain  $D_uRD_v$ , which is indeed Eulerian, since

$$D_uRD_v\mathbf{1} = D_uRv = rD_uv = rD_uD_v\mathbf{1} = rD_vD_u\mathbf{1} = rD_vu = D_vR^T u = D_vR^T D_u\mathbf{1}.$$

Since  $D_uRD_v$  is Eulerian, we can define the edge expansion of  $R$  similar to that for doubly stochastic matrices:

**Definition 2.0.4.** (*Edge expansion of irreducible nonnegative matrices*) Let  $R \in \mathbb{R}^{n \times n}$  be an irreducible nonnegative matrix with positive left and right eigenvectors  $u$  and  $v$  for the PF eigenvalue  $r$ . The *edge expansion of the cut  $S$*  is defined as

$$\phi_S(R) := \frac{\langle \mathbf{1}_S, D_uRD_v\mathbf{1}_{\bar{S}} \rangle}{\langle \mathbf{1}_S, D_uRD_v\mathbf{1} \rangle} \quad (2.0.5)$$

and the *edge expansion of  $R$*  is defined as

$$\phi(R) = \min_{S: \sum_{i \in S} u_i v_i \leq \frac{1}{2} \sum_i u_i v_i} \phi_S(R) = \min_{S: \sum_{i \in S} u_i v_i \leq \frac{1}{2} \sum_i u_i v_i} \frac{\sum_{i \in S, j \in \bar{S}} R_{i,j} \cdot u_i \cdot v_j}{\sum_{i \in S, j} R_{i,j} \cdot u_i \cdot v_j}.$$

◇

The edge expansion  $\phi(R)$  can be intuitively understood as the *measure of irreducibility of  $R$*  (though the correspondence is not exact in the strictest sense). If  $\phi(R)$  is high, say a constant or even  $1/\text{polylog}(n)$ , then  $R$  is well-connected (strongly). As  $\phi(R)$  becomes smaller, it implies there are two (strongly) disconnected components within  $R$ , or that  $R$  has a sink-like component.

Our next aim is to define  $\Delta(R)$  and  $\phi(R)$  for nonnegative matrices  $R$  that are not irreducible. We do this by considering the ball of irreducible matrices in a small ball around  $R$ , and taking the limit of the infimum to get a well-defined quantity.

**Definition 2.0.6.** (Spectral gap and Edge Expansion of any nonnegative matrix) Let  $E$  be the set of all irreducible nonnegative matrices. For any nonnegative matrix  $R$ , let

$$R_\epsilon = \{H : H \in E, \|R - H\|_F \leq \epsilon\}.$$

Then we define the spectral gap of  $R$  as

$$\Delta(R) = \lim_{\epsilon \rightarrow 0} \inf_{H \in R_\epsilon} \Delta(H),$$

and the edge expansion of  $R$  as

$$\phi(R) = \lim_{\epsilon \rightarrow 0} \inf_{H \in R_\epsilon} \phi(H).$$

◇

The first simple thing we can say is the following.

**Lemma 2.0.7.** *Let  $R$  be a nonnegative matrix. If  $R$  is irreducible, then  $\phi(R) > 0$ .*

*Proof.* Since  $R$  is irreducible, the left and right PF eigenvectors  $u$  and  $v$  are positive. For the sake of contradiction, if  $\phi(R) = 0$ , there is some  $S$  with  $\phi_S(R) = 0$ , implying that  $\langle \mathbf{1}_S, D_u R D_v \mathbf{1}_{\bar{S}} \rangle = 0$ , and since  $u$  and  $v$  are positive, it implies that  $R_{i,j} = 0$  for  $i \in S, j \in \bar{S}$ , and similarly  $R_{i,j} = 0$  for  $i \in \bar{S}, j \in S$  since  $D_u R D_v$  is Eulerian. This implies there is no path from  $i \in S$  to  $j \in \bar{S}$ , implying  $R$  is not irreducible, a contradiction. □

According to the Perron-Frobenius theorem (part 3), if  $R$  is irreducible then  $\operatorname{Re} \lambda_2(R) < \lambda_1(R)$ . However, since irreducibility implies positivity of edge expansion from Lemma 2.0.7, it means that the limiting case of Theorem 1.4.1 showing that  $\phi(R) > 0 \Leftrightarrow \Delta(R) > 0$  implies that we get a much stronger and tighter statement than the Perron-Frobenius theorem.



*Chapter 3*

GENERALIZATIONS OF THE PERRON-FROBENIUS THEOREM  
AND THE CHEEGER-BUSER INEQUALITIES

Human reason has the peculiar fate in one species of its cognitions that it is burdened with questions which it cannot dismiss, since they are given to it as problems by the nature of reason itself, but which it also cannot answer, since they transcend every capacity of human reason.

~ Immanuel Kant, *Critique of Pure Reason*

The aim of this section is to prove our main Theorem 1.4.1. As stated in the Introduction, there are two well known theorems in Spectral Theory. The first is the Perron-Frobenius Theorem, which provides us, among other results, a *qualitative* statement connecting the edge expansion of matrices and their second eigenvalue. More specifically, it tells us that for any irreducible nonnegative matrix  $R$  – for which it is always the case that  $\phi(R) > 0$  – the spectral gap  $\Delta(R) > 0$ . The second are the Cheeger-Buser inequalities as follows.

**Theorem 3.0.1.** (*Cheeger-Buser Inequality* [[Che70](#); [Bus82](#); [AM85](#); [SJ89](#); [Dod84](#); [Nil91](#)]) *Let  $R$  be a reversible nonnegative matrix. Then*

$$\frac{1}{2} \cdot \Delta(R) \leq \phi(R) \leq \sqrt{2 \cdot \Delta(R)}.$$

This gap in our understanding, between the qualitative result for the nonreversible case and a quantitative result for the reversible case, is the primary focus of this section. Our main aim in theorem 1.4.1 is to show an inequality similar to the form above but for *any* nonnegative matrix (not necessarily reversible).

We will prove Theorem 1.4.1, for the case of irreducible nonnegative matrices first, and extend it to all matrices (not necessary irreducible) in Section 3.8. We restate the main theorem that we want to prove in this chapter.

**Theorem 3.0.2.** *Let  $R$  be an irreducible nonnegative matrix. Then*

$$\frac{1}{15} \cdot \frac{\Delta(R)}{n} \leq \phi(R) \leq \sqrt{2 \cdot \Delta(R)}.$$

The upper bound on  $\phi(R)$  akin to Cheeger's inequality follows by a straightforward extension of Fiedler's proof for doubly stochastic matrices [Fie95], and the lower bound will require substantial work.

However, before we go into the details of the proof of Theorem 1.4.1, we will first prove the Cheeger-Buser Inequalities both for completeness and concreteness for our definition of 2.0.4 which is different from some sources. We will start by proving a crucial lemma that will be used in all subsequent sections.

**Lemma 3.0.3.** *Let  $R$  be an irreducible nonnegative matrix with positive (left and right) eigenvectors  $u$  and  $v$  for the PF eigenvalue 1, normalized so that  $\langle u, v \rangle = 1$ . Define  $A = D_u^{\frac{1}{2}} D_v^{-\frac{1}{2}} R D_u^{-\frac{1}{2}} D_v^{\frac{1}{2}}$ . Then the following hold for  $A$ :*

1.  $\phi(A) = \phi(R)$ .
2. For every  $i$ ,  $\lambda_i(A) = \lambda_i(R)$ .
3.  $\|A\|_2 = 1$ .
4. If  $R$  is reversible, i.e.  $D_u R D_v = D_v R^T D_u$ , then  $A$  is symmetric.

*Proof.* Let the matrix  $A$  be as defined, and let  $w = D_u^{\frac{1}{2}} D_v^{\frac{1}{2}} \mathbf{1}$ . Then it is easily checked that  $Aw = w$  and  $A^T w = w$ . Further,

$$\langle w, w \rangle = \langle D_u^{\frac{1}{2}} D_v^{\frac{1}{2}} \mathbf{1}, D_u^{\frac{1}{2}} D_v^{\frac{1}{2}} \mathbf{1} \rangle = \langle D_u \mathbf{1}, D_v \mathbf{1} \rangle = \langle u, v \rangle = 1$$

where we used the fact that the matrices  $D_u^{\frac{1}{2}}$  and  $D_v^{\frac{1}{2}}$  are diagonal, and so they commute, and are unchanged by taking transposes. Let  $S$  be any set. The condition  $\sum_{i \in S} u_i \cdot v_i \leq \frac{1}{2}$  translates to  $\sum_{i \in S} w_i^2 \leq \frac{1}{2}$  since  $u_i \cdot v_i = w_i^2$ . Thus, for any set  $S$  for

which  $\sum_{i \in S} u_i \cdot v_i = \sum_{i \in S} w_i^2 \leq \frac{1}{2}$ ,

$$\begin{aligned}
\phi_S(R) &= \frac{\langle \mathbf{1}_S, D_u R D_v \mathbf{1}_{\bar{S}} \rangle}{\langle \mathbf{1}_S, D_u D_v \mathbf{1}_{\bar{S}} \rangle} \\
&= \frac{\langle \mathbf{1}_S, D_u D_u^{-\frac{1}{2}} D_v^{\frac{1}{2}} A D_u^{\frac{1}{2}} D_v^{-\frac{1}{2}} D_v \mathbf{1}_{\bar{S}} \rangle}{\langle \mathbf{1}_S, D_u^{\frac{1}{2}} D_v^{\frac{1}{2}} D_u^{\frac{1}{2}} D_v^{\frac{1}{2}} \mathbf{1}_S \rangle} \\
&= \frac{\langle \mathbf{1}_S, D_u^{\frac{1}{2}} D_v^{\frac{1}{2}} A D_u^{\frac{1}{2}} D_v^{\frac{1}{2}} \mathbf{1}_{\bar{S}} \rangle}{\langle \mathbf{1}_S, D_u^{\frac{1}{2}} D_v^{\frac{1}{2}} D_u^{\frac{1}{2}} D_v^{\frac{1}{2}} \mathbf{1}_S \rangle} \\
&= \frac{\langle \mathbf{1}_S, D_w A D_w \mathbf{1}_{\bar{S}} \rangle}{\langle \mathbf{1}_S, D_w^2 \mathbf{1}_S \rangle} \\
&= \phi_S(A)
\end{aligned}$$

and (1) holds. Further, since  $A$  is a similarity transform of  $R$ , all eigenvalues are preserved and (2) holds. For (3), consider the matrix  $H = A^T A$ . Since  $w$  is the positive left and right eigenvector for  $A$ , i.e.  $Aw = w$  and  $A^T w = w$ , we have  $Hw = w$ . But since  $A$  was nonnegative, so is  $H$ , and since it has a positive eigenvector  $w$  for eigenvalue 1, by Perron-Frobenius (Theorem 2.0.1, part 2),  $H$  has PF eigenvalue 1. But  $\lambda_i(H) = \sigma_i^2(A)$ , where  $\sigma_i(A)$  is the  $i$ 'th largest singular value of  $A$ . Thus, we get  $\sigma_1^2(A) = \lambda_1(H) = 1$ , and thus  $\|A\|_2 = 1$ . For (4),

$$\begin{aligned}
D_u R D_v &= D_v R^T D_u \Leftrightarrow \\
D_u D_u^{-\frac{1}{2}} D_v^{\frac{1}{2}} A D_u^{\frac{1}{2}} D_v^{-\frac{1}{2}} D_v &= D_v D_u^{\frac{1}{2}} D_v^{-\frac{1}{2}} A^T D_u^{-\frac{1}{2}} D_v^{\frac{1}{2}} \Leftrightarrow \\
D_u^{\frac{1}{2}} D_v^{\frac{1}{2}} A D_u^{\frac{1}{2}} D_v^{\frac{1}{2}} &= D_u^{\frac{1}{2}} D_v^{\frac{1}{2}} A^T D_u^{\frac{1}{2}} D_v^{\frac{1}{2}} \Leftrightarrow \\
A &= A^T
\end{aligned}$$

as required.  $\square$

Given Lemma 3.0.3, we can restrict to showing proofs for  $A$  instead of  $R$ , since both the spectral gap and edge expansion remain unaffected.

We will prove the Cheeger-Buser Inequalities. There are many well-known proofs in literature, but the definition of  $\phi(R)$  for general matrices has often been unsatisfying (although it works technically), and we show complete proofs for our Definition 2.0.4 of  $\phi(R)$  which is the same definition as in [Mih89]. This exposition will also be helpful in contrasting with similar lemmas for the nonreversible case.

### 3.1 Buser Inequality – the lower bound on $\phi(R)$

We start by showing the lower bound on  $\phi(R)$  for reversible  $R$ . To achieve this, note from the preliminaries that for the case of reversible  $R$ , the definition of  $\phi(R)$  for reducible  $R$  for exactly as in the irreducible case, and thus we show the theorem for irreducible reversible  $R$ . For any such  $R$ , note from the Perron-Frobenius Theorem 2.0.1 that  $\lambda_1(R) > 0$ , and by rescaling the matrix with a constant – which does not change  $\Delta(R)$  or  $\phi(R)$  (Lemma 3.0.3) – we assume that  $\lambda_1(R) = 1$ . Further, we will work with  $A = D_u^{\frac{1}{2}} D_v^{-\frac{1}{2}} R D_u^{-\frac{1}{2}} D_v^{\frac{1}{2}}$  which is symmetric since  $R$  is reversible from Lemma 3.0.3, is irreducible, and it has the same spectral gap and edge expansion. Thus, we will show a lower bound on  $\phi(A)$  where we assume  $Aw = w$  and  $A^T w = w$  for a positive  $w$  (Theorem 2.0.1). The lower bound easily follows from the spectral decomposition of  $A$ . Note that the following lemma does not require  $A$  to be reversible.

**Lemma 3.1.1.** *Let  $A$  be any irreducible nonnegative matrix with largest eigenvalue 1 and positive left and right eigenvector  $w$ . If  $\langle v, Av \rangle \leq \gamma \langle v, v \rangle$  with  $0 \leq \gamma \leq 1$  for every vector  $v$  with  $v \perp w$ , then*

$$\frac{1 - \gamma}{2} \leq \phi(A)$$

*Proof.* Let  $A = ww^* + B$  with  $Bw = 0$ , then  $\langle v, Av \rangle = \langle v, Bv \rangle$ , and for any set  $S$ , let  $D_w 1_S = c_0 w + v$  where  $v \perp w$ . Then

$$\langle w, D_w 1_S \rangle = c_0$$

and

$$\langle D_w 1_S, D_w 1_S \rangle = |c_0|^2 + \langle v, v \rangle$$

and note that

$$\langle w, D_w 1_S \rangle = \langle D_w 1_S, D_w 1_S \rangle = \langle D_w 1, D_w 1_S \rangle.$$

Then for any set  $S$  with  $\langle D_w 1_S, D_w 1_S \rangle \leq 1/2$ , we have

$$\begin{aligned}
\phi_S(A) &= \frac{\langle D_w 1_{\bar{S}}, AD_w 1_S \rangle}{\langle D_w 1, D_w 1_S \rangle} \\
&= 1 - \frac{\langle D_w 1_S, AD_w 1_S \rangle}{\langle D_w 1, D_w 1_S \rangle} \\
&= 1 - \frac{\langle c_0 w + v, A(c_0 w + v) \rangle}{\langle D_w 1, D_w 1_S \rangle} \\
&= 1 - \frac{\langle c_0 w + v, c_0 w + Av \rangle}{\langle D_w 1, D_w 1_S \rangle} \\
&= 1 - \frac{|c_0|^2 + \langle v, Av \rangle}{\langle D_w 1, D_w 1_S \rangle} \\
&\geq 1 - \frac{|c_0|^2 + \gamma \langle v, v \rangle}{\langle D_w 1, D_w 1_S \rangle} \\
&= 1 - \frac{\langle D_w 1_S, D_w 1_S \rangle^2 + \gamma(\langle D_w 1_S, D_w 1_S \rangle - \langle D_w 1_S, D_w 1_S \rangle^2)}{\langle D_w 1, D_w 1_S \rangle} \\
&= 1 - (\gamma + (1 - \gamma)\langle D_w 1_S, D_w 1_S \rangle) \\
&\quad [\text{since } \langle D_w 1_S, D_w 1_S \rangle \leq 1/2] \\
&\geq \frac{1 - \gamma}{2}
\end{aligned}$$

as required.  $\square$

The Buser inequality easily follows from the following.

**Lemma 3.1.2.** *For any  $v \perp w$ ,  $\langle v, Av \rangle \leq \lambda_2(A)\langle v, v \rangle$*

*Proof.* Let  $u_1 = w, u_2, u_3, \dots, u_n$  be an orthogonal set of eigenvectors for  $A$  (See Preliminaries 2), and let  $v = \sum_i c_i u_i$  with  $c_1 = 0$  since  $v \perp w$ , and

$$\langle v, Av \rangle = \left\langle \sum_i c_i u_i, A \sum_i c_i u_i \right\rangle = \left\langle \sum_i c_i u_i, \sum_i c_i \lambda_i u_i \right\rangle = \sum_{i \geq 2} c_i^2 \lambda_i \leq \lambda_2 \sum_i c_i^2 = \lambda_2 \langle v, v \rangle$$

as required.  $\square$

Combining Lemma 3.1.1 and Lemma 3.1.2 gives the lower bound on  $\phi(A)$  in Theorem 3.0.1.

### 3.2 Cheeger Inequality – the upper bound on $\phi(R)$

We now proceed with the upper bound on  $\phi(A)$  which is relatively complicated. Our proof method is similar to that in [Mih89], [Chu07] and going earlier to [AM85].

**Lemma 3.2.1.**  $\phi(A) \leq \sqrt{2 \cdot \Delta(A)}$

*Proof.* Let  $v$  be the eigenvector for eigenvalue  $\lambda_2(A)$  with  $v \perp w$  and assume  $\langle w, w \rangle = 1$ . Then we have that

$$1 - \lambda_2 = \frac{\langle v, (I - A)v \rangle}{\langle v, v \rangle}$$

Let  $u = D_w^{-1}v - c \cdot \mathbf{1}$ , and note that  $\langle D_w u, D_w u \rangle = \langle v, v \rangle + c^2$  since  $v \perp w$ . Our aim is to choose  $c$  in order to divide the positive and negative entries of  $u$  into groups  $S$  and  $\bar{S}$ , such that  $\sum_{i \in S} w_i^2 \leq 1/2$  and  $\sum_{i \in \bar{S}} w_i^2 \leq 1/2$ . To achieve this, without loss of generality, assume that the entries of  $D_w^{-1}v$  are arranged in decreasing order (as indices go from 1 to  $n$ ), and let  $r$  be the smallest index such that  $\sum_{i=1}^r w_i^2 > \frac{1}{2}$ . Thus  $\sum_{i=1}^{r-1} w_i^2 \leq \frac{1}{2}$  and  $\sum_{i=r+1}^n w_i^2 \leq \frac{1}{2}$  since  $\sum_i w_i^2 = 1$ . We then choose  $c = v_r/w_r$ , and this gives us  $u_i \geq 0$  for  $i < r$ ,  $u_r = 0$ , and  $u_i \leq 0$  for  $i > r$ . Thus, let  $x$  be the vector with  $x_i = u_i$  for  $i < r$  and 0 otherwise,  $y_i = -u_i$  for  $i > r$  and 0 otherwise, we get  $u = x - y$ , with the property that  $\sum_i w_i^2 \leq 1/2$  when  $i$  runs over nonzero entries of  $x$  or  $y$ , and  $\langle x, y \rangle = 0$ . Thus, we have that

$$\begin{aligned} 1 - \lambda_2 &= \frac{\langle v, (I - A)v \rangle}{\langle v, v \rangle} \\ &= \frac{\langle D_w u, (I - A)D_w u \rangle}{\langle D_w u, D_w u \rangle + c^2} \\ &\quad [\text{since } (I - A)w = 0 \text{ and } (I - A)^T w = 0] \\ &\geq \frac{\langle D_w x, (I - A)D_w x \rangle + \langle D_w y, (I - A)D_w y \rangle - 2\langle D_w x, (I - A)D_w y \rangle}{\langle D_w x, D_w x \rangle + \langle D_w y, D_w y \rangle} \\ &\geq \frac{\langle D_w x, (I - A)D_w x \rangle + \langle D_w y, (I - A)D_w y \rangle}{\langle D_w x, D_w x \rangle + \langle D_w y, D_w y \rangle} \\ &\quad [\text{since } 2\langle D_w x, A \rangle D_w y \geq 0] \\ &\geq \frac{\langle D_w x, (I - A)D_w x \rangle}{\langle D_w x, D_w x \rangle} \end{aligned} \tag{3.2.2}$$

where we assume in the last line that  $\frac{\langle D_w x, (I - A)D_w x \rangle}{\langle D_w x, D_w x \rangle} \leq \frac{\langle D_w y, (I - A)D_w y \rangle}{\langle D_w y, D_w y \rangle}$ . Note that  $Aw = w$  and  $A^T w = w$ , so for any  $i$ ,  $w_i^2 = \sum_j a_{i,j} w_i w_j$ , for any  $j$ ,

$w_j^2 = \sum_i a_{i,j} w_i w_j$ . Let  $a'_{i,j} = a_{i,j} w_i w_j$ . So

$$\begin{aligned}
\langle D_w x, D_w x \rangle &= \sum_i w_i^2 x_i^2 = 1/2 \left( \sum_i w_i^2 x_i^2 + \sum_j w_j^2 x_j^2 \right) \\
&= \frac{1}{2} \cdot \left( \sum_{i,j} a_{i,j} w_j w_i x_i^2 + \sum_{j,i} a_{i,j} w_i w_j x_j^2 \right) \\
&= \frac{1}{2} \cdot \sum_{i,j} a_{i,j} w_i w_j (x_i^2 + x_j^2) \\
&\geq \frac{1}{4} \cdot \sum_{i,j} a'_{i,j} (x_i + x_j)^2
\end{aligned}$$

and

$$\langle D_w x, (I - A) D_w x \rangle = \frac{1}{2} \sum_{i,j} a'_{i,j} (x_i - x_j)^2$$

multiplying LHS of the two equations, we get

$$\begin{aligned}
\langle D_w x, D_w x \rangle \langle D_w x, (I - A) D_w x \rangle &\geq \frac{1}{8} \sum_{i,j} a'_{i,j} (x_i + x_j)^2 \sum_{i,j} a'_{i,j} (x_i - x_j)^2 \\
&\geq \frac{1}{8} \left( \sum_{i,j} \sqrt{a'_{i,j}} |x_i - x_j| \cdot \sqrt{a'_{i,j}} |x_i + x_j| \right)^2 \\
&\quad \text{[Cauchy-Shwarz]} \\
&= \frac{1}{8} \left( \sum_{i,j} a'_{i,j} |(x_i^2 - x_j^2)| \right)^2
\end{aligned}$$

Since  $x_i \geq x_j$  for  $i < j$ , then for  $m'_{i,j} = a'_{i,j} + a'_{j,i}$

$$\begin{aligned}
\sum_{i,j} a'_{i,j} \left| (x_i^2 - x_j^2) \right| &= \sum_{i < j} m'_{i,j} (x_i^2 - x_j^2) \\
&= \sum_{i=1}^n \sum_{j=i+1}^n \sum_{k=i}^{j-1} m'_{i,j} (x_k^2 - x_{k+1}^2) \\
&= \sum_{i=1}^n \sum_{k=i}^{n-1} \sum_{j=k+1}^n m'_{i,j} (x_k^2 - x_{k+1}^2) \\
&= \sum_{k=1}^{n-1} \sum_{i=1}^k \sum_{j=k+1}^n m'_{i,j} (x_k^2 - x_{k+1}^2) \\
&= \sum_{k=1}^{r-1} (x_k^2 - x_{k+1}^2) \sum_{i=1}^k \sum_{j=k+1}^n m'_{i,j} \\
&\quad \text{[since for } k \geq r, x_k = 0\text{]} \\
&= 2 \sum_{k=1}^{r-1} (x_k^2 - x_{k+1}^2) \cdot \phi_k \cdot \mu_k
\end{aligned}$$

[factor of 2 since  $m_{i,j}$  is already sum of two entries,

$$\text{and } \mu_k = \sum_{i=1}^k w_i^2 \leq 1/2 \text{ for any } k \leq r]$$

$$\geq 2\alpha \cdot \sum_{k=1}^{r-1} (x_k^2 - x_{k+1}^2) \cdot \mu_k$$

[letting  $\alpha = \min_k \phi_k$ ]

$$= 2\alpha \cdot \sum_{k=1}^{r-1} w_k^2 x_k^2$$

$$= 2\alpha \cdot \langle D_w x, D_w x \rangle$$



which finally gives after combining everything,

$$\begin{aligned}
1 - \lambda_2 &= \frac{\langle v, (I - A)v \rangle}{\langle v, v \rangle} \\
&\geq \frac{\langle D_w x, (I - A)D_w x \rangle}{\langle D_w x, D_w x \rangle} \\
&\quad \text{[from equation 3.2.2]} \\
&\geq \frac{1}{8} \cdot \frac{(2\alpha \cdot \langle D_w x, D_w x \rangle)^2}{\langle D_w x, D_w x \rangle^2} \\
&= \frac{1}{2} \cdot \alpha^2
\end{aligned}$$

as required.  $\square$

### 3.3 Tightness of the Cheeger-Buser Inequality

It follows from straightforward calculations that for the Hypercube on  $n$  vertices  $H_n$  where  $n$  is a power of 2, we get

$$\phi(H_n) = \frac{1}{2} \cdot \Delta(H_n)$$

showing that the Buser inequality is *exactly* tight, and for the undirected cycle  $C_n$  on  $n$  vertices, we get that

$$\phi(C_n) \geq \sqrt{\Delta(C_n)}$$

showing that the Cheeger inequality is tight up to the constant. We proceed to prove the upper bound on  $\phi(R)$  in Theorem 3.0.2.

### 3.4 Fiedler's Proof – Upper bound on $\phi(R)$ in terms of $\Delta(R)$

Given Cheeger's inequality (Lemma 3.2.1), the upper bound on  $\phi(R)$  is relatively straightforward. We show the bound for  $A$  defined in Lemma 3.0.3.

**Lemma 3.4.1.** (*Extension of Fiedler [Fie95]*) *Let  $R$  be an irreducible nonnegative matrix with positive (left and right) eigenvectors  $u$  and  $v$  for eigenvalue 1, and let  $A = D_u^{\frac{1}{2}} D_v^{-\frac{1}{2}} R D_u^{-\frac{1}{2}} D_v^{\frac{1}{2}}$ . Then*

$$\phi(A) \leq \sqrt{2 \cdot \Delta(A)}$$

*Proof.* Given  $R$  as stated, and letting

$$A = D_u^{\frac{1}{2}} D_v^{-\frac{1}{2}} R D_u^{-\frac{1}{2}} D_v^{\frac{1}{2}},$$

note that

$$w = D_u^{\frac{1}{2}} D_v^{\frac{1}{2}} \mathbf{1},$$

where we use positive square roots for the entries in the diagonal matrices. Since  $A$  has  $w$  as both the left and right eigenvector for eigenvalue 1, so does  $M = \frac{A+A^T}{2}$ .

As explained before Definition 2.0.4 for edge expansion of general nonnegative matrices,  $D_wAD_w$  is Eulerian, since  $D_wAD_w\mathbf{1} = D_wA\mathbf{1} = D_ww = D_w^2\mathbf{1} = D_ww = D_wA^T\mathbf{1} = D_wA^TD_w\mathbf{1}$ . Thus, for any  $S$ ,

$$\langle \mathbf{1}_S, D_wAD_w\mathbf{1}_{\bar{S}} \rangle = \langle \mathbf{1}_{\bar{S}}, D_wAD_w\mathbf{1}_S \rangle = \langle \mathbf{1}_S, D_wA^TD_w\mathbf{1}_{\bar{S}} \rangle,$$

and thus for any set  $S$  for which  $\sum_{i \in S} w_i^2 \leq \frac{1}{2} \sum_i w_i^2$ ,

$$\phi_S(A) = \frac{\langle \mathbf{1}_S, D_wAD_w\mathbf{1}_{\bar{S}} \rangle}{\langle \mathbf{1}_S, D_wAD_w\mathbf{1} \rangle} = \frac{1}{2} \cdot \frac{\langle \mathbf{1}_S, D_wAD_w\mathbf{1}_{\bar{S}} \rangle + \langle \mathbf{1}_S, D_wA^TD_w\mathbf{1}_{\bar{S}} \rangle}{\langle \mathbf{1}_S, D_wAD_w\mathbf{1} \rangle} = \phi_S(M)$$

and thus

$$\phi(A) = \phi(M). \quad (3.4.2)$$

For any matrix  $H$ , let

$$R_H(x) = \frac{\langle x, Hx \rangle}{\langle x, x \rangle}.$$

For every  $x \in \mathbb{C}^n$ ,

$$\operatorname{Re}R_A(x) = R_M(x), \quad (3.4.3)$$

since  $A$  and  $\langle x, x \rangle$  are nonnegative and we can write

$$R_M(x) = \frac{1}{2} \frac{\langle x, Ax \rangle}{\langle x, x \rangle} + \frac{1}{2} \frac{\langle x, A^*x \rangle}{\langle x, x \rangle} = \frac{1}{2} \frac{\langle x, Ax \rangle}{\langle x, x \rangle} + \frac{1}{2} \frac{\langle Ax, x \rangle}{\langle x, x \rangle} = \frac{1}{2} \frac{\langle x, Ax \rangle}{\langle x, x \rangle} + \frac{1}{2} \frac{\langle x, Ax \rangle^*}{\langle x, x \rangle} = \operatorname{Re}R_A(x).$$

Also,

$$\operatorname{Re}\lambda_2(A) \leq \lambda_2(M). \quad (3.4.4)$$

To see this, first note that  $\lambda_2(A) < 1$  since  $A$  is irreducible. Thus, since  $\lambda_2(A) \neq 1$ , then let  $v$  be the eigenvector corresponding to  $\lambda_2(A)$ . Then since  $Aw = w$ , we have that

$$Av = \lambda_2(A)v \Rightarrow \langle w, Av \rangle = \langle w, \lambda_2(A)v \rangle \Leftrightarrow \langle A^T w, v \rangle = \lambda_2(A)\langle w, v \rangle \Leftrightarrow (1 - \lambda_2(A))\langle w, v \rangle = 0$$

which implies that  $v \perp w$ . Thus, we have that

$$\operatorname{Re}\lambda_2(A) = \operatorname{Re} \frac{\langle v, Av \rangle}{\langle v, v \rangle} = \frac{\langle v, Mv \rangle}{\langle v, v \rangle} \leq \max_{u \perp w} \frac{\langle u, Mu \rangle}{\langle u, u \rangle} = \lambda_2(M)$$

where the second equality uses equation 3.4.3, and the last equality follows from the variational characterization of eigenvalues stated in the Preliminaries 2. Thus, using equation 3.4.4, equation 3.4.2 and Cheeger's inequality for  $M$  (Theorem 3.0.1), we get

$$\phi(A) = \phi(M) \leq \sqrt{2 \cdot (1 - \lambda_2(M))} \leq \sqrt{2 \cdot (1 - \operatorname{Re}\lambda_2(A))} = \sqrt{2 \cdot \Delta(A)}$$

as required.  $\square$

### 3.5 Role of singular values

In this section, we try and obtain a lower bound on  $\phi$  by mimicking the proof of Buser's inequality in Theorem 3.0.1. The following lemma immediately follows.

**Lemma 3.5.1.** *Let  $A$  be an irreducible nonnegative matrix with largest eigenvalue 1 and  $w$  the corresponding positive left and right eigenvector. Then*

$$\frac{1 - \sigma_2(A)}{2} \leq \phi(A),$$

where  $\sigma_2(A)$  is the second largest singular value of  $A$ .

*Proof.* The proof immediately follows by noting that for  $v \perp w$ ,  $\langle v, Av \rangle \leq \sigma_2(A) \langle v, v \rangle$  by basic linear algebra, and using lemmas 3.1.1 gives the result.  $\square$

We note that Lemma 3.5.1 is not very meaningful in the following sense – let  $A$  be a directed cycle, then  $\sigma_2(A) = 1$  but  $\phi(A) \approx 1/n$ , showing the bound is not continuous. A larger gap can be obtained by de Bruijn matrices – discussed in Section 4.4 – for which  $\sigma_2(A) = 1$  but  $\phi(A) \approx 1/\log n$ .

Another thought might be to first ensure that  $A$  is lazy, or write  $A' = \frac{1}{2}A + \frac{1}{2}I$ , in which case  $\sigma_2(A')$  might become more meaningful for  $\phi(A') = \frac{1}{2}\phi(A)$ . However, noting that  $A = w \cdot w^T + B$  and  $A^T = w \cdot w^T + B^T$ , we have that the second largest eigenvalue of  $\tilde{A} = \frac{1}{2}(A + A^T)$

$$\frac{1}{2}(A + A^T) = w \cdot w^T + \frac{1}{2}(B + B^T)$$

is exactly the largest eigenvalue of  $\tilde{B} = \frac{1}{2}(B + B^T)$ . Further, since  $A$  is such that  $\|A\|_2 = 1$  from Lemma 3.0.3 since it has the same left and right eigenvector  $w$  for eigenvalue 1, it implies that  $\sigma_2(A) = \|B\|_2$ . Thus, let  $x$  with  $\|x\|_2 = 1$  be the eigenvector for the largest eigenvalue of  $\frac{1}{2}(B + B^T)$ , then

$$\lambda_2\left(\frac{1}{2}(A + A^T)\right) = \langle x, \frac{1}{2}(B + B^T)x \rangle \leq \frac{1}{2}\|x\|_2\|Bx\|_2 + \frac{1}{2}\|x\|_2\|B^T x\|_2 = \|B\|_2 = \sigma_2(A).$$

Thus, using easy cheeger, we would have

$$\frac{1}{2} - \frac{1}{2}\sigma_2(A) \leq \frac{1}{2} - \frac{1}{4}\lambda_2(A + A^T) \leq \phi(A),$$

and singular values are again not meaningful since the lower bound provided by them is weaker.

### 3.6 Limits of perturbation theory

In this section, we discuss one perturbation bound to illustrate the difficulty in proving a lower bound on  $\phi(R)$  in terms of the spectral gap using tools from perturbation theory, and also illuminate the contrast with Theorem 1.4.1. The Baur-Fike bounds state the following.

**Lemma 3.6.1.** (*Baur-Fike [BF60]*) *Let  $A$  be any diagonalizable matrix with such that  $A = VGV^{-1}$  is the Jordan form for  $A$  with  $\mathcal{K}_p(A) = \|V\|_p\|V^{-1}\|_p$ . Let  $E$  be a perturbation of  $A$ , such that  $A' = A + E$ . Then for every eigenvalue  $\mu$  of  $A'$ , there is an eigenvalue  $\lambda$  of  $A$  such that*

$$|\mu - \lambda| \leq \mathcal{K}_p(A) \cdot \|E\|_p.$$

The proof is simple but we do not rewrite it here. Note that to contrast with our Theorem 1.4.1, let  $S$  be the set that achieves  $\phi$  for  $A$  (assume it has largest eigenvalue 1), and let  $A'$  be two disconnected components where the mass going out and coming into the set  $S$  has been removed and put back within the sets to ensure that the largest eigenvalue of  $A'$  is 1. Note that  $\lambda_2(A') = \lambda_2(A) = 1 = \lambda_1(A)$ , and thus, from the above lemma, we get that

$$\Delta(A) \leq \mathcal{K}_p(A) \cdot \|E\|_p.$$

Note that even if we could have a bound where  $\|E\|_p \approx \phi(A)$ , the dependence of  $\mathcal{K}(A)$  cannot be avoided, and further, it is still limited to diagonalizable matrices. An extension to general matrices was obtained by Saad [Saa11].

**Lemma 3.6.2.** (*Baur-Fike extension by Saad [Saa11]*) *Let  $A$  be any matrix (not necessarily diagonalizable), and let  $\mathcal{K}_2(A) = \|V\|_2\|V^{-1}\|_2$  for the Jordan decomposition  $A = VGV^{-1}$ . Let  $E$  be a perturbation of  $A$ , such that  $A' = A + E$ . Then for every eigenvalue  $\mu$  of  $A'$ , there is an eigenvalue  $\lambda$  of  $A$  such that*

$$1 \leq \frac{1}{|\lambda - \mu|} \sum_{i=0}^{l-1} \left( \frac{1}{|\lambda - \mu|} \right)^i \mathcal{K}_2(A) \|E\|_2$$

where  $l$  is the size of the largest Jordan block.

We can reprove the lemma using Schur decomposition instead of the Jordan decomposition, and we get the following.

**Lemma 3.6.3.** *Let  $A$  be any matrix (not necessarily diagonalizable) with largest singular value  $\sigma = \|A\|_2$ . Let  $E$  be a perturbation of  $A$ , such that  $A' = A + E$ . Then for every eigenvalue  $\mu$  of  $A'$ , there is an eigenvalue  $\lambda$  of  $A$  such that*

$$1 \leq \frac{1}{|\lambda - \mu|} \left( 1 + \frac{\sigma}{|\lambda - \mu|} \right)^{n-1} \|E\|_2.$$

*Proof.* Let  $A = UTU^*$  be the Schur decomposition of  $A$ . Let  $T$  be an upper triangular matrix with  $|T_{i,i}| \geq \alpha > 0$  implying that  $T$  is invertible, and  $\|T\| \leq \sigma$ . Let maximum entry at distance  $k$  from diagonal in  $T^{-1}$  be  $\gamma_k$ . Note that for the diagonal entries of  $T^{-1}$ , we have that  $|T^{-1}(k, k)| \leq \frac{1}{\alpha}$ . Thus  $\gamma_0 \leq \frac{1}{\alpha}$ . Assume for  $k \geq 1$ ,

$$\gamma_k \leq \frac{\sigma}{\alpha^2} \left( 1 + \frac{\sigma}{\alpha} \right)^{k-1}.$$

For  $k = 1$ , it is easy to verify that for any row  $r$ ,

$$T^{-1}(r, r)T(r, r+1) + T^{-1}(r, r+1)T(r+1, r+1) = 0$$

and thus

$$|T^{-1}(r, r+1)| \leq \frac{|T^{-1}(r, r)| \cdot |T(r, r+1)|}{|T(r+1, r+1)|} \leq \frac{\frac{1}{\alpha} \cdot \sigma}{\alpha} = \frac{\sigma}{\alpha^2}$$

as required. Assume the above equation holds for all  $\gamma_l$  for  $l \leq k$ , we will show the equation for  $\gamma_{k+1}$ . Consider any entry  $x$  in  $T^{-1}$  at distance  $x = k + 1$  from the diagonal. Then since  $T^{-1}T = I$ , we get that for some fixed row  $r$ , and column  $r + x$ ,

$$\begin{aligned} \sum_j T^{-1}(r, j)T(j, r+x) &= 0 \\ \sum_{j=r}^{r+x} T^{-1}(r, j)T(j, r+x) &= 0 \\ \sum_{j=r}^{r+x-1} T^{-1}(r, j)T(j, r+x) + T^{-1}(r, r+x)T(r+x, r+x) &= 0 \end{aligned}$$

and thus

$$\begin{aligned}
|T^{-1}(r, r+x)| &\leq \frac{1}{T(r+x, r+x)} \sum_{j=r}^{r+x-1} |T^{-1}(r, j)| \cdot |T(j, r+x)| \\
&\leq \frac{1}{\alpha} \left( \frac{\sigma}{\alpha} + \sum_{j=r+1}^{r+x-1} \gamma_{j-r} \cdot \sigma \right) \\
&= \frac{\sigma}{\alpha} \left( \frac{1}{\alpha} + \sum_{j-r=1}^{j-r=x-1} \gamma_{j-r} \right) \\
&= \frac{\sigma}{\alpha} \left( \frac{1}{\alpha} + \sum_{l=1}^{l=k} \gamma_l \right) \\
&= \frac{\sigma}{\alpha} \left( \frac{1}{\alpha} + \sum_{l=1}^{l=k} \frac{\sigma}{\alpha^2} \left( 1 + \frac{\sigma}{\alpha} \right)^{l-1} \right) \\
&= \frac{\sigma}{\alpha} \left( \frac{1}{\alpha} + \frac{\sigma}{\alpha^2} \frac{\left( 1 + \frac{\sigma}{\alpha} \right)^k - 1}{\left( 1 + \frac{\sigma}{\alpha} \right) - 1} \right) \\
&= \frac{\sigma}{\alpha^2} \left( 1 + \frac{\sigma}{\alpha} \right)^k \\
&= \gamma_{k+1}.
\end{aligned}$$

Thus we have

$$\|T^{-1}\|_2 \leq n \sum_{i=0}^{n-1} \gamma_i \leq \frac{1}{\alpha} \left( 1 + \frac{\sigma}{\alpha} \right)^{n-1} \quad (3.6.4)$$

and reproving Baur-Fike using Schur decomposition, we get that for some eigenvalue  $\mu$  of  $A + E$  and corresponding eigenvector  $v$ , we have

$$(A + E)v = \mu v,$$

$$1 \leq \|(A - \mu I)^{-1}\|_2 \|E\|_2,$$

and thus, writing  $A = UTU^*$ , we get from equation 3.6.4 that the eigenvalue  $\lambda$  of  $A$  closed to  $\mu$  is such that,

$$1 \leq \frac{1}{|\lambda - \mu|} \left( 1 + \frac{\|A\|_2}{|\lambda - \mu|} \right)^{n-1} \|E\|_2.$$

Similarly, expanding  $A = VGV^{-1}$  with the Jordan decomposition, we get by expanding each block using

$$(|\lambda - \mu|I + E)^{-1} = \frac{1}{|\lambda - \mu|} \sum_{i=0}^{l-1} \left( \frac{1}{|\lambda - \mu|} \right)^i,$$

that

$$1 \leq \frac{1}{|\lambda - \mu|} \sum_{i=0}^{l-1} \left( \frac{1}{|\lambda - \mu|} \right)^i \mathcal{K}_2(A) \|E\|_2.$$

□

Thus, for general matrices, there is a loss of a factor of  $\exp(n)$ , and a further loss of a factor of  $\mathcal{K}(A)$  if Lemma 3.6.3 is used, or  $\sigma(A)$  if Lemma 3.6.3 is used. Thus for general matrices, these give extremely weak lower bounds for  $\phi$  even if we choose  $E$  appropriately. Thus we need different ideas.

### 3.7 Lower bound on $\phi(R)$ in terms of $\Delta(R)$

As a consequence of the discussion in the previous two sections, we want to obtain a more meaningful bound than that provided by singular values and also one that is independent of the condition numbers or exponential factors or singular values, so that combined with Lemma 3.4.1, it provides us with a complete generalization of the Perron-Frobenius theorem. The lower bound will be the result of a sequence of lemmas that we state next. Before that, we want to give an overview of the proof. For ease of understanding, we will discuss it for the case of double stochastic matrices – which have the uniform distribution as the fixed point – and they turn out to be a sufficiently rich special case that contains the properties of the general case.

Consider an irreducible doubly stochastic matrix  $A$ . Note that all our spectral reasoning so far relied crucially on the spectral decomposition of some matrix in all of our Lemmas 3.2.1, 3.0.1, 3.5.1. However, we cannot use it for showing a result which has form as in Theorem 1.4.1 for the lower bound on  $\phi(A)$  since  $A$  cannot be diagonalized by a unitary, and attempting to mimic the proof of Buser's inequality (Section 3.1) only gives us a lemma similar to 3.5.1. As discussed in the previous section, other theorems in literature which could be used in limited contexts – Baur-Fike for instance in cases where  $A$  is diagonalizable, however extending them using the Schur or Jordan decomposition to general non-diagonalizable matrices or using other tools from perturbation theory gives lower bounds with factors exponential in  $n$ , and/or a dependence on the eigenvalue/eigenvector condition numbers of  $A$ , and/or a dependence on the largest singular value of  $A$ , as shown in Lemma 3.6.3 by using the Schur decomposition instead of the Jordan decomposition. The singular values and the eigenvalue condition numbers of  $A$  are less meaningful if  $A$  is doubly stochastic, but they become dominant when we consider general matrices as required in Theorem 1.4.1.

The key idea that unlocks the entire proof is to try and understand  $\phi(A^2)$  and  $\phi(A^k)$ . It turns out that  $\phi(A^k) \leq k \cdot \phi(A)$ . Note that this helps us lower bound the edge expansion of  $A$  by understanding the edge expansion of  $A^k$ . Write  $A = J + UTU^*$  where  $J = \frac{1}{n}\mathbf{1} \cdot \mathbf{1}^T$ , and  $U$  is the unitary and  $T$  the upper triangular matrix in the Schur decomposition of  $A - J$ . Further, it is simple to see that  $A^k = J + UT^kU^*$ . We need to find a sufficiently small  $k$  such that the expansion of  $A^k$  is easy to bound. To do this, we will try to ensure that for some  $k$ ,  $\|T^k\| \approx 0$ , and thus  $\phi(A^k) \approx \phi(J) = \text{constant}$ .

Note that since the eigenspace corresponding to the largest eigenvalue 1 is removed in  $J$ , the diagonal of  $T$  contains all the eigenvalues of  $A$  with eigenvalue 1 replaced by 0. Let the eigenvalue with largest magnitude be  $\lambda_m$  and assume that  $|\lambda_m| < 1$ . If we raise  $T^{1/1-|\lambda_m|}$ , then it is clear that every entry in its diagonal will be about  $e^{-1}$ , and the diagonal will exponentially decrease by taking further powers. Thus the diagonal entries of  $T^{\log n/(1-|\lambda_m|)}$  will all be inverse polynomially small, and assume at this point that they are approximately 0. Thus, the matrix will now behave in a manner similar to a nilpotent matrix, and it will follow that  $\|T^{n \log n/(1-|\lambda_m|)}\| \approx 0$ . Thus for  $k \approx \frac{n \cdot \log n}{1 - |\lambda_m|}$ , we will have

$$\phi(A) \geq \frac{1}{k} \phi(A^k) \approx \frac{1}{k} \phi(J) \approx \frac{1 - |\lambda_m|}{n \cdot \log n},$$

qualitatively giving us the kind of bound that we need. There are many technical caveats that produce a dependence on the largest singular value of  $A$  and the eigenvalue condition number of the largest eigenvalue of  $A$ , but a careful analysis (with sufficient tricks) helps us avoid both the factors, and also helps us remove the factor of  $\log n$  and transform the dependence from  $|\lambda_m|$  to  $\text{Re}\lambda_2$ .

We proceed now to prove the lower bound in Theorem 3.0.2.

The first lemma states that  $\phi$  is sub-multiplicative in the following sense.

**Lemma 3.7.1.** *(Submultiplicativity of  $\phi_S$ ) Let  $R$  and  $B$  be nonnegative matrices that have the same left and right eigenvectors  $u$  and  $v$  for eigenvalue 1. Then for every cut  $S$ , we have that*

$$\phi_S(RB) \leq \phi_S(R) + \phi_S(B).$$

*Proof.* Let

$$\gamma_S(R) = \langle \mathbf{1}_{\bar{S}}, D_u R D_v \mathbf{1}_S \rangle + \langle \mathbf{1}_S, D_u R D_v \mathbf{1}_{\bar{S}} \rangle$$

and similarly  $\gamma_S(B)$ . Without loss of generality, we assume that the largest eigenvalue of  $R$  and  $B$  is 1, since the edge expansion does not change by scaling 3.0.3. Then for



every cut  $S$ , we will show that

$$\gamma_S(RB) \leq \gamma_S(R + B) = \gamma_S(R) + \gamma_S(B).$$

Fix any cut  $S$ . Assume  $R = \begin{bmatrix} P & Q \\ H & V \end{bmatrix}$  and  $B = \begin{bmatrix} X & Y \\ Z & W \end{bmatrix}$  naturally divided based on cut  $S$ . For any vector  $u$ , let  $D_u$  be the diagonal matrix with  $u$  on the diagonal. Since  $Rv = v$ ,  $R^T u = u$ ,  $Bv = v$ ,  $B^T u = u$ , we have

$$P^T D_{u_S} \mathbf{1} + H^T D_{u_{\bar{S}}} \mathbf{1} = D_{u_S} \mathbf{1}, \quad (3.7.2)$$

$$Z D_{v_S} \mathbf{1} + W D_{v_{\bar{S}}} \mathbf{1} = D_{v_{\bar{S}}} \mathbf{1}, \quad (3.7.3)$$

$$X D_{v_S} \mathbf{1} + Y D_{v_{\bar{S}}} \mathbf{1} = D_{v_S} \mathbf{1}, \quad (3.7.4)$$

$$Q^T D_{u_S} \mathbf{1} + V^T D_{u_{\bar{S}}} \mathbf{1} = D_{u_{\bar{S}}} \mathbf{1}, \quad (3.7.5)$$

where  $u$  is divided into  $u_S$  and  $u_{\bar{S}}$  and  $v$  into  $v_S$  and  $v_{\bar{S}}$  naturally based on the cut  $S$ . Further, in the equations above and in what follows, the vector  $\mathbf{1}$  is the all 1's vector with dimension either  $|S|$  or  $|\bar{S}|$  which should be clear from the context of the equations, and we avoid using different vectors to keep the notation simpler. Then we have from the definition of  $\gamma_S$ ,

$$\begin{aligned} \gamma_S(R) &= \langle \mathbf{1}_{\bar{S}}, D_u R D_v \mathbf{1}_S \rangle + \langle \mathbf{1}_S, D_u R D_v \mathbf{1}_{\bar{S}} \rangle \\ &= \langle \mathbf{1}, D_{u_S} Q D_{v_{\bar{S}}} \mathbf{1} \rangle + \langle \mathbf{1}, D_{u_{\bar{S}}} H D_{v_S} \mathbf{1} \rangle \end{aligned}$$

and similarly

$$\gamma_S(B) = \langle \mathbf{1}, D_{u_S} Y D_{v_{\bar{S}}} \mathbf{1} \rangle + \langle \mathbf{1}, D_{u_{\bar{S}}} Z D_{v_S} \mathbf{1} \rangle.$$

The matrix  $RB$  also has  $u$  and  $v$  as the left and right eigenvectors for eigenvalue 1 respectively, and thus,

$$\begin{aligned}
\gamma_S(RB) &= \langle \mathbf{1}, D_{u_S} P Y D_{v_S} \mathbf{1} \rangle + \langle \mathbf{1}, D_{u_S} Q W D_{v_S} \mathbf{1} \rangle + \langle \mathbf{1}, D_{u_S} H X D_{v_S} \mathbf{1} \rangle + \langle \mathbf{1}, D_{u_S} V Z D_{v_S} \mathbf{1} \rangle \\
&= \langle P^T D_{u_S} \mathbf{1}, Y D_{v_S} \mathbf{1} \rangle + \langle \mathbf{1}, D_{u_S} Q W D_{v_S} \mathbf{1} \rangle + \langle \mathbf{1}, D_{u_S} H X D_{v_S} \mathbf{1} \rangle + \langle V^T D_{u_S} \mathbf{1}, Z D_{v_S} \mathbf{1} \rangle \\
&= \langle D_{u_S} \mathbf{1} - H^T D_{u_S} \mathbf{1}, Y D_{v_S} \mathbf{1} \rangle + \langle \mathbf{1}, D_{u_S} Q (D_{v_S} \mathbf{1} - Z D_{v_S} \mathbf{1}) \rangle \\
&\quad + \langle \mathbf{1}, D_{u_S} H (D_{v_S} \mathbf{1} - Y D_{v_S} \mathbf{1}) \rangle + \langle D_{u_S} \mathbf{1} - Q^T D_{u_S} \mathbf{1}, Z D_{v_S} \mathbf{1} \rangle \\
&\quad \text{[from equations 3.7.2, 3.7.3, 3.7.4, 3.7.5 above]} \\
&= \langle D_{u_S} \mathbf{1}, Y D_{v_S} \mathbf{1} \rangle + \langle \mathbf{1}, D_{u_S} Q D_{v_S} \mathbf{1} \rangle - \langle H^T D_{u_S} \mathbf{1}, Y D_{v_S} \mathbf{1} \rangle - \langle \mathbf{1}, D_{u_S} Q Z D_{v_S} \mathbf{1} \rangle \\
&\quad + \langle \mathbf{1}, D_{u_S} H D_{v_S} \mathbf{1} \rangle + \langle D_{u_S} \mathbf{1}, Z D_{v_S} \mathbf{1} \rangle - \langle \mathbf{1}, D_{u_S} H Y D_{v_S} \mathbf{1} \rangle - \langle Q^T D_{u_S} \mathbf{1}, Z D_{v_S} \mathbf{1} \rangle \\
&\leq \langle D_{u_S} \mathbf{1}, Y D_{v_S} \mathbf{1} \rangle + \langle \mathbf{1}, D_{u_S} Q D_{v_S} \mathbf{1} \rangle + \langle \mathbf{1}, D_{u_S} H D_{v_S} \mathbf{1} \rangle + \langle D_{u_S} \mathbf{1}, Z D_{v_S} \mathbf{1} \rangle \\
&\quad \text{[since every entry of the matrices is nonnegative, and thus each of the terms above]} \\
&= \gamma_S(R) + \gamma_S(B)
\end{aligned}$$

as required. Note that since  $R$  and  $B$  have the same left and right eigenvectors, so does  $RB$ , and since  $\langle \mathbf{1}_{\bar{S}}, D_u R D_v \mathbf{1}_S \rangle = \langle \mathbf{1}_S, D_u R D_v \mathbf{1}_{\bar{S}} \rangle$ , we exactly have that

$$\phi_S(R) = \frac{1}{2} \frac{\gamma_S(R)}{\sum_{i \in S} u_i v_i}$$

which gives the lemma.  $\square$

The following lemma follows directly as a corollary of Lemma 3.7.1, and is essentially the heart of the entire proof.

**Lemma 3.7.6.** (Submultiplicativity of  $\phi$ ) *Let  $R \in \mathbb{R}^{n \times n}$  be an irreducible nonnegative matrix with left and right eigenvectors  $u$  and  $v$  for the PF eigenvalue 1. Then*

$$\phi(R^k) \leq k \cdot \phi(R).$$

*Proof.* Noting that  $R^k$  has  $u$  and  $v$  as left and right eigenvectors for any  $k$ , we inductively get using Lemma 3.7.1 that

$$\phi_S(R^k) \leq \phi_S(R) + \phi_S(R^{k-1}) \leq \phi_S(R) + (k-1) \cdot \phi_S(R) = k \cdot \phi_S(R),$$

and we get by letting  $S$  be the set that minimizes  $\phi(R)$ , that

$$\phi(R^k) \leq k \cdot \phi(R).$$

$\square$

For the case of *symmetric* doubly stochastic matrices  $R$ , Lemma 3.7.6 follows from a theorem of Blakley and Roy [BR65]. (It does not fall into the framework of an extension of that result to the nonsymmetric case [Pat12]). Lemma 3.7.6 helps to lower bound  $\phi(R)$  by taking powers of  $R$ , which is useful since we can take sufficient powers in order to make the matrix simple enough that its edge expansion is easily calculated.

The next two lemmas follow by technical calculations.

**Lemma 3.7.7.** (*Bounded norm of powers*) *Let  $T \in \mathbb{C}^{n \times n}$  be an upper triangular matrix with  $\|T\|_2 = \sigma$  and for every  $i$ ,  $|T_{i,i}| \leq \alpha < 1$ . Then*

$$\|T^k\|_2 \leq n \cdot \sigma^n \cdot \binom{k+n}{n} \cdot \alpha^{k-n}.$$

*Proof.* Let  $g_r(k)$  denote the maximum of the absolute value of entries at distance  $r$  from the diagonal in  $T^k$ , where the diagonal is at distance 0 from the diagonal, the off-diagonal is at distance 1 from the diagonal and so on. More formally,

$$g_r(k) = \max_i |T^k(i, i+r)|.$$

We will inductively show that for  $\alpha \leq 1$ , and  $r \geq 1$ ,

$$g_r(k) \leq \binom{k+r}{r} \cdot \alpha^{k-r} \cdot \sigma^r, \quad (3.7.8)$$

where  $\sigma = \|T\|_2$ . First note that for  $r = 0$ , since  $T$  is upper triangular, the diagonal of  $T^k$  is  $\alpha^k$ , and thus the hypothesis holds for  $r = 0$  and all  $k \geq 1$ . Further, for  $k = 1$ , if  $r = 0$ , then  $g_0(1) \leq \alpha$  and if  $r \geq 1$ , then  $g_r(1) \leq \|T\|_2 \leq \sigma$  and the inductive hypothesis holds also in this case, since  $r \geq k$  and  $\alpha^{k-r} \geq 1$ . For the inductive step, assume that for all  $r \geq 1$  and all  $j \leq k-1$ ,  $g_r(j) \leq \binom{j+r}{r} \cdot \alpha^{j-r} \cdot \sigma^r$ . We will show the calculation for  $g_r(k)$ .

Since  $|a+b| \leq |a|+|b|$ ,

$$\begin{aligned} g_r(k) &\leq \sum_{i=0}^r g_{r-i}(1) \cdot g_i(k-1) \\ &= g_0(1) \cdot g_r(k-1) + \sum_{i=0}^{r-1} g_{r-i}(1) \cdot g_i(k-1). \end{aligned}$$

The first term can be written as,

$$\begin{aligned}
g_0(1) \cdot g_r(k-1) &= \alpha \cdot \binom{k-1+r}{r} \cdot \alpha^{k-1-r} \cdot \sigma^r \\
&\quad [\text{using that } g_0(1) \leq \alpha \text{ and the inductive hypothesis for the second term}] \\
&\leq \alpha^{k-r} \cdot \sigma^r \cdot \binom{k+r}{r} \cdot \frac{\binom{k-1+r}{r}}{\binom{k+r}{r}} \\
&\leq \frac{k}{k+r} \cdot \binom{k+r}{r} \cdot \alpha^{k-r} \cdot \sigma^r
\end{aligned} \tag{3.7.9}$$

and the second term as

$$\begin{aligned}
g_r(k) &\leq \sum_{i=0}^{r-1} g_{r-i}(1) \cdot g_i(k-1) \\
&\leq \sigma \cdot \sum_{i=0}^{r-1} \binom{k-1+i}{i} \cdot \alpha^{k-1-i} \cdot \sigma^i \\
&\quad [\text{using } g_{r-i}(1) \leq \sigma \text{ and the inductive hypothesis for the second term}] \\
&\leq \sigma^r \cdot \alpha^{k-r} \cdot \binom{k+r}{r} \cdot \sum_{i=0}^{r-1} \frac{\binom{k-1+i}{i}}{\binom{k+r}{r}} \cdot \alpha^{r-1-i} \\
&\quad [\text{using } \sigma^i \leq \sigma^{r-1} \text{ since } \sigma \geq 1 \text{ and } i \leq r-1] \\
&\leq \sigma^r \cdot \alpha^{k-r} \cdot \binom{k+r}{r} \cdot \sum_{i=0}^{r-1} \frac{\binom{k-1+i}{i}}{\binom{k+r}{r}} \\
&\quad [\text{using } \alpha \leq 1 \text{ and } i \leq r-1]
\end{aligned}$$

We will now show that the quantity inside the summation is at most  $\frac{r}{k+r}$ . Inductively, for  $r = 1$ , the statement is true, and assume that for any other  $r$ ,

$$\sum_{i=0}^{r-1} \frac{\binom{k-1+i}{i}}{\binom{k+r}{r}} \leq \frac{r}{k+r}.$$

Then we have

$$\begin{aligned}
\sum_{i=0}^r \frac{\binom{k-1+i}{i}}{\binom{k+r+1}{r+1}} &= \frac{\binom{k+r}{r}}{\binom{k+r+1}{r+1}} \cdot \sum_{i=0}^{r-1} \frac{\binom{k-1+i}{i}}{\binom{k+r}{r}} + \frac{\binom{k-1+r}{k}}{\binom{k+r+1}{r+1}} \\
&\leq \frac{r+1}{k+r+1} \cdot \frac{r}{k+r} + \frac{(r+1) \cdot k}{(k+r+1) \cdot (k+r)} \\
&= \frac{r+1}{k+r+1}
\end{aligned}$$

Thus we get that the second term is at most  $\sigma^r \cdot \alpha^{k-r} \cdot \binom{k+r}{r} \cdot \frac{r}{k+r}$ , and combining it with the first term (equation 3.7.9), it completes the inductive hypothesis.

Noting that the operator norm is at most the Frobenius norm, and since  $g_r(k)$  is increasing in  $r$  and the maximum value of  $r$  is  $n$ , we get using equation 3.7.8,

$$\begin{aligned} \|T^k\|_2 &\leq \sqrt{\sum_{i,j} |T^k(i,j)|^2} \\ &\leq n \cdot \sigma^n \cdot \alpha^{k-n} \cdot \binom{k+n}{n} \end{aligned}$$

as required.  $\square$

Using Lemma 3.7.7, we can show the following lemma for the special case of upper triangular matrices with operator norm at most 1.

**Lemma 3.7.10.** *Let  $T \in \mathbb{C}^{n \times n}$  be an upper triangular matrix with  $\|T\|_2 \leq 1$  and  $|T_{i,i}| \leq \alpha < 1$  for every  $i$ . Assume  $T^k$  is well defined for every real  $k$ . Then  $\|T^k\| \leq \epsilon$  for*

$$k \geq \frac{4n + 2 \ln(\frac{n}{\epsilon})}{\ln\left(\frac{1}{\alpha}\right)}.$$

*Proof.* Let  $X = T^{k_1}$ , where  $k_1 = \frac{c_1}{\ln(\frac{1}{\alpha})}$  for  $\alpha < 1$ . Then  $\|X\|_2 \leq \|T\|_2^{k_1} \leq 1$ , and for every  $i$ ,

$$|X_{i,i}| \leq |T_{i,i}|^{k_1} \leq |\lambda_m|^{c_1/\ln(\frac{1}{\alpha})} = e^{-c_1}.$$

Using Lemma 3.7.7 for  $X$  with  $\sigma = 1$  and  $\beta = e^{-c_1}$ , we get that for  $k_2 = c_2 \cdot n$ ,

$$\begin{aligned} \|X^{k_2}\| &\leq n \cdot \binom{k_2+n}{n} \cdot e^{-c_1(k_2-n)} \\ &\leq n \cdot e^n \cdot (c_2+1)^n \cdot e^{-c_1(c_2-1)n} \\ &\quad \text{[using } \binom{a}{b} \leq \left(\frac{ea}{b}\right)^b \text{]} \\ &= \exp\left(n \cdot \left(\frac{\ln n}{n} + \ln(c_2+1) + 1 + c_1 - c_1c_2\right)\right) \end{aligned}$$

and to have this quantity less than  $\epsilon$ , we require

$$\begin{aligned} &\exp\left(n \cdot \left(\frac{\ln n}{n} + \ln(c_2+1) + 1 + c_1 - c_1c_2\right)\right) \leq \epsilon \\ \Leftrightarrow &\left(\frac{1}{\epsilon}\right)^{\frac{1}{n}} \leq \exp\left(-1 \cdot \left(\frac{\ln n}{n} + \ln(c_2+1) + 1 + c_1 - c_1c_2\right)\right) \\ \Leftrightarrow &\frac{1}{n} \ln \frac{n}{\epsilon} + 1 + c_1 + \ln(c_2+1) \leq c_1c_2 \end{aligned} \tag{3.7.11}$$

and we set

$$c_1 = 1 + \frac{1}{2.51} \cdot \frac{1}{n} \ln\left(\frac{n}{\epsilon}\right)$$

and  $c_2 = 3.51$  which always satisfies inequality 3.7.11. As a consequence, for

$$\begin{aligned} k &= k_1 \cdot k_2 \\ &= \frac{c_1 \cdot c_2 \cdot n}{\ln\left(\frac{1}{\alpha}\right)} \\ &= \frac{3.51 \cdot n + 1.385 \cdot \ln\left(\frac{n}{\epsilon}\right)}{\ln\left(\frac{1}{\alpha}\right)} \end{aligned}$$

we get,

$$\|T^k\|_2 \leq \|X^{k_2}\| \leq \epsilon$$

as required. □

Given lemmas 3.7.6 and 3.7.10, we can lower bound  $\phi(R)$  in terms of  $\ln\left(\frac{1}{|\lambda_m|}\right)$  (where  $\lambda_m$  is the nontrivial eigenvalue that is maximum in magnitude). Our aim is to lower bound  $\phi(R)$  by  $\phi(R^k)$ , but since the norm of  $R^k$  increases by powering, we cannot use the lemmas directly, since we do not want a dependence on  $\sigma(R)$  in the final bound. To handle this, we transform  $R$  to  $A$ , such that  $\phi(R) = \phi(A)$ , the eigenvalues of  $R$  and  $A$  are the same, but  $\sigma(A) = \|A\|_2 = 1$  irrespective of the norm of  $R$ , using Lemma 3.0.3.

Given Lemma 3.0.3, we lower bound  $\phi(A)$  using  $\phi(A^k)$  in terms of  $1 - |\lambda_m(A)|$ , to obtain the corresponding bounds for  $R$ .

**Lemma 3.7.12.** *Let  $R$  be an irreducible nonnegative matrix with positive (left and right) eigenvectors  $u$  and  $v$  for the PF eigenvalue 1, normalized so that  $\langle u, v \rangle = 1$ . Let  $\lambda_m$  be the nontrivial eigenvalue of  $R$  that is maximum in magnitude, and let  $R^k$  be well-defined for every real  $k$ . Then*

$$\frac{1}{15} \cdot \frac{\ln\left(\frac{1}{|\lambda_m|}\right)}{n} \leq \phi(R).$$

*Proof.* From the given  $R$  with positive left and right eigenvectors  $u$  and  $v$  for eigenvalue 1 as stated, let  $A = D_u^{\frac{1}{2}} D_v^{-\frac{1}{2}} R D_u^{-\frac{1}{2}} D_v^{\frac{1}{2}}$  and  $w = D_u^{\frac{1}{2}} D_v^{\frac{1}{2}} \mathbf{1}$  as in Lemma 3.0.3. Note that  $w$  is positive, and

$$\langle w, w \rangle = \langle D_u^{\frac{1}{2}} D_v^{\frac{1}{2}} \mathbf{1}, D_u^{\frac{1}{2}} D_v^{\frac{1}{2}} \mathbf{1} \rangle = \langle u, v \rangle = 1.$$

Further,  $Aw = w$  and  $A^T w = w$ , and since  $A^k = D_u^{\frac{1}{2}} D_v^{-\frac{1}{2}} R^k D_u^{-\frac{1}{2}} D_v^{\frac{1}{2}}$  it is well-defined for every real  $k$ .

Let  $A = w \cdot w^T + B$ . Since  $(w \cdot w^T)^2 = w \cdot w^T$  and  $Bw \cdot w^T = w \cdot w^T B = 0$ , we get

$$A^k = w \cdot w^T + B^k.$$

Let  $B = UTU^*$  be the Schur decomposition of  $B$ , where the diagonal of  $T$  contains all but the stochastic eigenvalue of  $A$ , which is replaced by 0, since  $w$  is both the left and right eigenvector for eigenvalue 1 of  $A$ , and that space is removed in  $w \cdot w^T$ . Further, the maximum diagonal entry of  $T$  is at most  $|\lambda_m|$  where  $\lambda_m$  is the nontrivial eigenvalue of  $A$  (or  $R$ ) that is maximum in magnitude. Note that  $|\lambda_m| < 1$  since  $A$  (and  $R$ ) is irreducible. Since  $w \cdot w^T B = Bw \cdot w^T = 0$  and  $\|A\|_2 \leq 1$  from Lemma 3.0.3, we have that  $\|B\|_2 \leq 1$ .

Thus, using Lemma 3.7.10 (in fact, the last lines in the proof of Lemma 3.7.10), for

$$k \geq \frac{3.51 \cdot n + 1.385 \cdot \ln\left(\frac{n}{\epsilon}\right)}{\ln\left(\frac{1}{|\lambda_m|}\right)},$$

we get that

$$\|B^k\|_2 = \|T^k\|_2 \leq \epsilon,$$

and for  $e_i$  being the vector with 1 at position  $i$  and zeros elsewhere, we get using Cauchy-Schwarz

$$|B^k(i, j)| = |\langle e_i, B^k e_j \rangle| \leq \|e_i\|_2 \|B\|_2 \|e_j\|_2 \leq \epsilon.$$

Further, note that  $B^k w = 0$  and  $w^T B^k = 0$ . This means that for any  $i$  and  $S \subseteq [n]$ ,

$$\sum_{j \in S} B^k(i, j) w_j = - \sum_{j \in \bar{S}} B^k(i, j) w_j$$

Thus, for any set  $S$  for which  $\sum_{i \in S} w_i^2 \leq \frac{1}{2}$ , then

$$\begin{aligned}
\phi_S(A^k) &= \frac{\langle \mathbf{1}_S, D_w A^k D_w \mathbf{1}_{\bar{S}} \rangle}{\langle \mathbf{1}_S, D_w D_w \mathbf{1} \rangle} \\
&= \frac{\sum_{i \in S, j \in \bar{S}} A^k(i, j) \cdot w_i \cdot w_j}{\sum_{i \in S} w_i^2} \\
&= \frac{\sum_{i \in S, j \in \bar{S}} (w \cdot w^T(i, j) + B^k(i, j)) \cdot w_i \cdot w_j}{\sum_{i \in S} w_i^2} \\
&= \frac{\sum_{i \in S} w_i^2 \sum_{j \in \bar{S}} w_j^2 - \sum_{i \in S, j \in S} B^k(i, j) \cdot w_i \cdot w_j}{\sum_{i \in S} w_i^2} \\
&\geq \sum_{j \in \bar{S}} w_j^2 - \epsilon \frac{(\sum w_i^2)^2}{\sum_{i \in S} w_i^2} \\
&\geq \frac{1}{2}(1 - \epsilon)
\end{aligned}$$

since  $\sum_{i \in S} w_i^2 \leq \frac{1}{2}$ . Note that this holds for *every* set  $S$ . Thus, we get that for

$$k \geq \frac{3.51n + 1.385 \cdot \ln\left(\frac{n}{\epsilon}\right)}{\ln\left(\frac{1}{|\lambda_m|}\right)}$$

the edge expansion

$$\phi(A^k) \geq \frac{1}{2}(1 - \epsilon),$$

and thus using Lemma 3.7.6, we get that

$$\phi(A) \geq \frac{1}{k} \cdot \phi(A^k) \geq \frac{1 - \epsilon}{2} \cdot \frac{\ln\left(\frac{1}{|\lambda_m|}\right)}{3.51 \cdot n + 1.385 \cdot \ln(n/\epsilon)}$$

and setting  $\epsilon = \frac{1}{2 \cdot e}$ , and using  $\ln(e \cdot x) \leq x$ , we get that

$$\phi(A) \geq \frac{1}{15} \cdot \frac{\ln\left(\frac{1}{|\lambda_m|}\right)}{n},$$

and it carries to  $R$  due to Lemma 3.0.3. □

We almost have the proof that we seek, but we need to take care of two issues. We need a dependence on  $\text{Re}\lambda_2$  instead of  $|\lambda_m|$ , and we need to ensure that we can take real powers of the underlying matrix on which the lemmas are applied. To solve both the issues, we will now focus on the exponential version of  $R$ , or  $E_R = \exp(R - I)$ . We note the following properties of this matrix.



**Lemma 3.7.13.** *Let  $E_R$  be the exponential version of  $R$ , i.e.  $E_R = \exp(R - I)$ . Then the following hold for  $E_R$ .*

1.  $E_A = D_u^{\frac{1}{2}} D_v^{-\frac{1}{2}} E_R D_u^{-\frac{1}{2}} D_v^{\frac{1}{2}}$  for  $A = D_u^{\frac{1}{2}} D_v^{-\frac{1}{2}} R D_u^{-\frac{1}{2}} D_v^{\frac{1}{2}}$
2. *The largest eigenvalue of  $E_R$  is 1, the left and right eigenvectors of  $E_R$  and  $R$  are same, and  $E_R$  is irreducible.*
3.  $(E_R)^k$  is well-defined for all real  $k$
4.  $\phi(E_R^t) \leq t \cdot \phi(R)$

*Proof.* The first three properties are straightforward and follow from the definitions. For the last property, we show for  $A$  and it will be implied for  $R$  by Lemma 3.0.3. For any set  $S$ , we can write

$$\begin{aligned}
\phi_S(E_A^t) &= \phi_S(\exp(t(A - I))) \\
&= e^{-t} \phi_S\left(\sum_{i=0}^{\infty} \frac{1}{i!} t^i A^i\right) \\
&= e^{-t} \left( \phi_S(I) + \sum_{i=1}^{\infty} \frac{t^i \cdot \phi_S(A^i)}{i!} \right) \\
&\leq e^{-t} \left( 0 + \sum_{i=1}^{\infty} i \frac{t^i \cdot \phi_S(A)}{i!} \right) \\
&\quad \text{[using Lemma 3.7.6]} \\
&= e^{-1} \left( t \cdot \phi_S(A) \sum_{i=1}^{\infty} \frac{t^{i-1}}{(i-1)!} \right) \\
&= t \cdot \phi_S(A)
\end{aligned}$$

and thus

$$\phi(E_A) \leq t \cdot \phi(A)$$

as required, and it extends to  $R$  by Lemma 3.0.3.  $\square$

Given Lemma 3.7.12, we use the exponential version of  $R$  to obtain the lower bound on edge expansion in Theorem 3.0.2, restated below.

**Lemma 3.7.14.** *Let  $R$  be an irreducible nonnegative matrix with positive (left and right) eigenvectors  $u$  and  $v$  for the PF eigenvalue 1, normalized so that  $\langle u, v \rangle = 1$ . Then*

$$\frac{1}{15} \cdot \frac{1 - \operatorname{Re}\lambda_2(R)}{n} \leq \phi(R).$$

*Proof.* We show the theorem for  $A$  and it extends to  $R$  by Lemma 3.0.3. Note that for every eigenvalue  $\lambda = a + i \cdot b$  of  $A$ , the corresponding eigenvalue of  $E_A$  is

$$\begin{aligned}\exp(\lambda - 1) &= \exp(a - 1) \exp(i \cdot b) \\ |\exp(\lambda - 1)| &= \exp(a - 1).\end{aligned}$$

Thus, to maximize the magnitude  $|\exp(\lambda - 1)|$  of the eigenvalue of  $E_A$ , we need to maximize  $\exp(a - 1)$ , and since  $a < 1$  as  $A$  is irreducible, the value  $|\exp(\lambda - 1)|$  is maximized when  $a$  is closest to 1. In other words, letting  $\lambda_m(E_A)$  be the eigenvalue of  $E_A$  that is largest in magnitude, we have that

$$|\lambda_m(E_A)| = \exp(\operatorname{Re}\lambda_2(A) - 1).$$

Applying Lemma 3.7.12 on  $E_A$ , we get that

$$\phi(E_A) \geq \frac{1}{15} \cdot \frac{\ln\left(\frac{1}{|\lambda_m(E_A)|}\right)}{n} = \frac{1}{15} \cdot \frac{1 - \operatorname{Re}\lambda_2(A)}{n},$$

and from Lemma 3.7.13, we finally get

$$\phi(A) \geq \frac{1}{15} \cdot \frac{1 - \operatorname{Re}\lambda_2(A)}{n}$$

as required, and it extends to  $R$  through Lemma 3.0.3.  $\square$

This completes the proof of our first main theorem, the lower bound on  $\phi$  for irreducible nonnegative matrices. A simple extension to all matrices follows after extending the definition of the spectral gap and edge expansion .

### 3.8 Extension of Theorem 3.0.2 to all nonnegative matrices

A simple lemma follows from the definition of  $\liminf$ .

**Lemma 3.8.1.** *Let  $p : E \rightarrow \mathbb{R}$  and  $q : E \rightarrow \mathbb{R}$  be two functions such that for all  $H \in E$ ,  $p(H) \leq q(H)$ . Then for all  $R$ ,*

$$\liminf_{\epsilon \rightarrow 0} \inf_{H \in R_\epsilon} p(H) \leq \liminf_{\epsilon \rightarrow 0} \inf_{H \in R_\epsilon} q(H).$$

*Proof.* Note that if  $R \in E$ , it holds trivially. Assume  $R \notin E$ . Fix  $\epsilon$ . Let  $a_\epsilon = \inf_{H \in R_\epsilon} p(H)$  and  $b_\epsilon = \inf_{H \in R_\epsilon} q(H)$ . First we claim that  $a_\epsilon \leq b_\epsilon$ . For the sake of contradiction, assume

$$a_\epsilon > b_\epsilon. \tag{3.8.2}$$

Let  $\delta_\epsilon = (a_\epsilon - b_\epsilon)/2 > 0$ , then there exists  $T \in E$  such that  $q(T) \leq b_\epsilon + \delta_\epsilon$  (else  $\inf_{H \in R_\epsilon} q(H) \geq b_\epsilon + \delta_\epsilon > b_\epsilon$ ). Further,

$$a_\epsilon \leq p(T) \leq q(T) \leq b_\epsilon + \delta_\epsilon$$

or  $a_\epsilon \leq b_\epsilon$ , a contradiction to 3.8.2. Thus,  $a_\epsilon \leq b_\epsilon$ .

Now let  $c_\epsilon = a_\epsilon - b_\epsilon$ , and we know that for all  $\epsilon > 0$ ,  $c_\epsilon \leq 0$ . It follows that

$$\lim_{\epsilon \rightarrow 0} c_\epsilon \leq 0 \tag{3.8.3}$$

Again for the sake of contradiction assume the contrary, i.e.  $\lim_{\epsilon \rightarrow 0} c_\epsilon > 0$  and  $\delta = \frac{1}{2} \lim_{\epsilon \rightarrow 0} c_\epsilon > 0$ . By the definition of limit, there exists  $\epsilon > 0$  such that  $c_\epsilon > \delta$ , or  $c_\epsilon > 0$ , a contradiction to 3.8.3. Thus the lemma follows.  $\square$

**Claim 3.8.4.** *The main Theorem 3.0.2 holds for all nonnegative matrices  $R$ .*

*Proof.* Follows from Lemma 3.8.1 after setting  $p$  and  $q$  appropriately.  $\square$

This concludes the proof of our main Theorem 1.4.1.

*Chapter 4*

## CONSTRUCTIONS OF NONREVERSIBLE CHAINS

We have now perceived, that all the explanations commonly given of nature are mere modes of imagining, and do not indicate the true nature of anything, but only the constitution of the imagination. I do not attribute to nature either beauty or deformity, order or confusion. Only in relation to our imagination can things be called beautiful or ugly, well-ordered or confused.

~ Baruch Spinoza, *Ethics*

The starting point of this section is to understand the optimality of Theorem 1.4.1. The main difference between Theorem 1.4.1 and the Cheeger-Buser inequality 3.0.1 is the loss of a factor of  $n$  in the nonreversible case, and we want to understand whether this loss is indeed necessary or whether it is a relic of the limitations of our proof techniques. We will also seek constructions of *doubly stochastic* matrices with these properties, to test the optimality of our theorem even in the case of a uniform principal eigenvector for the nonnegative matrix, where one might expect a  $\text{polylog}(n)$  loss instead of a loss of  $n$  in Theorem 1.4.1. We remark that we explain in detail in Sections 4.5, 4.6, 4.7 and 4.9 how we arrive at our constructions in Sections 4.8 and 4.10 so that they do not seem mysterious. Although brevity is the hallmark of wit, we think comprehensiveness is the hallmark of understanding, and we'll adhere to the latter for the most part, and as a consequence detail the thought process to arrive at our constructions, which might be instructive in a search for other similar constructions.

Before we proceed towards constructions, we need to understand the *non-expansion* of graphs.

#### 4.1 Non-expansion

The quantity edge expansion  $\phi$  as defined in 2.0.4 has been extensively studied in the last 70 years within combinatorics and spectral theory, albeit mostly for reversible matrices, and undirected graphs (or symmetric matrices) with a few edges (or few nonzero entries in the matrix) and constant expansion – also called (combinatorial) expanders – have many remarkable, and almost magical properties (see [HLW06]), making them a fundamental combinatorial object from which many optimal (up to lower order terms) pseudorandom objects can be constructed, such as error-correcting codes and pseudorandom generators amongst others, and further they serve as a building block in a large number of constructions within mathematics.

What we seek now is a direction opposite to that of expansion of graphs – the *non-expansion* of graphs. This is uninteresting for undirected graphs, since non-expansion of symmetric matrices simply implies a small spectral gap due to the Cheeger-Buser inequality 3.0.1, and it is elementary to construct such graphs. However, for the case of directed graphs (or irreversible matrices), the property of non-expansion is non-trivial, since at the outset, it is possible for a nonreversible matrix to have constant spectral gap but edge expansion that diminishes with the matrix size.

All the constructions that we present in this section are of non-expanding irreversible matrices, and although they go furthest from the remarkable and highly sought-after property of constant expansion, they are truly beautiful in a different and unique manner and deserve study in their own right. Our aim of this section is two-fold – to analyze and give an exposition of a few interesting known constructions, and present new constructions that are *exponentially* better with regards to the lower bound in Theorem 1.4.1, and with regards to the non-expansion of graphs as defined next. In fact, even the sub-optimal (in the sense of the lower bound in Theorem 1.4.1) constructions will have many interesting and aesthetically pleasing properties. To systematize exposition, we define the following quantity.

**Definition 4.1.1.** Let  $E_n$  be the set of all  $n \times n$  doubly stochastic matrices. For any  $A \in E_n$ , define the non-expansion of  $A$  as

$$\Gamma(A) = \frac{\phi(A)}{1 - \operatorname{Re}\lambda_2(A)}$$

and overriding notation, define

$$\Gamma(n) = \inf_{A \in E_n} \Gamma(A).$$

◇

**Lemma 4.1.2.** *For nonreversible matrices,  $\frac{1}{15n} \leq \Gamma(n) \leq \frac{1}{2}$  and for reversible matrices,  $\Gamma^{rev}(n) = \frac{1}{2}$*

*Proof.* The lower bounds follow from Theorem 1.4.1 and the Cheeger-Buser inequality 3.0.1, and the upper bound follows by taking the hypercube on  $n$  vertices in  $E_n$ , as discussed in Section 3.3. □

## 4.2 Beyond 1/2

The first immediate question is to find a doubly stochastic  $A$  such that  $\Gamma(A) < \frac{1}{2}$ , since we know that for any symmetric  $A$ ,  $\Gamma(A) \geq \frac{1}{2}$  from 4.1.2. In fact, it is not difficult to find such matrices numerically. A straightforward manner of achieving this is to start with  $J$ , and for some random  $(i, j)$  and  $(k, l)$ , and random  $\delta$ , set  $A_{i,j} \pm \delta$ ,  $A_{k,l} \pm \delta$ ,  $A_{i,l} \mp \delta$ , and  $A_{k,j} \mp \delta$  (where the range of  $\delta$  is chosen to ensure the entries of  $A$  do not become negative). With this simple algorithm, it is possible to find many examples that beat 1/2, and the following example was constructed after observing some of these matrices.

**Lemma 4.2.1.** *(Beyond 1/2) Let the matrix  $A$  be as follows (where the  $\cdot$  are zeros):*

$$A = \begin{bmatrix} \cdot & \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \\ \cdot & \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \\ \cdot & \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \\ 1 & \cdot & \cdot & \cdot \end{bmatrix}.$$

Then  $\Gamma(A) = \frac{1}{3} < \frac{1}{2}$ , improving upon 4.1.2.

*Proof.* Note that  $A$  is doubly stochastic, and for  $S = \{2, 3\}$ ,  $\phi(A) = \phi_S(A) = \frac{1}{3}$ , and all nontrivial eigenvalues of  $A$  are 0. Thus, the lemma follows. □

**Remark 4.2.2.** (Symmetry about the opposite diagonal) The matrix  $A$  in Lemma 4.2.1 represents an interesting chain, whose adjacency matrix is *symmetric about the opposite diagonal*. Although this property seems unrelated to edge expansion or eigenvalues, it will curiously appear again in our final example. ◇

### 4.3 Affine-linear constructions

There are many affine-linear constructions known in literature, and one such construction is a result of Maria Klawe [Kla84]. In fact, the purpose of Klawe's paper was indeed to show non-expansion of certain constructions of  $d$ -regular graphs, albeit undirected, but it was observed by Umesh Vazirani [Vaz17] in the 80's that there is a natural way to orient the edges to create directed graphs with  $d/2$  in-and-out degrees with similar expansion properties, and we learned of this construction from him. There is an entire family of constructions with different parameters, but all are equivalent for us from the perspective of minimizing  $\Gamma(n)$ . We state one specific (and neat) construction below.

**Construction 4.3.1.** (Klawe-Vazirani [Kla84; Vaz17]) Let  $n > 2$  be a prime, and create the graph on  $n$  vertices with in-degree and out-degree 2 by connecting every vertex  $v \in \mathbb{Z}/n$  to two vertices,  $1 + v$  and  $2v$ , each with edge-weight  $1/2$ .  $\diamond$

**Example 4.3.2.** An example for  $n = 7$  is shown below for right multiplication by a vector (take the transpose of the matrix for left multiplication):

$$A_{KV} = \begin{bmatrix} \frac{1}{2} & \cdot & \cdot & \cdot & \cdot & \cdot & \frac{1}{2} \\ \frac{1}{2} & \cdot & \cdot & \cdot & \frac{1}{2} & \cdot & \cdot \\ \cdot & 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \frac{1}{2} & \cdot & \cdot & \frac{1}{2} & \cdot \\ \cdot & \cdot & \frac{1}{2} & \frac{1}{2} & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \frac{1}{2} & \cdot & \frac{1}{2} \\ \cdot & \cdot & \cdot & \frac{1}{2} & \cdot & \frac{1}{2} & \cdot \end{bmatrix}.$$

$\diamond$

We note the following properties of these graphs.

**Lemma 4.3.3.** *The matrices  $A_{KV}$  in Construction 4.3.1 have the following properties:*

1. *The matrices have one eigenvalue 1, one eigenvalue 0, and  $n - 2$  eigenvalues  $\lambda$  such that  $\lambda = \frac{1}{2} \exp\left(\frac{2\pi I}{n-1} \cdot k\right)$  for  $k = 1, \dots, n - 2$ .*
2. *[Kla84]  $\phi(A) \leq c \cdot \left(\frac{\log \log n}{\log n}\right)^{1/5}$  where  $c$  is a constant.*
3.  *$\Gamma(n) \in O\left(\frac{\log \log n}{\log n}\right)^{1/5}$  improving upon 4.2.1.*

*Proof.* (1) Let the matrix be as follows:  $A = \frac{1}{2}(A' + A'')$  where  $A'$  is the directed cycle on  $n$  vertices and  $A''$  represent the cycle (since  $n > 2$  is a prime) that goes from vertex  $i$  to  $(2 \cdot i) \bmod n$ . Considering the matrices corresponding to right multiplication by a vector with vertices  $\{0, \dots, n-1\}$ , we have  $A'_{i,i-1} = 1$  and otherwise  $A'_{i,j} = 0$ , and  $A''_{i,j} = 1$  if  $i = 2 \cdot j$ , and else  $A''_{i,j} = 0$ . Let  $U$  denote the Fourier transform over the field  $\mathbb{Z}_n$ , with  $U_{i,j} = \frac{1}{\sqrt{n}} \omega^{i \cdot j}$  where  $\omega = \exp(2\pi I/n)$  is the  $n$ 'th root of unity and  $I = \sqrt{-1}$ . Let  $B = U^* A U$ ,  $B' = U^* A' U$ , and  $B'' = U^* A'' U$ . Note that  $B'$  is a diagonal matrix with  $B'_{i,i} = \omega^i$  and 0 otherwise. Similarly,

$$B''_{i,j} = \langle U_i, A'' U_j \rangle = \frac{1}{n} \sum_{k=0}^{n-1} \omega^{-i \cdot k} \omega^{j \cdot (k/2)} = \frac{1}{n} \sum_{k=0}^{n-1} \omega^{(j/2-i) \cdot k}$$

and thus  $B''_{i,2 \cdot i} = 1$  and 0 otherwise. Note  $B_{0,0} = 1$  and  $B_{0,j} = 0$  and  $B_{i,0} = 0$  for all  $i, j$ , which is the trivial block corresponding to eigenvalue 1, and the rest of the eigenvalues of  $B$  are in the  $(n-1) \times (n-1)$  block. For any such eigenvalue  $\lambda$  and corresponding eigenvector  $v$  of  $B$ , we have for  $1 \leq i \leq n-1$  that

$$\frac{1}{2}(\omega^i v_i + v_{2 \cdot i}) = \lambda v_i$$

or

$$(2\lambda - \omega^i)v_i = v_{2 \cdot i}.$$

Note that  $(2\lambda - \omega^i) \neq 0$ , else  $v$  will be the all zeros vector. Thus, we get that the equation

$$\prod_{i=1}^{n-1} (2\lambda - \omega^i) = 1, \quad (4.3.4)$$

whose roots will be the non-trivial eigenvalues of  $B$  and  $A$ . Note that  $\lambda = 0$  is a root, since  $\prod_{i=1}^{n-1} \omega^i = 1$  and  $(-1)^{n-1} = 1$  since  $n$  is a prime. We claim that the remaining  $n-2$  roots are all such that  $|\lambda| = \frac{1}{2}$  with  $\lambda \neq \frac{1}{2}$ , i.e.  $\lambda = \frac{1}{2} \exp(2\pi k \cdot I/(n-1))$  for  $k \in [n-1]$ . To see this, assume  $2\lambda \neq 1$ , and multiplying and dividing equation 4.3.4 by  $(2\lambda - 1)$ , we get that

$$1 = \frac{\prod_{i=0}^{n-1} (2\lambda - \omega^i)}{2\lambda - 1} = \frac{(2\lambda)^n - 1}{2\lambda - 1}$$

or

$$2\lambda = (2\lambda)^n$$

proving the claim.



(2) Let  $s(A) = \frac{A + A^T}{2}$ . It is shown in [Kla84] [Theorem 2.1] that the vertex expansion  $\mu(s(A))$  is bounded as follows:

$$\mu(s(A)) \leq c_1 \cdot \left( \frac{\log \log n}{\log n} \right)^{1/5}.$$

Note that since the degree of  $s(A)$  is 4, we get that

$$\phi(A) = \phi(s(A)) \leq 4 \cdot c_1 \left( \frac{\log \log n}{\log n} \right)^{1/5}$$

which proves the claim.

(3) Since  $\operatorname{Re} \lambda_2 \leq \frac{1}{2}$ , we get the claimed bound on  $\Gamma(n)$  from (1) and (2).  $\square$

In fact, there are many different affine-linear constructions that are known. Recall that Alon and Boppana [Alo86; Nil91] showed that for any infinite family of  $d$ -regular undirected graphs, the adjacency matrices, normalized to be doubly stochastic and with eigenvalues  $1 = \lambda_1 \geq \lambda_2 \geq \dots \geq -1$ , have  $\lambda_2 \geq \frac{2\sqrt{d-1}}{d} - o(1)$ . Feng and Li [Li92] showed that undirectedness is essential to this bound: they provide a construction of cyclically-directed  $r$ -partite ( $r \geq 2$ )  $d$ -regular digraphs (with  $n = kr$  vertices for  $k > d$ ,  $\gcd(k, d) = 1$ ), whose normalized adjacency matrices have (apart from  $r$  “trivial” eigenvalues), only eigenvalues of norm  $\leq 1/d$ . The construction is of an affine-linear nature quite similar to the matrices in Klawe-Vazirani, and to our knowledge does not give an upper bound on  $\Gamma$  any stronger than those.

#### 4.4 The de Bruijn construction

One of the most beautiful constructions is the de Bruijn graphs or (implicitly) the de Bruijn sequences. Consider the following problem: Let  $s$  be a string of bits such that every  $x \in \{0, 1\}^3$  appears as a continuous substring within  $s$  exactly once. The earliest reference to such a string comes from a Sanskrit prosody in the work of Pingala [Bro69], and one such string  $s$  is  $s = \text{yamātārājabhānasalagām}$ , in which each three-syllable pattern occurs starting at its name: ‘yamātā’ has a short–long–long pattern, ‘mātārā’ has a long–long–long pattern, and so on, until ‘salagām’ which has a short–short–long pattern. In general, a de Bruijn sequence  $\text{dB}(n, k)$  is a string containing every  $n$ -letter sequence from an alphabet of size  $k$  exactly once as a contiguous subsequence, and the prosody contains a string in  $\text{dB}(3, 2)$ . These were described by de Bruijn [Bru46] and I J Good [Goo46] independently, and previously by Camille Flye Sainte-Marie for an alphabet of size 2 [Bru75]. These sequences

have also been called “shortest random-like sequences” by Karl Popper [Pop05].

**Construction 4.4.1.** (de Bruijn [Bru46]) Define de Bruijn graphs on vertices  $\{0, 1\}^k$  and let every vertex  $|a\rangle = |a_1 a_2 \cdots a_k\rangle$ , have two outgoing edges to vertices  $|a_2 \cdots a_k 0\rangle$  and  $|a_2 \cdots a_k 1\rangle$  with weight  $1/2$  each. In words, starting with a  $k$ -bit vertex  $v$ , uniformly go to one of the following two vertices: shift  $v$  one bit to the left, and append 0 or 1 uniformly.  $\diamond$

**Example 4.4.2.** For  $k = 3$  ( $n = 8$ ), the adjacency matrix (for right-multiplication by a vector) looks like the following:

$$A_{dB} = \begin{bmatrix} \frac{1}{2} & \cdot & \cdot & \cdot & \frac{1}{2} & \cdot & \cdot & \cdot \\ \frac{1}{2} & \cdot & \cdot & \cdot & \frac{1}{2} & \cdot & \cdot & \cdot \\ \cdot & \frac{1}{2} & \cdot & \cdot & \cdot & \frac{1}{2} & \cdot & \cdot \\ \cdot & \frac{1}{2} & \cdot & \cdot & \cdot & \frac{1}{2} & \cdot & \cdot \\ \cdot & \cdot & \frac{1}{2} & \cdot & \cdot & \cdot & \frac{1}{2} & \cdot \\ \cdot & \cdot & \frac{1}{2} & \cdot & \cdot & \cdot & \frac{1}{2} & \cdot \\ \cdot & \cdot & \cdot & \frac{1}{2} & \cdot & \cdot & \cdot & \frac{1}{2} \\ \cdot & \cdot & \cdot & \frac{1}{2} & \cdot & \cdot & \cdot & \frac{1}{2} \end{bmatrix}.$$

$\diamond$

In fact, it is possible to construct many different matrices with different shifts and different base fields instead of  $\mathbb{F}_2$ , but all the constructions have similar properties.

The matrices in construction 4.4.1 have many remarkable and beautiful properties. The first observation is that the walk mixes exactly in  $k$  steps, or  $A^k = J$ , since after  $k$  steps, the vertex that is reached is completely uniform independent of the starting vertex. In fact, the most remarkable thing about these matrices is that all the (nontrivial) eigenvalues are 0. This implies that each of the Jordan blocks are of size at most  $k$  and nilpotent. Further, half the singular values are 1, and the other half are all 0. And the remarkable thing is that the edge expansion of these matrices is  $O(1/k) = O(1/\log n)$ , which shows that  $\Gamma(n) \in O(1/\log n)$ . The edge expansion of these matrices was studied in [DT98], but it does not give the actual non-expanding set. In the following lemma, we completely explore and prove every property of de Bruijn matrices.

**Lemma 4.4.3.** *Let  $A$  be the de Bruijn matrix on  $n = 2^k$  vertices. Then the following hold for  $A$ :*

1.  $\frac{1}{2 \log n} \leq \phi(A) \leq \frac{8}{\log n}$
2.  $A$  is doubly stochastic, and all the nontrivial eigenvalues of  $A$  are zero.
3.  $\Gamma(n) \leq \frac{8}{\log n} \in O\left(\frac{1}{\log n}\right)$ , improving upon 4.3.3
4. The Jordan and Schur forms are the same, and  $A$  has the trivial block of size 1 for eigenvalue 1, and it has exactly  $2^{k-1-r}$  Jordan blocks of size  $r \in [k-1]$  and one block of size  $k$  for the 0 eigenvalues.
5.  $A$  has  $n/2$  singular values that are 1, and  $n/2$  singular values that are 0.

*Proof.* (1) Let  $S$  be the set of all  $k$ -bit strings that have  $r = \lceil k/2 \rceil$  contiguous ones. Let  $S = \bigcup_{i=r}^k T_i$  where  $T_i$  is the set of all strings that have ones at all the  $r$  positions ending at  $i$ , and there is no  $j > i$  with the same property, i.e. there is no  $j > i$  such that the substring  $[j-r+1, j]$  is all ones. Then note that the  $T_i$ 's are disjoint. Further, the definition of  $T_i$  implies that the  $r$  positions ending at  $i$  are all ones, and the  $i+1$ 'st position (except for  $T_k$ ) is 0. In fact, these two constraints are *sufficient* to define the  $T_i$ 's and ensure that they do not overlap, since to overlap, there must be a string with  $r$  contiguous ones ending at  $i$  and  $r$  contiguous ones ending at  $j$ , but if the  $i+1$  position in the string is 0, then there are  $k-r-1 < k/2 \leq r$  positions left for  $r$  ones, which is an impossibility.

Thus, for  $T_i$ , all strings have  $r+1$  positions fixed – the indices  $i-r+1$  to  $i$  contain 1, and the position  $i+1$  contains 0. Note that the positions  $\leq i-r$  could be any bits, and also all positions  $> i+1$ , since the length of the suffix is  $k-(i+1) < r$  for all  $i \geq r$ . Thus, we get that  $|T_i| = 2^{k-r-1}$  for  $r \leq i \leq k-1$ , and  $|T_k| = 2^{k-r}$ . Since  $\frac{k}{2} \leq r \leq \frac{k}{2} + 1$ , we have

$$\begin{aligned}
 |S| &= (k-r) \cdot 2^{k-r-1} + 2^{k-r} \\
 &\leq \frac{k}{2} 2^{k/2-1} + 2^{k/2} \\
 &\leq \frac{5}{4} \cdot k \cdot 2^{k/2} \\
 &\ll 2^{k-1} \\
 &= \frac{n}{2}
 \end{aligned}$$

and thus,  $S$  is a valid set to consider for determining  $\phi$ . Moreover,

$$\begin{aligned} |S| &= (k - r) \cdot 2^{k-r-1} + 2^{k-r} \\ &\geq \left(\frac{k}{2} - 1\right) 2^{k/2-2} + 2^{k/2-1} \\ &\geq \frac{k}{8} 2^{k/2} \end{aligned}$$

The key property of all the sets is the following: for any  $i > r$ , the vertices in the sets  $T_i$  have all outgoing edges inside the set  $S$ , i.e. there are no edges from the vertices in the set  $T_i$  to  $\bar{S}$ , since the strings will always have a contiguous substring of  $r$  ones after a one-bit left shift. The only set that could have edges to  $\bar{S}$  is  $T_r$ , and it could have at most  $2 \cdot |T_r|$  outgoing edges. Thus, we get that

$$\phi_S(A) \leq \frac{2 \cdot |T_r|}{|S|} \leq \frac{2 \cdot 2^{k/2-1}}{\frac{1}{8} \cdot k \cdot 2^{k/2}} \leq \frac{8}{k}$$

as required.

Further, since  $A^k = J$  from (2), we have from 3.7.6 that  $\phi(A^k) \leq k \cdot \phi(A)$  or

$$\phi(A) \geq \frac{1}{2k}.$$

(2) It is straightforward to see from the definition that  $A\mathbf{1} = \mathbf{1}$  and  $A^T\mathbf{1} = \mathbf{1}$  and thus  $A$  is doubly stochastic. Let  $a = a_1a_2 \cdots a_k$  be a  $k$ -bit string, let  $|a\rangle$  denote the corresponding standard basis vector in an  $n$ -dimensional space, and for any  $S \subseteq [k]$ , let  $a_S = \sum_{i \in S} a_i$  and

$$v_S = \sum_a (-1)^{a_S} |a\rangle.$$

Let  $V = \{v_S : S \subseteq [k]\}$  and  $W = \{v_S : 1 \in S, S \subseteq [k]\}$ . Then we show that for any  $v_S \in W$ ,

$$Av_S = 0.$$

Note that by definition,

$$A|a_1 \dots a_k\rangle = \frac{1}{2}|a_2 \dots a_k 0\rangle + \frac{1}{2}|a_2 \dots a_k 1\rangle$$

By direct calculation, we have letting  $T = S \setminus \{1\}$ ,

$$\begin{aligned}
Av_S &= \sum_a (-1)^{a_S} A|a_1 \cdots a_k\rangle \\
&= \sum_a (-1)^{a_1} (-1)^{a_T} A|a_1 \cdots a_k\rangle \\
&= \frac{1}{2} \sum_a (-1)^{a_T} (-1)^{a_1} (|a_2 \cdots a_k 0\rangle + |a_2 \cdots a_k 1\rangle) \\
&= \frac{1}{2} \sum_{a_2, \dots, a_k=0}^1 (-1)^{a_T} (|a_2 \cdots a_k 0\rangle + |a_2 \cdots a_k 1\rangle) \sum_{a_1=0}^1 (-1)^{a_1} \\
&= 0
\end{aligned}$$

as claimed. Further, for  $S \neq T$ , let  $U = (S \setminus (S \cap T)) \cup (T \setminus (S \cap T)) \neq \emptyset$ , then it is simple to see that

$$\langle v_S, v_T \rangle = \sum_a \sum_b (-1)^{a_S} (-1)^{b_T} \langle a|b \rangle = \sum_a (-1)^{a_S} (-1)^{a_T} = \sum_a (-1)^{a_U} = 0.$$

Thus the  $v_S$  are all orthogonal, and  $|W| = 2^{n-1}$ , and since  $Av_S = 0$  for  $v_S \in W$ , it implies that the kernel  $W$  of  $A$  has dimension  $n - 1$ . Since  $A$  has 1 as the trivial eigenvalue for  $v_\emptyset$ , it means that all the nontrivial eigenvalues of  $A$  are 0.

(3) Combining (1) and (2) gives the bound on gamma since  $\lambda_2(A) = 0$ .

(4) We will use notation from (2). The set  $V$  as defined contains orthogonal vectors as shown in (2), and if we express  $A$  in the basis of the vectors in  $V$ , we get a matrix of Jordan blocks, and as such both the Jordan and Schur forms of  $A$  will exactly be the same (since the vectors of  $V$  form a unitary matrix). Our aim is to now understand the effect of  $A$  on vectors not in  $W$ . This will help us understand the chain of generalized eigenvectors. Consider  $S \subseteq [k]$  where  $S = \{i_1, \dots, i_r\}$  with  $i_1 < i_2 < \dots < i_r$ , and let  $T = \{i_1 - 1, i_2 - 1, \dots, i_r - 1\}$ . Let  $a = a_1 \dots a_k$ ,  $b = b_1 \dots b_k$  with  $b_i = a_i + 1$  and  $b_k = 0$ , and  $c = c_1 \dots c_k$  with  $c_i = a_i + 1$  with  $c_k = 1$ . Then note that if  $i_1 = 1$ , then

from part (2),  $Av_S = 0$ , and if  $i_1 > 1$ , then

$$\begin{aligned}
Av_S &= A \sum_a (-1)^{as} |a_1 \dots a_r\rangle \\
&= \frac{1}{2} \sum_a (-1)^{as} |a_2 \dots a_r 0\rangle + \frac{1}{2} \sum_a (-1)^{as} |a_2 \dots a_r 1\rangle \\
&= \sum_{a_2, \dots, a_k=0}^1 (-1)^{as} |a_2 \dots a_r 0\rangle + \sum_{a_2, \dots, a_k=0}^1 (-1)^{as} |a_2 \dots a_r 1\rangle \\
&\quad [\text{since } 1 \notin S] \\
&= \sum_{b_1, \dots, b_{k-1}=0}^1 (-1)^{b_T} |b\rangle + \sum_{c_1, \dots, c_{k-1}=0}^1 (-1)^{c_T} |c\rangle \\
&= \sum_a (-1)^{a_T} |a\rangle \\
&= v_T.
\end{aligned}$$

Thus, for any  $S \subseteq [k]$  denote  $S + j = \{i \in [k] : i - j \in S\}$ , and let  $1 \in S$  and  $\max S = r$ , then we have for  $1 \leq j \leq k - r$

$$Av_{S+j} = v_{S+j-1}$$

giving us a chain of  $k + 1 - r$  vectors that end with a vector in the kernel. Thus, this forms one specific Jordan block. In general, we have that any vector  $v_S$  will belong to a Jordan block of size  $k - (\max S - \min S)$ . To count the number of distinct Jordan blocks, consider  $S$  such that  $1 \in S$ . Then the vector  $v_S$  in the kernel will be the last vector in the chain that starts with  $v_{S+k-\max S}$ , in a block of size  $k + 1 - \max S$ . Thus, for each  $r \in [k - 1]$ , the number of Jordan blocks of size  $r$  is the number of vectors  $v_S$  with  $1 \in S$  and  $k + 1 - r \in S$ , which is exactly  $2^{k-1-r}$ . Further, the only block of size  $k$  is obtained for the chain ending in  $v_{\{1\}}$ , and there is the trivial block of size 1 corresponding to  $v_\emptyset$ . As a sanity check, if we sum the sizes of all blocks, we get

$$\sum_{r=1}^{k-1} r \cdot 2^{k-1-r} + k + 1 = 2^k \left(1 - 2^{-(k-1)} - (k-1)2^{-k}\right) + k + 1 = 2^k = n$$

as expected.

(5) Note that with the unitary  $U$  formed by the vectors from  $V = \{v_S : S \subseteq [k]\}$  (after suitably normalizing), we get that  $A = UTU^*$  where  $T$  is a collection of Jordan blocks as shown in (4) above. Since a Jordan block of size  $r$  can be converted to a diagonal matrix of size  $r$  with  $r - 1$  ones and one zero entry by multiplying with

a permutation matrix, we get that  $T = DP$  where  $P$  is a permutation matrix that converts each Jordan block to a diagonal matrix. Thus we have the singular value decomposition of  $A = UDPU^* = UDQ$  since  $Q$  is a unitary. To count the number of zeros on the diagonal in  $D$ , note that each nontrivial Jordan block contributes exactly one 0, and thus the total number of zeros is equal to the number of nontrivial Jordan blocks, which is exactly

$$\sum_{r=1}^{k-1} 2^{k-1-r} + 1 = 2^{k-1} = \frac{n}{2}$$

implying that there are  $n - n/2$  ones on the diagonal. Thus  $A$  has  $n/2$  singular values that are 1 and  $n/2$  singular values that are 0.  $\square$

The beautiful thing about this construction is that it is extremely simple to describe, and still has the remarkable properties in the lemma above. Also, this construction is the benchmark for other constructions, and although it does not achieve a low enough value of  $\Gamma(n)$  that would be sufficient for Theorem 1.4.1, it will be the starting point for the construction in Section 4.5.

Our aim now will be to beat the upper bound on  $\Gamma$  in Lemma 4.4.3, and understand if our lower bound on  $\phi$  in Theorem 1.4.1 is tight or whether it is exponentially worse than the truth. Note that if it is true that

$$\Gamma(n) \in \Omega\left(\frac{1}{\text{polylog}(n)}\right),$$

it would mean that our techniques of proof of Theorem 1.4.1 are extremely weak, and different techniques will be required to get a tighter bound. From a utilitarian perspective, it would imply that the spectral gap is a good estimate for  $\phi$  (up to  $\text{polylog}(n)$  terms which are essentially negligible in succinctly defined chains where the input length is  $O(\log n)$ ) even in the nonreversible case. Towards this end, we will try to find constructions of matrices that try to surpass the upper bound on  $\Gamma$  in Lemma 4.4.3.

## 4.5 Constraints on the Search Space

At this point, we are in search of a doubly stochastic matrix  $A$  that helps to improve the bound in Lemma 4.4.3. Since the search space (all doubly stochastic matrices) is difficult to understand in terms of non-expansion, we will systematically try to impose meaningful constraints on it to arrive at the type and form of matrices that

we want. Towards this end, our first question, that will turn out to be sufficient to be the last, is to understand the following:

**Main question:** *How small can the edge expansion of a doubly stochastic matrix be if all its nontrivial eigenvalues are 0?*

If we can show that  $\Gamma(n) \in \Omega(1/\log n)$  for all  $n \times n$  matrices that have all eigenvalues 0, then it will imply that de Bruijn matrices are optimal in the sense of non-expansion as described in Definition 4.1.1 in Section 4.1, that is, they have the least edge expansion amongst all matrices that have all (nontrivial) eigenvalues 0. This will be our first constraint, and further, this restriction is also sufficiently general in the following sense.

**Constraint 1:** Restrict all nontrivial eigenvalues to 0

**Justification:** The rationale behind choosing all eigenvalues 0 is as follows – As seen in the first steps in the proof of Lemma 3.7.10, if for a doubly stochastic matrix  $A$ , every nontrivial eigenvalue has magnitude at most  $1 - c$  for some constant  $c$ , then powering just  $O(\log n)$  times will make the diagonal entries inverse polynomially small in magnitude, and thus it would seem that the matrix should have behavior similar to matrices with all eigenvalues 0. Thus, if  $A$  had all eigenvalues with magnitude less than  $1 - c$ , we can simply consider the matrix  $A^k$  with  $k \in O(\log n)$  as our starting matrix, and we know that its expansion will be at most  $O(\log n)$  times the expansion of  $A$  (from lemma 3.7.6), and thus if  $A$  had small expansion – about  $O(1/\sqrt{n})$  –  $A^k$  will have similar expansion (albeit off by a factor of  $\log n$ ). Given any doubly stochastic  $A$  with  $\text{Re}\lambda_2 < 1$ , it is simple to ensure that  $|\lambda_i| \leq 1 - c$  for some specific  $c$  by lazification, i.e. by considering  $\exp(t \cdot (A - I))$  or  $\frac{1}{2}(A + I)$ , which is essentially the first step in the proof of Lemma 3.7.14 or the lower bound in Theorem 1.4.1

Restricting to matrices with all 0 (nontrivial) eigenvalues, our primary concern throughout will be the matrix  $B = A - J$ . If all nontrivial eigenvalues of  $A$  are 0, it means all eigenvalues of  $B$  are 0, and we will further write the Schur form of  $B$  as  $B = UTU^*$  where  $U$  is a unitary and  $T$  is upper triangular and all its diagonal entries are 0.



**Lemma 4.5.1.** *If  $A = J + B$  has all (nontrivial) eigenvalues 0, then  $B^{n-1} = 0$ .*

*Proof.* The proof is immediate since  $T$  is nilpotent.  $\square$

Note that the entries in the rows and columns of the matrix  $A$  will always sum to 1, since we have removed the all ones eigenvector in  $J$  and we ensure that the first column of  $U$  is the vector  $1/\sqrt{n} \cdot \mathbf{1}$ , which would imply all other columns of  $U$  are orthogonal to the vector  $\mathbf{1}$  (since  $U$  is a unitary), which would further give us  $B\mathbf{1} = 0$  and  $B^T\mathbf{1} = 0$ . Also, there is another useful consequence of constraint 1 (4.5) – since all the eigenvalues of  $A$  are real, we can restrict to real unitary matrices  $U$  (by looking at the process of obtaining a Schur decomposition, since  $A$  is real and has real eigenvalues). This actually gives us our second condition:

**(Implied) Constraint 2:** The unitary  $U$  is real, and has  $\frac{1}{\sqrt{n}}\mathbf{1}$  as the first column.

Given this observation, the next step is to look at the proof of Lemma 3.7.10. In Lemma 3.7.10, the main aim was to upper bound  $k$  for which  $T^k \approx 0$  and it was seen that a value of  $k$  about  $n/1 - \text{Re}\lambda_2$  was sufficient. Our main aim is to now find a construction of matrices such that this lemma is tight. In other words, we now seek a construction of  $T$  (and  $B$ ) such that for sufficiently small  $k$ , the norm  $\|T^k\|_2$  is sufficiently far from zero. Consider the de Bruijn matrices and the matrix  $B_{dB} = A_{dB} - J$ . We know that  $B_{dB}^k = 0$  for  $k = \log n$ . Further from Lemma 4.4.3, since  $\phi(A_{dB}) \leq 8/k$ , it also implies that for any  $j \ll k$ ,  $\|B^j\| \gg 0$ , since otherwise from the proof of Lemma 4.4.3, we would get that  $\phi(A) > 1/j$ , which would be a contradiction.

It is not difficult to construct a  $T$  such that  $T^k \gg 0$  for  $k \in o(n)$ . For instance, it is simple to obtain this if we let the Schur form be one large Jordan block, that is,  $T$  is simply the matrix with 1's above the diagonal.

$$T = \begin{bmatrix} \mathbf{0} & 0 & 0 & 0 & 0 & 0 \\ 0 & \mathbf{0} & 1 & 0 & 0 & 0 \\ 0 & 0 & \mathbf{0} & 1 & 0 & 0 \\ 0 & 0 & 0 & \ddots & \ddots & 0 \\ 0 & 0 & 0 & 0 & \mathbf{0} & 1 \\ 0 & 0 & 0 & 0 & 0 & \mathbf{0} \end{bmatrix}, T^2 = \begin{bmatrix} \mathbf{0} & 0 & 0 & 0 & 0 & 0 \\ 0 & \mathbf{0} & 0 & 1 & 0 & 0 \\ 0 & 0 & \mathbf{0} & 0 & \ddots & 0 \\ 0 & 0 & 0 & \ddots & \ddots & 1 \\ 0 & 0 & 0 & 0 & \mathbf{0} & 0 \\ 0 & 0 & 0 & 0 & 0 & \mathbf{0} \end{bmatrix}, T^3 = \begin{bmatrix} \mathbf{0} & 0 & 0 & 0 & 0 & 0 \\ 0 & \mathbf{0} & 0 & 0 & 1 & 0 \\ 0 & 0 & \mathbf{0} & 0 & \ddots & 1 \\ 0 & 0 & 0 & \ddots & \ddots & 0 \\ 0 & 0 & 0 & 0 & \mathbf{0} & 0 \\ 0 & 0 & 0 & 0 & 0 & \mathbf{0} \end{bmatrix}$$

For this matrix, it is clear that  $\|T^k\| = 1$  for any  $k < n - 1$ , since the diagonal consisting of ones keeps shifting away from the main diagonal with higher powers of  $T$ . However, the immediate problem in choosing the  $T$  mentioned above is that there might not be any unitary  $U$  such that  $J + UTU^* = A$  is a nonnegative matrix. In fact, this is one of the primary problems with constructing these matrices – ensuring that they are positive. Note that the entries in the rows and columns of the matrix will always sum to 1 due to condition 2. At this point, it is difficult to find a unitary  $U$  that transforms the matrix  $T$  above to a doubly stochastic matrix, and we will need to modify  $T$  in some manner. Note that essentially, the only requirement for  $T$  is that it is upper triangular with diagonal entries 0, but having a completely general  $T$  is extremely difficult to handle. Thus, our next relaxation/constraint of  $T$  will be as follows:

**Constraint 3:** For  $A = J + UTU^*$ , let  $T$  have some number  $r$  above the diagonal instead of 1, and let the rest of the entries in  $T$  be 0.

$$T = \begin{bmatrix} \mathbf{0} & 0 & 0 & 0 & 0 & 0 \\ 0 & \mathbf{0} & r & 0 & 0 & 0 \\ 0 & 0 & \mathbf{0} & r & 0 & 0 \\ 0 & 0 & 0 & \ddots & \ddots & 0 \\ 0 & 0 & 0 & 0 & \mathbf{0} & r \\ 0 & 0 & 0 & 0 & 0 & \mathbf{0} \end{bmatrix}, T^2 = \begin{bmatrix} \mathbf{0} & 0 & 0 & 0 & 0 & 0 \\ 0 & \mathbf{0} & 0 & r^2 & 0 & 0 \\ 0 & 0 & \mathbf{0} & 0 & \ddots & 0 \\ 0 & 0 & 0 & \ddots & \ddots & r^2 \\ 0 & 0 & 0 & 0 & \mathbf{0} & 0 \\ 0 & 0 & 0 & 0 & 0 & \mathbf{0} \end{bmatrix}, T^3 = \begin{bmatrix} \mathbf{0} & 0 & 0 & 0 & 0 & 0 \\ 0 & \mathbf{0} & 0 & 0 & r^3 & 0 \\ 0 & 0 & \mathbf{0} & 0 & \ddots & r^3 \\ 0 & 0 & 0 & \ddots & \ddots & 0 \\ 0 & 0 & 0 & 0 & \mathbf{0} & 0 \\ 0 & 0 & 0 & 0 & 0 & \mathbf{0} \end{bmatrix}$$

Note that for  $r \approx 1 - 1/n$ , since  $\|T^k\| = r^k$ , for any  $k < n/2$ , we would have that  $\|T^k\| = r^k \gtrsim e^{-1/2}$  which is much larger than 0. Thus if we can transform  $T$  to a doubly stochastic matrix using any valid unitary  $U$  with  $r \approx 1 - 1/n$ , we will get the type of matrix that we are looking for. At this point, instead of fixing  $r$  to being

about  $O(1/n)$  far from 1, our aim will be to have a matrix  $T$  for which there is *some* unitary that transforms it to a doubly stochastic matrix and has  $r$  as large as possible.

Also, the rationale for  $T$  having non-zero entries only on the off-diagonal is as follows: In any upper triangular matrix  $T$  in which the diagonal has zeros, the off-diagonal entries *affect* the entries in powers of  $T$  the most, since entries far from the diagonal will become ineffective after a few powers of  $T$ . Thus, choosing  $T$  with the non-zeros pattern of a Jordan block will not be far from optimal.

Note that our structure of  $T$  gives the following lemma which helps to illustrate the main issue with trying to have constructions that beat the upper bound on  $\Gamma$  in Lemma 4.4.3.

**Lemma 4.5.2.** *Let  $A = J + UTU^*$  be a doubly stochastic matrix with  $T$  being the all zeros matrix but with entry  $r$  in the off-diagonal entries from row 2 to  $n - 1$ . Then*

$$r^2 = \frac{\sum A_{i,j}^2 - 1}{n - 2}$$

*Proof.* Looking at the trace of  $AA^T$ , we get

$$\sum_{i,j} A_{i,j}^2 = \text{Tr}(AA^T) = 1 + r^2(n - 2)$$

which gives the lemma. □

Note that from this lemma, it might seem that maximizing  $r$  is a simple task – maximizing the sum of squares of entries of  $A$ , and it is easy to construct such an  $A$ , for instance  $A = (1 - p)I + pJ$  for an appropriate  $p$ . This illustrates two issues. The lemma does not use our constraints on  $A$  – nonnegativity, and the fact that all nontrivial eigenvalues 0. This is the primary issue in all attempts of construction of the intended matrices.

**Problems with simulation.** We would also like to re-state, and mentioned in the introduction, that it is not possible to use simulations and find different  $A$ 's that are doubly stochastic has have small expansion but large spectral gap, and its even harder to simulate  $T$  and  $U$  to have the type of properties that we care about. The main issue is the extreme sensitivity of these matrices to small perturbations, and in fact this actually is our very aim – to find matrices that *are* heavily affected (in terms of change in eigenvalues) by a small perturbations (which corresponds to a

small change in the expansion). Since simulations with finite number of bits act as perturbations themselves, it would be unlikely to arrive at such matrices numerically.

#### 4.6 Special Cases of specific matrices satisfying constraints

To get started on our aim of finding  $T$  with a large value of  $r$  and some unitary that transforms it to a doubly stochastic matrix, we are going to start with a very simple case. We were averse to looking at specific small examples initially, since it seemed that for any finite  $n$  (sufficiently small enough, say  $n \leq 12$ ), the values of edge expansion and the spectral gaps would be off by large constant factors, and would essentially be uninformative since they are scalar values. However, it turned out that these matrices indicated something that we did not initially expect.

Consider the case of  $n = 3$ . Let our  $T$  and  $U$  be as follows:

$$T = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & r \\ 0 & 0 & 0 \end{bmatrix}, \quad U = \begin{bmatrix} \frac{1}{\sqrt{3}} & a_1 & b_1 \\ \frac{1}{\sqrt{3}} & a_2 & b_2 \\ \frac{1}{\sqrt{3}} & a_3 & b_3 \end{bmatrix}$$

where the  $a_i$ 's and  $b_i$ 's are real, as stated in constraint 4.5. We can now treat these as 3 points in the x-y plane, and get the following equations using the fact that  $U$  is a unitary:

$$a_1 + a_2 + a_3 = 0$$

$$b_1 + b_2 + b_3 = 0$$

$$a_1^2 + b_1^2 = \frac{2}{3}$$

$$a_2^2 + b_2^2 = \frac{2}{3}$$

$$a_3^2 + b_3^2 = \frac{2}{3}$$

The last three equations tell us that each of the three points are on a circle of radius  $t = \sqrt{2/3}$ , and the first two equations tells us that the vector  $(a_3, b_3) = -(a_1, b_1) - (a_2, b_2)$ . Since all the three points are on the circle, it implies that the third point lies on the bisector of the angle between the vectors from the origin to the

first and second points. However, since the equations are completely symmetric, it implies that this must be satisfied by all three points, and thus it shows that the three points lie at the corners of an equilateral triangle. Thus, we get that the points are at an angle of  $2\pi/3$  from each other, and this gives

$$\begin{aligned}(a_1, b_1) &= (a, b) \\(a_2, b_2) &= \left(-\frac{1}{2}a - \frac{\sqrt{3}}{2}b, -\frac{1}{2}b + \frac{\sqrt{3}}{2}a\right) \\(a_3, b_3) &= \left(-\frac{1}{2}a + \frac{\sqrt{3}}{2}b, -\frac{1}{2}b - \frac{\sqrt{3}}{2}a\right)\end{aligned}$$

Thus we have our unitary  $U$ , and we need to choose  $(a, b)$  (with  $a^2 + b^2 = \frac{2}{3}$ ) in order to choose as large a value of  $r$  as possible keeping the matrix nonnegative. Note that due to the structure of  $T$  and  $U$ , we get that the entries  $B_{i,j} = r \cdot a_i \cdot b_j$ , and we need to ensure  $B_{i,j} + \frac{1}{3} \geq 0$ . Thus our problem becomes solving the following:

**maximize**  $r$

$$\text{s.t. } B_{i,j} + \frac{1}{3} \geq 0 \text{ for all } i, j, \text{ and } a^2 + b^2 = \frac{2}{3}.$$

It turns out that the solution to the above problem is obtained by

$$a = b = \frac{1}{\sqrt{3}}$$

giving

$$r = \frac{\sqrt{3} + 1}{\sqrt{3} + 2}.$$

Note that at this point, we have a doubly stochastic matrix  $A$  with all eigenvalues 0, with a specific value of  $r$  that is obtained, but all these numbers could be off by large factors and are essentially meaningless.

What is indeed meaningful, is to look at the unitary  $U$ :

$$U = \begin{bmatrix} \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} \\ \frac{1}{\sqrt{3}} & -\frac{1}{2}\left(1 + \frac{1}{\sqrt{3}}\right) & \frac{1}{2}\left(1 - \frac{1}{\sqrt{3}}\right) \\ \frac{1}{\sqrt{3}} & -\frac{1}{2}\left(1 - \frac{1}{\sqrt{3}}\right) & -\frac{1}{2}\left(1 + \frac{1}{\sqrt{3}}\right) \end{bmatrix}$$

The fascinating thing is that in addition to having the first column as a multiple of  $\mathbf{1}$ , even the first row in  $U$  is a multiple of the all ones vector. And  $U$  indicates a rotation in space of  $T$  and is a vector unlike the numbers  $\phi$ ,  $r$ ,  $\lambda_2$  that are scalars, it indicates that the maximum value of  $r$  is obtained in the direction of the all 1's vector. This gives us our next crucial constraint:

**Constraint 4:** The maximum value of  $r$  is obtained when  $U$  has the first row containing the all ones vector.

#### 4.7 The general case and relevant reasoning

We now wish to understand how large the value of  $r$  can be, for any unitary with the first row and column vectors that are multiples of the all ones vector. Indeed, we can show the following:

**Lemma 4.7.1.** *Let  $A = J + UTU^*$  be a doubly stochastic matrix where  $T$  contains zeros on the diagonal and  $r$  on the off-diagonal entries (from row 2 to  $n$ ) and  $U$  be some real unitary with the first row and column being a multiple of the all ones vector. Then*

$$r \in 1 - \Omega\left(\frac{1}{\sqrt{n}}\right).$$

*Proof.* Let the  $k$ 'th column of  $U$  be  $u_k$ , where  $u_{i,k}$  represents the  $i$ 'th entry of column  $k$  or  $(i, k)$ 'th entry of  $U$ , then based on our choice of  $T$  and the conditions on  $U$ , we get

$$A = J + r \cdot \sum_{k=2}^{n-1} u_k u_{k+1}^*$$

and

$$A_{i,j} = \frac{1}{n} + r \sum_{k=2}^{n-1} u_{i,k} u_{j,k+1}$$

since the unitaries are real as observed in constraint 4.5. Note that every entry in the first row and column of  $U$  is  $\frac{1}{\sqrt{n}}$ , and thus  $u_{i,1} = \frac{1}{\sqrt{n}}$  for all  $i$ ,  $u_{1,k} = \frac{1}{\sqrt{n}}$  for all  $k$ , and since the first row and column of  $U$  are multiples of the all ones vector, the sum of entries in any other row or column of  $U$  is 0. Thus we get that

$$A_{1,1} = \frac{1}{n} + r \cdot \frac{n-2}{n}$$

$$1 - A_{1,1} = 1 - \frac{1}{n} - r + \frac{2r}{n}$$

and for  $j \geq 2$ ,

$$\begin{aligned}
A_{1,j} &= \frac{1}{n} + r \sum_{k=2}^{n-1} u_{1,k} u_{j,k+1} \\
&= \frac{1}{n} + \frac{r}{\sqrt{n}} \sum_{k=2}^{n-1} u_{j,k+1} \\
&= \frac{1}{n} + \frac{r}{\sqrt{n}} (-u_{j,1} - u_{j,2}) \\
&\quad [\text{since } \sum_{k=1}^n u_{j,k} = 0] \\
&= \frac{1-r}{n} - \frac{r}{\sqrt{n}} \cdot u_{j,2}
\end{aligned}$$

which gives for  $j \geq 2$

$$u_{j,2} = \frac{\sqrt{n}}{r} \cdot \left( \frac{1-r}{n} - A_{1,j} \right).$$

Now consider  $u_2$  (or the second column of  $U$ ), then we have

$$\begin{aligned}
1 &= \sum_{j=1}^n u_{j,2}^2 \\
&= \frac{1}{n} + \frac{n}{r^2} \sum_{j=2}^n \left( \frac{1-r}{n} - A_{1,j} \right)^2 \\
\frac{n-1}{n^2} \cdot r^2 &= \frac{n-1}{n^2} \cdot (1-r)^2 + \sum_{j=2}^n A_{1,j}^2 - 2 \cdot \frac{1-r}{n} \cdot \sum_{j=2}^n A_{1,j} \quad (4.7.2)
\end{aligned}$$

Note that since the matrix is double stochastic,  $\sum_{j=2}^n A_{1,j} = 1 - A_{1,1}$  and each  $A_{1,j} \geq 0$ , and we get

$$\sum_{j=2}^n A_{1,j}^2 \leq \left( \sum_{j=2}^n A_{1,j} \right)^2 = (1 - A_{1,1})^2$$

Replacing these in equation 4.7.2, we get

$$\begin{aligned}
\frac{n-1}{n^2} \cdot r^2 &\leq \frac{n-1}{n^2} \cdot (1-r)^2 + (1 - A_{1,1})^2 - 2 \cdot \frac{1-r}{n} \cdot (1 - A_{1,1}) \\
\frac{n-1}{n^2} \cdot r^2 &\leq \frac{n-1}{n^2} \cdot (1-r)^2 + (1 - A_{1,1}) \left( 1 - A_{1,1} - 2 \cdot \frac{1-r}{n} \right) \\
(n-1)(2r-1) &\leq (n(1-r) + 2r-1)(n(1-r) + 4r-3) \\
0 &\leq (n^2 - 6n + 8)r^2 + (-2n^2 + 8n - 8)r + n^2 - 3n + 2
\end{aligned}$$

and since  $r \leq 1$  – else the matrix will have norm larger than 1 and will not be doubly stochastic, see Lemma 3.0.3, the valid range of  $r$  solving the above quadratic is obtained by

$$r \leq 1 - \frac{\sqrt{n} + 2}{n - 4}$$

which implies that

$$r \in 1 - \Omega\left(\frac{1}{\sqrt{n}}\right)$$

and completes the proof.  $\square$

Looking at Lemma 4.7.1 again, and seeing what it says, we see that after fixing the first row of our unitary matrix to the all ones vector, given the form of  $T$  that we have fixed, the best value of  $r$  that we can hope to achieve is about  $1 - \frac{1}{\sqrt{n}}$ , and this will be our aim henceforth. Note that if possible, this will give us an *exponential* improvement over the deBruin construction for  $\Gamma(n)$  in Lemma 4.4.3. Thus, to get a maximum value of  $r$ , our optimization problem becomes the following:

**maximize**  $r$

**such that:**

$$\frac{1}{n} + r \sum_{k=2}^{n-1} u_{i,k} u_{j,k+1} \geq 0 \text{ for all } 2 \leq i, j \leq n,$$

$$\frac{1}{n} + \frac{r}{\sqrt{n}} \sum_{k=2}^{n-1} u_{j,k+1} \geq 0 \text{ for all } 2 \leq j \leq n$$

$$\frac{1}{n} + \frac{r}{\sqrt{n}} \sum_{k=2}^{n-1} u_{i,k} \geq 0 \text{ for all } 2 \leq i \leq n$$

$$u_{i,k} = \langle e_i, U e_k \rangle$$

$$UU^T = U^T U = I.$$

$$u_{1,j} = \frac{1}{\sqrt{n}}, u_{i,1} = \frac{1}{\sqrt{n}}, \text{ for all } 1 \leq i, j \leq n.$$

Although we can attempt and solve the above problem, it is unwieldy and the conditions on the  $(n - 1)^2$  variables in  $U$  make it almost intractable. To solve this issue and understand how the solutions to this problem would look like, we will simplify it by fixing other entries of the unitary  $U$ . This fixing will be mildly creative and empirical, based on our observations in the  $n = 3$  and other cases with small  $n$ . Note that intuitively, the unitary is a rotation in space, of two distinct ‘‘Schur’’



blocks, where a Schur block is same as a Jordan block except that the off-diagonal entries are  $r$  and not 1. The first is the trivial block containing only the eigenvalue 1, and the second block is of size  $n - 1$  and contains the remaining eigenvalues. Since only two types of actions are performed on the Schur blocks, we are going to set the entries (at positions greater than 1) in any column of the unitary  $U$  to consist only of *two* distinct values. With this restriction, since  $U$  has  $1/\sqrt{n}$  in the first row and column and since  $U$  has to be unitary, there is exactly one unitary matrix that has only two distinct values in each column, and it turns out to be a *symmetric* unitary, with  $U_{i,i} = \alpha$ , and  $U_{i,j} = \beta$  for  $2 \leq i, j \leq n$ .

Having fixed the unitary matrix  $U$ , and the upper triangular matrix  $T$ , our aim is to choose an  $r$  as large as possible such that the resulting matrix  $A$  is nonnegative. Thus, the optimization problem 4.7 becomes:

**maximize**  $r$

**such that:**

$$\frac{1}{n} + r \sum_{k=2}^{n-1} u_{i,k} u_{j,k+1} \geq 0 \text{ for all } 2 \leq i, j \leq n$$

$$\frac{1}{n} + \frac{r}{\sqrt{n}} \sum_{k=2}^{n-1} u_{j,k+1} \geq 0 \text{ for all } 2 \leq j \leq n$$

$$\frac{1}{n} + \frac{r}{\sqrt{n}} \sum_{k=2}^{n-1} u_{i,k} \geq 0 \text{ for all } 2 \leq i \leq n$$

Subject to the constraints provided by these inequalities, we aim to *minimize*  $\phi$  or *maximize*  $r$ . Due to our restrictions on  $U$ , the cut  $S = \{1\}$  in the resulting matrix  $A$  is special, and we solve the above problem by *minimizing* the edge expansion  $1 - A_{1,1}$  of this cut. With the set of possible values that  $r$  can take, we note that a set of extreme points of the resulting optimization problem of minimizing  $1 - A_{1,1}$  or maximizing  $A_{1,1}$  are obtained if we *force* the values of all the entries  $A_{1,i}$  for  $3 \leq i \leq n$  to 0. We then maximize  $r$  for the resulting matrix (indeed, there are exactly two possible doubly stochastic matrices at this point), and the result is the following construction.

#### 4.8 Rootn matrices – fixing the spectral gap and minimizing edge expansion

**Construction 4.8.1.** Let  $m = \sqrt{n}$ ,

$$a_n = \frac{m^2 + m - 1}{m \cdot (m + 2)}, \quad b_n = \frac{m + 1}{m \cdot (m + 2)}, \quad c_n = \frac{1}{m \cdot (m + 1)},$$

$$d_n = \frac{m^3 + 2m^2 + m + 1}{m \cdot (m + 1) \cdot (m + 2)}, \quad e_n = \frac{1}{m \cdot (m + 1) \cdot (m + 2)}, \quad f_n = \frac{2m + 3}{m \cdot (m + 1) \cdot (m + 2)},$$

and define the  $n \times n$  matrix

$$A_n = \begin{bmatrix} a_n & b_n & 0 & 0 & 0 & 0 & 0 & \cdots & 0 \\ 0 & c_n & d_n & e_n & e_n & e_n & e_n & \cdots & e_n \\ 0 & c_n & e_n & d_n & e_n & e_n & e_n & \cdots & e_n \\ 0 & c_n & e_n & e_n & d_n & e_n & e_n & \cdots & e_n \\ 0 & c_n & e_n & e_n & e_n & d_n & e_n & \cdots & e_n \\ 0 & c_n & e_n & e_n & e_n & e_n & d_n & \cdots & e_n \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & c_n & e_n & e_n & e_n & e_n & e_n & \cdots & d_n \\ b_n & f_n & c_n & c_n & c_n & c_n & c_n & \cdots & c_n \end{bmatrix}$$

◇

**Example 4.8.2.** Construction 4.8 for  $n = 9$  looks like the following:

$$A_9 = \frac{1}{60} \begin{bmatrix} 44 & 16 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 5 & 49 & 1 & 1 & 1 & 1 & 1 & 1 \\ 0 & 5 & 1 & 49 & 1 & 1 & 1 & 1 & 1 \\ 0 & 5 & 1 & 1 & 49 & 1 & 1 & 1 & 1 \\ 0 & 5 & 1 & 1 & 1 & 49 & 1 & 1 & 1 \\ 0 & 5 & 1 & 1 & 1 & 1 & 49 & 1 & 1 \\ 0 & 5 & 1 & 1 & 1 & 1 & 1 & 49 & 1 \\ 0 & 5 & 1 & 1 & 1 & 1 & 1 & 1 & 49 \\ 16 & 9 & 5 & 5 & 5 & 5 & 5 & 5 & 5 \end{bmatrix}.$$

Note  $\lambda_2(A_9) = 0$ , and  $\phi(A_9) = \frac{16}{60} < \frac{1}{\sqrt{9}}$ .

◇

**Theorem 4.8.3.** *The following hold for the matrices  $A_n$  in construction 4.8:*

1.  $A_n$  is doubly stochastic.

2. Every nontrivial eigenvalue of  $A_n$  is 0.

3. The edge expansion is bounded as

$$\frac{1}{6\sqrt{n}} \leq \phi(A_n) \leq \frac{1}{\sqrt{n}}.$$

4. As a consequence of 1,2,3,

$$\phi(A_n) \leq \frac{1 - \operatorname{Re}\lambda_2(A_n)}{\sqrt{n}}$$

and thus

$$\Gamma(n) \leq \frac{1}{\sqrt{n}},$$

exponentially improving upon the bound in Lemma 4.4.3.

*Proof.* The following calculations are easy to check, to see that  $A_n$  is a doubly stochastic matrix:

1.  $a_n \geq 0, b_n \geq 0, c_n \geq 0, d_n \geq 0, e_n \geq 0, f_n \geq 0$ .
2.  $a_n + b_n = 1$ .
3.  $c_n + d_n + (n-3)e_n = 1$ .
4.  $b_n + f_n + (n-2)c_n = 1$ .

This completes the proof of (1).

$A_n$  is triangularized as  $T_n$  by the unitary  $U_n$ , i.e.

$$A_n = U_n T_n U_n^*,$$

with  $T_n$  and  $U_n$  defined as follows. Recall that  $m = \sqrt{n}$ . Let

$$r_n = 1 - \frac{1}{m+2},$$

$$\alpha_n = \frac{-n^2 + 2n - \sqrt{n}}{n \cdot (n-1)} = -1 + \frac{1}{m \cdot (m+1)},$$

$$\beta_n = \frac{n - \sqrt{n}}{n \cdot (n-1)} = \frac{1}{m \cdot (m+1)},$$

$$T_n = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & r_n & 0 & 0 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 0 & r_n & 0 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 0 & 0 & r_n & 0 & 0 & \cdots & 0 \\ 0 & 0 & 0 & 0 & 0 & r_n & 0 & \cdots & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & r_n & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \ddots & \vdots \\ 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & r_n \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix},$$

and

$$U_n = \begin{bmatrix} \frac{1}{\sqrt{n}} & \frac{1}{\sqrt{n}} & \frac{1}{\sqrt{n}} & \frac{1}{\sqrt{n}} & \frac{1}{\sqrt{n}} & \frac{1}{\sqrt{n}} & \cdots & \frac{1}{\sqrt{n}} & \frac{1}{\sqrt{n}} \\ \frac{1}{\sqrt{n}} & \alpha_n & \beta_n & \beta_n & \beta_n & \beta_n & \cdots & \beta_n & \beta_n \\ \frac{1}{\sqrt{n}} & \beta_n & \alpha_n & \beta_n & \beta_n & \beta_n & \cdots & \beta_n & \beta_n \\ \frac{1}{\sqrt{n}} & \beta_n & \beta_n & \alpha_n & \beta_n & \beta_n & \cdots & \beta_n & \beta_n \\ \frac{1}{\sqrt{n}} & \beta_n & \beta_n & \beta_n & \alpha_n & \beta_n & \cdots & \beta_n & \beta_n \\ \frac{1}{\sqrt{n}} & \beta_n & \beta_n & \beta_n & \beta_n & \alpha_n & \cdots & \beta_n & \beta_n \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ \frac{1}{\sqrt{n}} & \beta_n & \beta_n & \beta_n & \beta_n & \beta_n & \cdots & \alpha_n & \beta_n \\ \frac{1}{\sqrt{n}} & \beta_n & \beta_n & \beta_n & \beta_n & \beta_n & \cdots & \beta_n & \alpha_n \end{bmatrix}.$$

To show that  $U_n$  is a unitary, the following calculations can be easily checked:

1.  $\frac{1}{n} + \alpha_n^2 + (n-2) \cdot \beta_n^2 = 1.$
2.  $\frac{1}{\sqrt{n}} + \alpha_n + (n-2) \cdot \beta_n = 0.$
3.  $\frac{1}{n} + 2 \cdot \alpha_n \cdot \beta_n + (n-3) \cdot \beta_n^2 = 0.$

Also, to see that  $A_n = U_n T_n U_n^*$ , the following calculations are again easy to check:

1.

$$A_n(1, 1) = a_n = \langle u_1, T u_1 \rangle = \frac{1}{n} + \frac{1}{n} \cdot (n-2) \cdot r_n.$$

2.

$$A_n(1, 2) = b_n = \langle u_1, T u_2 \rangle = \frac{1}{n} + \frac{1}{\sqrt{n}} \cdot (n-2) \cdot r_n \cdot \beta_n.$$

3.

$$A_n(n, 1) = b_n = \langle u_n, T u_1 \rangle = \frac{1}{n} + \frac{1}{\sqrt{n}} \cdot (n-2) \cdot r_n \cdot \beta_n.$$

4. For  $3 \leq j \leq n$ ,

$$A_n(1, j) = 0 = \langle u_1, Tu_j \rangle = \frac{1}{n} + \frac{1}{\sqrt{n}} \cdot \alpha_n \cdot r_n + (n-3) \cdot \frac{1}{\sqrt{n}} \cdot \beta_n \cdot r_n.$$

5. For  $2 \leq i \leq n-1$ ,

$$A_n(i, 1) = 0 = \langle u_i, Tu_1 \rangle = \frac{1}{n} + \frac{1}{\sqrt{n}} \cdot \alpha_n \cdot r_n + \frac{1}{\sqrt{n}} \cdot (n-3) \cdot \beta_n \cdot r_n.$$

6. For  $2 \leq i \leq n-1$ ,

$$A_n(i, 2) = c_n = \langle u_i, Tu_2 \rangle = \frac{1}{n} + \alpha_n \cdot \beta_n \cdot r_n + (n-3) \cdot \beta_n^2 \cdot r_n.$$

7. For  $3 \leq j \leq n$ ,

$$A_n(n, j) = c_n = \langle u_n, Tu_j \rangle = \frac{1}{n} + \alpha_n \cdot \beta_n \cdot r_n + (n-3) \cdot \beta_n^2 \cdot r_n.$$

8. For  $2 \leq i \leq n-1$ ,

$$A_n(i, i+1) = d_n = \langle u_i, Tu_{i+1} \rangle = \frac{1}{n} + \alpha_n^2 \cdot r_n + (n-3) \cdot \beta_n^2 \cdot r_n.$$

9. For  $2 \leq i \leq n-2$ ,  $3 \leq j \leq n$ ,  $i+1 \neq j$ ,

$$A_n(i, j) = e_n = \langle u_i, Tu_j \rangle = \frac{1}{n} + 2 \cdot \alpha_n \cdot \beta_n \cdot r_n + (n-4) \cdot \beta_n^2 \cdot r_n.$$

10.

$$A_n(n, 2) = f_n = \langle u_n, Tu_2 \rangle = \frac{1}{n} + (n-2) \cdot r_n \cdot \beta_n^2.$$

We thus get a Schur decomposition for  $A_n$ , and since the diagonal of  $T_n$  contains only zeros except the trivial eigenvalue 1, we get that all nontrivial eigenvalues of  $A_n$  are zero. This completes the proof of (2).

If we let the set  $S = \{1\}$ , then we get that

$$\phi(A_n) \leq \phi_S(A_n) = b_n < \frac{1}{\sqrt{n}}.$$

Further, since  $T_n$  can be written as  $\Pi_n D_n$ , where  $D_n(1, 1) = 1$ ,  $D_n(i, i) = r_n$  for  $i = 2$  to  $n-1$ , and  $D_n(n, n) = 0$  for some permutation  $\Pi_n$ , we get that  $A_n = (U_n \Pi_n) D_n U_n^*$  which gives a singular value decomposition for  $A_n$  since  $U_n \Pi_n$  and  $U_n^*$  are unitaries. Thus,  $A_n$  has exactly one singular value that is 1,  $n-2$  singular values that are  $r_n$ , and one singular value that is 0. Thus, from Lemma 3.5.1, we get that

$$\phi(A) \geq \frac{1-r_n}{2} = \frac{1}{2 \cdot (\sqrt{n}+2)} \geq \frac{1}{6\sqrt{n}}$$

and this completes the proof of (3).  $\square$

**Remark 4.8.4.** We remark that for the matrices  $A_n$  constructed in Theorem 4.8.3, it holds that

$$\phi(A_n) \leq \frac{1 - |\lambda_i(A)|}{\sqrt{n}}$$

for any  $i \neq 1$ , giving a stronger guarantee than that required for Theorem 1.4.1.

◇

We reiterate that it would be unlikely to arrive at such a construction by algorithmic simulation, since the eigenvalues of the matrices  $A_n$  are extremely sensitive. Although  $\lambda_2(A_n) = 0$ , if we shift only  $O(1/\sqrt{n})$  of the mass in the matrix  $A_n$  to create a matrix  $A'_n$ , by replacing  $a_n$  with  $a'_n = a_n + b_n$ ,  $b_n$  with  $b'_n = 0$ ,  $f_n$  with  $f'_n = f_n + b_n$  and keeping  $c_n, d_n, e_n$  the same, then  $\lambda_2(A'_n) = 1$ . Thus, since perturbations of  $O(1/\sqrt{n})$  (which is tiny for large  $n$ ) cause the second eigenvalue to jump from 0 to 1 (and the spectral gap from 1 to 0), it would not be possible to make tiny changes to random matrices to arrive at a construction satisfying the required properties in Theorem 4.8.3.

#### 4.9 Observations from the construction of Rootn Matrices

At this point, we know that our lower bound on  $\phi$  in theorem 1.4.1 is close to optimal, and a loss of  $n^\alpha$  is necessary for  $\frac{1}{2} \leq \alpha \leq 1$ . Our aim now is to find a construction that achieves a bound  $\Gamma(n) \in O(1/n)$ . However, this is going to take us in a direction different from the one we have taken so far, but to begin in that direction, we need some observations from the construction of Rootn Matrices. Our first observation comes from observing the underlying markov chain. Observe that the Rootn matrices in construction 4.8 look approximately like the following, where  $\epsilon \in \Theta(1/\sqrt{n})$ .

$$A_n = \begin{bmatrix} 1 - \epsilon & \epsilon & 0 & 0 & 0 & 0 & 0 & \dots & 0 \\ 0 & \epsilon^2 & 1 - \epsilon & \epsilon^3 & \epsilon^3 & \epsilon^3 & \epsilon^3 & \dots & \epsilon^3 \\ 0 & \epsilon^2 & \epsilon^3 & 1 - \epsilon & \epsilon^3 & \epsilon^3 & \epsilon^3 & \dots & \epsilon^3 \\ 0 & \epsilon^2 & \epsilon^3 & \epsilon^3 & 1 - \epsilon & \epsilon^3 & \epsilon^3 & \dots & \epsilon^3 \\ 0 & \epsilon^2 & \epsilon^3 & \epsilon^3 & \epsilon^3 & 1 - \epsilon & \epsilon^3 & \dots & \epsilon^3 \\ 0 & \epsilon^2 & \epsilon^3 & \epsilon^3 & \epsilon^3 & \epsilon^3 & 1 - \epsilon & \dots & \epsilon^3 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & \epsilon^2 & \epsilon^3 & \epsilon^3 & \epsilon^3 & \epsilon^3 & \epsilon^3 & \dots & 1 - \epsilon \\ \epsilon & \epsilon^2 & \epsilon^2 & \epsilon^2 & \epsilon^2 & \epsilon^2 & \epsilon^2 & \dots & \epsilon^2 \end{bmatrix}.$$

Note that for any vertex  $k \in [3, n]$ , since  $A_{i,j}$  is the probability of going from vertex  $j$  to vertex  $i$  (for right multiplication by a vector), the chain from vertex  $k$  almost

always goes backward from  $k$  to  $k - 1$  with probability  $\approx 1 - \epsilon$ , and otherwise goes approximately uniformly to any other vertex except vertex 1. Thus,

**Observation:** The Rootn matrix in construction 4.8 is *almost* a cycle.

This observation in fact leads further to the following concrete lemma.

**Lemma 4.9.1.** *For the Rootn Matrix  $A_n$ , for any set  $S = \{i, i + 1, \dots, j\}$ ,*

$$\phi_S(A_n) \in O\left(\frac{1}{\sqrt{n}}\right)$$

*Proof.* This can immediately be observed by directly summing the entries in the matrix  $A$  in construction 4.8. □

The main observation from Lemma 4.9.1 is that although we pick a set of size  $n/2$ , say  $\{2, \dots, n/2 + 1\}$ , there is contribution from *exactly one entry*  $d_n$  of about 1 that is in the complement set, and the rest of the  $O(n^2)$  numbers contribute about  $O(\sqrt{n})$  mass that leaves the set, and thus the average mass leaving the set is approximately  $n^2 \epsilon^3 / (n/2) \in O(1/\sqrt{n})$ . Thus, if we had zeros above the diagonal instead of the entries  $e_n$ , for a set of size  $n/2$ , we would have contribution from *exactly one entry*  $d_n$  of about 1, and the resulting edge expansion of the matrix would become  $O(1/n)$  as we would want. Note that the entries  $e_n$  are less meaningful in terms of the expansion, since removing a factor of  $n \cdot e_n \cdot J$  from the matrix will only keep the entries  $d_n$  in the off-diagonal block.

This takes us in a novel direction, since by observing construction 4.8 and noting 4.9 and Lemma 4.9.1, we see that we can *fix the edge expansion of the matrix* and somehow *set the entries of the matrix to have desired eigenvalues*, going in a direction opposite to that which we had for construction of 4.8 Rootn Matrices. One simple manner to achieve this is to have the following matrix (discussed previously for another requirement) –

$$A_n = \begin{bmatrix} \mathbf{0} & 1 & 0 & 0 & 0 & 0 \\ 0 & \mathbf{0} & 1 & 0 & 0 & 0 \\ 0 & 0 & \mathbf{0} & 1 & 0 & 0 \\ 0 & 0 & 0 & \ddots & \ddots & 0 \\ 0 & 0 & 0 & 0 & \mathbf{0} & 1 \\ 0 & 0 & 0 & 0 & 0 & \mathbf{0} \end{bmatrix}$$

which has edge expansion  $O(1/n)$  and all eigenvalues are 0. The matrix however is not doubly stochastic, and making it so by putting  $A_{n,1} = 1$  makes it a cycle and which brings the spectral gap close to  $\phi^2$ , putting it strictly within the Cheeger regime (see Section 3.3). However, inspecting the heaviest permutation within the Rootn Matrix (construction 4.8) through observation 4.9, we can start by fixing the *structure* of the matrix to be following:

$$A_n = \begin{bmatrix} \mathbf{1} - \mathbf{r} & r & 0 & 0 & 0 & 0 \\ \cdot & \cdot & r & 0 & 0 & 0 \\ \cdot & \cdot & \cdot & r & 0 & 0 \\ \cdot & \cdot & \cdot & \ddots & \ddots & 0 \\ \cdot & \cdot & \cdot & \cdot & \cdot & r \\ \cdot & \cdot & \cdot & \cdot & \cdot & \mathbf{1} - \mathbf{r} \end{bmatrix}$$

Note that the matrix is almost exactly similar to the Rootn matrix in construction 4.8 as shown in observation 4.9, where the entries represented by  $\cdot$  are yet to be filled. Since the matrix has to be doubly stochastic,  $r \leq 1$ , and irrespective of the value of  $r$ ,

$$\phi(A_n) \in O(1/n),$$

since by considering the set  $S = \{1, \dots, n/2\}$ ,

$$\phi_S(A) = \frac{r}{n/2} \in O(1/n).$$

The key thing to note is that this is almost exactly similar to the structure of the triangular matrix in the Schur form, and in essence, is the same structure as for Rootn matrices. All we need to do is to fill the entries of  $A_n$  so that it remains doubly stochastic, and has the second eigenvalue much far from 1, which will give us  $\Gamma(n) \in O(1/n)$

However, having fixed this structure, even if we choose, say, a  $5 \times 5$  matrix, it seems difficult to set variables to obtain some desired eigenvalues, since the characteristic polynomial has degree  $\gg 5$ , and it will not have an analytic solution, which although not necessary, its lack makes the analysis of the matrix nearly impossible. The main idea is this – instead of trying to directly control the eigenvalues of the matrix, we try and *control the eigenvalues indirectly* by controlling the coefficients of the characteristic polynomial. For any given matrix  $A_n$ , let the coefficient of  $\lambda^{n-k}$  in the



characteristic polynomial be  $a_k$ , then

$$a_k = \frac{(-1)^k}{k!} \begin{vmatrix} \text{Tr}A & 1 & 0 & 0 & 0 & 0 \\ \text{Tr}A^2 & \text{Tr}A & 2 & 0 & 0 & 0 \\ \text{Tr}A^3 & \text{Tr}A^2 & \text{Tr}A & \ddots & 0 & 0 \\ \ddots & \text{Tr}A^3 & \text{Tr}A^2 & \text{Tr}A & k-2 & 0 \\ \text{Tr}A^{k-1} & \ddots & \text{Tr}A^3 & \text{Tr}A^2 & \text{Tr}A & k-1 \\ \text{Tr}A^k & \text{Tr}A^{k-1} & \ddots & \text{Tr}A^3 & \text{Tr}A^2 & \text{Tr}A \end{vmatrix}$$

where  $|\cdot|$  is the determinant. Thus, we realize that controlling the traces of the powers of the matrix  $A_n$  helps to control the coefficients of the characteristic polynomial, which in turn controls the eigenvalues. This is not surprising in retrospect, since  $\text{Tr}A^k = \sum \lambda_i^k$ , but just this fact is not very useful unless the values of  $\sum \lambda_i^k$  are simple. However, for us, with constraint 1 (4.5), to have all eigenvalues 0, we only need to set  $\text{Tr}A^k = 1$  for all  $k \geq 1$ , and this implies that the matrix has one (trivial) eigenvalue 1, and all other eigenvalues of the matrix will be 0. Thus, given the structure 4.9, we are going to set the remaining values to ensure that  $\text{Tr}A^k = 1$ .

To set the values concretely, note that the underlying graph of our matrix is the following, letting  $A_{i,j}$  be the weight of the edge from  $j \rightarrow i$  (for right multiplication by a vector): the only “back” edges in the graph are from vertex  $i$  to  $i-1$  (for  $i \geq 2$ ) of weight  $r$ , and all the other edges are “forward” edges that go from  $i$  to  $j$  ( $j \geq i$ ). Consider the combinatorial meaning of  $\text{Tr}A^k$ . It sums the weights of every length  $k$  path (walk) from any vertex to itself. Fix any vertex  $i$ , and consider any path of length  $k$  from  $i$  to itself. How far can this path go forward? Note that if the path went from  $i$  to  $i+k$  in one step, since it can only go back one vertex in one step, the path cannot go back to vertex  $i$  in  $k$  steps. Thus, the maximum that a path of length  $k$  starting at any vertex can go forward in one step is  $k-1$ . Thus, in  $\text{Tr}A^k$ , there is *exactly* one path of length  $k$  from vertex  $i$  to itself that goes back  $k-1$  steps, and it has weight  $r^{k-1}a_{i,i-k+1}$ . Similarly, the weight of any path of length  $k$  that goes back  $l$  steps (with  $l \leq k-1$ ) will be a term of the form  $r^l \cdot c$  where  $c$  is the product of other forward edges in the graph along the path. As a consequence, we get that for any  $k \geq 1$ ,

$$\text{Tr}A^k = \sum_{i=0}^{k-1} r^i w_i(k), \quad (4.9.2)$$

or that  $\text{Tr}A^k$  is a polynomial in  $r$  of degree  $k-1$  where  $w_i(k)$  are functions of all the other nonzero entries of  $A$ . As stated above, the coefficient of  $r^{k-1}$  in  $\text{Tr}A^k$  is easy to

find, and is exactly

$$[r^{k-1}] \text{Tr} A^k = w_{k-1}(k) = \sum_{j=k-1}^n a_{j,j-k+1}$$

and in particular, contains only those entries that are at a distance of  $k - 1$  from the diagonal. This key fact is extremely important, and we state it explicitly as a fact that we are going to exploit:

**Fact 4.9.3.** *For the structure of  $A$  as discussed (see 4.9), the coefficient of  $r^{k-1}$  in  $\text{Tr} A^k$  is linear in the entries of the matrix.*

The observation 4.9.3 suggests to us an *inductive* manner of assigning forward edge weights. Note that if we have set all edge weights that are at a distance of  $k - 2$  from the diagonal in  $A$  using only equations  $\text{Tr} A^l = 1$  for  $1 \leq l \leq k - 1$ , the then equation 4.9.2 becomes

$$\text{Tr} A^k = W + r^{k-1} \cdot \sum_{j=k-1}^n a_{j,j-k+1}$$

and setting it to 1 gives

$$\sum_{j=k-1}^n a_{j,j-k+1} = \frac{1 - W}{r^{k-1}}, \quad (4.9.4)$$

where  $W$  is the sum of weights of all paths that go at most  $k - 2$  times back.

Since  $A^n = J$ , we have  $n - 1$  independent equations,  $\text{Tr} A^k = 1$  for  $1 \leq k \leq n - 1$ . Given these  $n - 1$  equations, *if our matrix consists only of  $n - 1$  different variables, we will be able to set each variable using one equation*, and since we can use equation 4.9.4 (that comes from the equation  $\text{Tr} A^k = 1$ ) to set the variables at distance  $k - 1$  from the diagonal, it gives us our  $n - 2$  different variables. Thus, *we set all variables at distance  $k$  from the origin to have value  $c_k$* . This is the most important and final conclusion.

We further need to ensure that our matrix remains doubly stochastic, the first column and last row will have special values, but otherwise the values are set as stated. We

thus obtain the following matrix:

$$A_n = \begin{bmatrix} b_0 & r & 0 & 0 & 0 & 0 & 0 & \cdots & 0 \\ b_1 & c_0 & r & 0 & 0 & 0 & 0 & \cdots & 0 \\ b_2 & c_1 & c_0 & r & 0 & 0 & 0 & \cdots & 0 \\ b_3 & c_2 & c_1 & c_0 & r & 0 & 0 & \cdots & 0 \\ b_4 & c_3 & c_2 & c_1 & c_0 & r & 0 & \cdots & 0 \\ \vdots & \vdots & c_3 & c_2 & c_1 & c_0 & r & \cdots & 0 \\ b_{n-3} & c_{n-4} & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \vdots \\ b_{n-2} & c_{n-3} & c_{n-4} & \cdots & c_3 & c_2 & c_1 & c_0 & r \\ b_{n-1} & b_{n-2} & b_{n-3} & \cdots & b_4 & b_3 & b_2 & b_1 & b_0 \end{bmatrix}$$

where for  $0 \leq i \leq n-2$

$$b_i = 1 - r - \sum_{j=0}^{i-1} c_j$$

and

$$b_{n-1} = 1 - \sum_{i=0}^{n-2} b_i.$$

With this structure, we can set  $c_0$  using  $\text{Tr}A = 1$ , and  $c_1$  using  $\text{Tr}A^2 = 1$ , and so on  $c_{k-1}$  using  $\text{Tr}A^k = 1$ , and note that  $\text{Tr}A^k$  contains  $b_{k-1}$  but  $b_{k-1}$  does not depend on  $c_{k-1}$ . Thus, using equation 4.9.4, we get each of the values of  $c_k$  as functions (polynomials, albeit with negative exponents) of  $r$ . And finally, the magic value of  $r$  that we use to evaluate each of the  $c_k$ 's, and that which makes the entire construction work, is to set  $r$  to be the  $(n-1)$ 'th root of  $1/n$ :

$$r = \left(\frac{1}{n}\right)^{\frac{1}{n-1}}$$

The value of  $r$  can be obtained in multiple ways, for instance by using the equation  $\text{Tr}A^{n-1} = 1$  which will be a polynomial only in  $r$  since all of the  $a_i$ 's have already been fixed, and choosing the positive real root of  $r$  in the equation. Alternately it can be obtained by taking  $A^{n-1} = J$  and looking at the  $a_{1,n}$ . We thus arrive at the following construction.

#### 4.10 Chet Matrices – fixing the edge expansion and maximizing the spectral gap

**Construction 4.10.1.** For any  $n$ , let  $C_n$  have the following structure.

$$C_n = \begin{bmatrix} b_0 & r & 0 & 0 & 0 & 0 & 0 & \cdots & 0 \\ b_1 & c_0 & r & 0 & 0 & 0 & 0 & \cdots & 0 \\ b_2 & c_1 & c_0 & r & 0 & 0 & 0 & \cdots & 0 \\ b_3 & c_2 & c_1 & c_0 & r & 0 & 0 & \cdots & 0 \\ b_4 & c_3 & c_2 & c_1 & c_0 & r & 0 & \cdots & 0 \\ \vdots & \vdots & c_3 & c_2 & c_1 & c_0 & r & \cdots & 0 \\ b_{n-3} & c_{n-4} & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \vdots \\ b_{n-2} & c_{n-3} & c_{n-4} & \cdots & c_3 & c_2 & c_1 & c_0 & r \\ b_{n-1} & b_{n-2} & b_{n-3} & \cdots & b_4 & b_3 & b_2 & b_1 & b_0 \end{bmatrix}$$

where for  $0 \leq i \leq n-2$

$$b_i = 1 - r - \sum_{j=0}^{i-1} c_j$$

and

$$b_{n-1} = 1 - \sum_{i=0}^{n-2} b_i.$$

Let  $C_n|_k$  be the matrix with structure of  $C_n$ , in which all  $c_l$  with  $l \geq k$  are set to 0, and all  $b_l$  with  $l \geq k+1$  are set to 0. Inductively for  $k = 0$  to  $n-3$ , set the polynomials

$$c_k = \frac{1 - \text{Tr}(C_n|_k)^{k+1}}{(n-k-2) \cdot (k+1) \cdot r^k},$$

and set

$$r = n - \frac{1}{n-1}.$$

◇

We now show certain specific cases, so that we can actually compute and see how the matrices  $A_n$  look.

**Example 4.10.2.** For  $n = 5$ , we get

$$\begin{aligned}c_0 &= \frac{2}{3}r - \frac{1}{3} \\c_1 &= \frac{5}{6}r - \frac{1}{3} \cdot \frac{1}{r} \\c_2 &= \frac{55}{27}r + \frac{2}{9} \cdot \frac{1}{r} - \frac{20}{27} \cdot \frac{1}{r^2} \\r &= 5^{-1/4}\end{aligned}$$

and the matrix approximated to 5 decimal places looks like:

$$C_5 \approx \begin{bmatrix} 0.33126 & 0.66874 & & & \\ 0.21870 & 0.11249 & 0.66874 & & \\ 0.15993 & 0.05886 & 0.11249 & 0.66874 & \\ 0.12170 & 0.03820 & 0.05886 & 0.11249 & 0.66874 \\ 0.16810 & 0.12170 & 0.15993 & 0.21870 & 0.33126 \end{bmatrix}$$

◇

Similarly, we can write another example.

**Example 4.10.3.** For  $n = 8$ , we get

$$\begin{aligned}c_0 &= \frac{1}{6} \cdot (2r - 1) \\c_1 &= \frac{1}{5r} \cdot \left( \frac{4}{3}r^2 - \frac{7}{12} \right) \\c_2 &= \frac{1}{4r^2} \cdot \left( \frac{152}{135}r^3 + \frac{7}{45}r - \frac{14}{27} \right) \\c_3 &= \frac{1}{3r^3} \cdot \left( \frac{778}{675}r^4 + \frac{49}{900}r^2 + \frac{7}{27}r - \frac{1981}{3600} \right) \\c_4 &= \frac{1}{2r^4} \cdot \left( \frac{112}{75}r^5 + \frac{133}{4050}r^3 + \frac{7}{135}r^2 + \frac{1981}{5400}r - \frac{1043}{1620} \right) \\c_5 &= \frac{1}{r^5} \cdot \left( \frac{27056}{10125}r^6 + \frac{2863}{121500}r^4 + \frac{28}{1215}r^3 + \frac{1981}{81000}r^2 + \frac{1043}{2430}r - \frac{193417}{243000} \right) \\r &= 8^{-1/7}\end{aligned}$$

and the matrix approximated to 5 decimals looks like:

$$C_8 = \begin{bmatrix} 0.25700 & 0.74300 & & & & & & \\ 0.17601 & 0.08100 & 0.74300 & & & & & \\ 0.13489 & 0.041118 & 0.08100 & 0.74300 & & & & \\ 0.10823 & 0.02666 & 0.041118 & 0.08100 & 0.74300 & & & \\ 0.089011 & 0.019219 & 0.02666 & 0.041118 & 0.08100 & 0.74300 & & \\ 0.074311 & 0.014700 & 0.019219 & 0.02666 & 0.041118 & 0.08100 & 0.74300 & \\ 0.062608 & 0.011703 & 0.014700 & 0.019219 & 0.02666 & 0.041118 & 0.08100 & 0.74300 \\ 0.09800 & 0.062608 & 0.074311 & 0.089011 & 0.10823 & 0.13489 & 0.17601 & 0.25700 \end{bmatrix}$$

◇

We give the equations for  $n = 16$  in Appendix A.1

Given the construction in 4.10, we have the following theorem.

**Theorem 4.10.4.** *Let  $C_n$  be the matrix generated by algorithm 4.10. Then the following hold for  $C_n$ .*

1. (Conjecture) Every entry of  $C_n$  is nonnegative.
2. All nontrivial eigenvalues of  $C_n$  are 0.
3.  $\phi(C_n) \leq 2/n \in O(1/n)$
4. As a consequence of 2 and 3, we get

$$\Gamma(n) \in O\left(\frac{1}{n}\right)$$

improving the bound in Lemma 4.8.3 and combined with theorem 1.4.1, it implies that

$$\Gamma(n) \in \Theta\left(\frac{1}{n}\right)$$

and that the lower bound on  $\phi(R)$  in Theorem 1.4.1 is tight up to constants.

*Proof.* Part (1) of lemma is a conjecture and we assume it for the remaining parts. For (3), since  $C_n$  is nonnegative due to (1),  $\phi(C_n)$  is well defined, and considering  $S = \{1, \dots, n/2\}$  we have  $\phi_S(C_n) \leq \frac{r}{n/2} \leq \frac{2}{n} \in O(1/n)$ . For (2), since the sum of every row and column of  $A_n$  is 1, it has one eigenvalue 1 corresponding to the all ones eigenvector, and further since  $\text{Tr}C_n^k = \sum_{i=1}^n \lambda_i^k(C_n) = 1 + \sum_{i=2}^n \lambda_i^k(C_n) = 1$  for all  $k \geq 1$ , it implies all other eigenvalues of  $C_n$  except 1 are 0.

□

There is only one uncertainty about this construction, and that is to show that all  $c_i$  and  $b_i$  produced by algorithm 4.10 are nonnegative. We do not know how to show this at present, and this will be the main conjecture of this thesis, stated and discussed in Section 4.12. However, we try to list some of the properties of Chet Matrices first.

#### 4.11 Observations and Properties of Chet Matrices

We find Chet matrices beautiful enough to warrant their independent study, and we shall explore many of their properties.

**1. (Hessenberg-Toeplitz Structure)** Chet matrices have a Hessenberg-Toeplitz structure. Hessenberg matrices  $H_{k,l}$  are matrices for which all the entries that are below the diagonal at a distance greater than  $k$  and entries above the diagonal at a distance greater than  $l$  are zero. Further, the matrix has a Toeplitz-like structure where entries are the same along every diagonal, except the first column and the last row.

**2. (Permanent)** Let  $C'_n$  be the matrix which has all the entries of  $C_n$ , but the  $n - 1$  entries above the diagonal that are  $r$  are replaced by  $-r$ . Then

$$\text{permanent}(C_n) = \text{determinant}(C'_n)$$

and the proof follows from straightforward induction.

**3. (Approximate values)** The approximate values of the entries of  $C_n$ , by numerical and analytical observations, are as follows:

$$r \approx 1 - \frac{\log n}{n - 1}.$$

For the entries of  $C_n$ ,

$$c_i \in O\left(\frac{1}{i \cdot n}\right).$$

See Appendix A.4 for a figure of the above for  $n = 500$ . Thus, note that

$$\sum_{i=0}^{O(\log n)} c_i \in O\left(\frac{\log \log n}{n}\right),$$

and thus for  $i \in O(\log n)$ ,

$$b_i = 1 - r - \sum_{j=0}^i c_j \approx \frac{\log n - \log \log n}{n} > 0.$$

A weaker statement is possible to show directly.

**Lemma 4.11.1.** *For any Chet Matrix  $C_n$ , if  $c_i \geq 0$  and  $b_i \geq 0$  for  $i \in O(n/\ln n)$ , then for  $i \in O(n/\ln n)$ ,*

$$c_i \in O\left(\frac{1}{i \cdot (n-i)}\right).$$

*Proof.* The proof follows immediately by noting that since  $c_i$  is set by using  $\text{Tr}C_n^{i+1} = 1$ , we get that

$$1 = \text{Tr}C_n^{i+1} = S + r^i \cdot c_i \cdot i \cdot (n-i)$$

where  $S$  is the weighted sum of all other paths of length  $i+1$  that do not use  $c_i$ . Since  $S \geq 0$  by the assumption of  $b_i, c_i \geq 0$ , and

$$r^i = n^{-\frac{i}{n-1}} \geq \exp\left(-\frac{\ln n}{n-1} \cdot i\right) \in \Omega(1)$$

since  $i \in O(n/\ln n)$ , the claim immediately follows.  $\square$

**4. (Analytical values)** The first three entries, computed analytically for any  $n$ , are as follows. Let  $r = n^{-1/(n-1)}$ .

$$c_0(n) = \frac{2 \cdot r - 1}{n - 2}$$

$$c_1(n) = \frac{(2r^2 - 1) \cdot n + 1}{2(n-3)(n-2) \cdot r}$$

$$c_2(n) = \frac{(2r^3 - 1) \cdot n^3 + (-8r^3 + 3r + 4) \cdot n^2 + (12r^3 - 15r - 3) \cdot n + 12r}{3(n-4)(n-3)(n-2)^2 r^2}$$

It can be shown that these are always nonnegative.

**5. (Distinct entries)** An interesting thing about this construction, is that there are  $\Theta(n)$  distinct entries in the matrix, however for Rootn matrices in (construction 4.8), we only had 6 distinct entries in the matrix, and de Bruijn has only 2. Note that starting with the structure of the matrix in construction 4.8, and again using the equations  $\text{Tr}(A^k) = 1$  for  $k = 1$  to 6 since there are 6 distinct variables, we obtain the same values of the variables as obtained from the Schur transformation of the



matrix, avoiding the Schur decomposition entirely.

**6. (Route to the construction, and infinite similar constructions)** It is quite remarkable the path we took to arrive at construction 4.10. We started with wanting to understand the edge expansion of matrices with all eigenvalues 0 since it is not far from optimal (see Section 4.5), and ended up carefully choosing  $T$  and  $U$  in the schur decomposition of doubly stochastic matrices to arrive at Rootn Matrices (construction 4.8). The construction informed us of a possible structure of matrices to consider, and with that structure and subsequent reasoning we arrived at having  $\text{Tr}A^k = 1$  as our primary condition and diagonally setting the values in the matrix to arrive at Chet Matrices. At this point, we can start with any matrix with small edge expansion and use the same algorithm 4.10 to set values at distance  $k$  from the diagonal by using  $\text{Tr}A^k = 1$ . Moreover, we can construct infinite such matrices with the structure of Chet Matrices but with different values of  $r$  and the  $b_i$ 's and  $c_i$ 's, simply by choosing some set of eigenvalues – say  $\frac{1}{2}, \frac{1}{4}, \dots, \frac{1}{2^{n-1}}$  – and using corresponding trace inequalities.

**7. (Matrices from approximate equations)** Note that since it is difficult grasp how the coefficients of the polynomials of the entries  $c_i$  in the matrix are behaving, it is tempting to try and approximate the entries of the Chet matrices in construction 4.10 and see if the approximation works. However, it turns out that the eigenvalues of the matrix, as expected, are extremely sensitive, and the spectral gap quickly diminishes to zero with approximation. Another idea, is to instead approximate the equations themselves instead of the matrix entries, by letting  $\text{Tr}A^k \approx 1$ . However, it is simple to show that this cannot work.

**Lemma 4.11.2.** *There are doubly stochastic matrices  $A$  with  $\text{Tr}A^k \approx 1$  but  $\text{Re}\lambda_2(A) \approx 1$ .*

*Proof.* Consider the adjacency matrix  $C$  of the graph which consists of 1 isolated vertex, and a directed cycle of length  $n - 1$ . Note that  $C$  is doubly stochastic and disconnected. The eigenvalues of  $C$  are  $1, \omega_i$  for  $i = 0$  to  $n - 2$ , where  $\omega_i = e^{\frac{2\pi \cdot i}{n-1}}$ . Let  $A = \alpha J + (1 - \alpha)C$ . Note that the eigenvalues of  $A$  are  $1, (1 - \alpha)\omega_i$ , for  $0 \leq i \leq n - 2$ , since the eigenvector for the first eigenvalue 1 is the all ones vector, and  $J$  is a projection on it. The other eigenvalue that was 1, corresponding to  $\omega_0$ , is in the space orthogonal to the all ones vector and just shrinks by a factor of  $(1 - \alpha)$ . Let  $\alpha = \frac{2 \log n}{n - 1}$ , then the second eigenvalue of  $A$  is  $\lambda_2 = 1 - \alpha = 1 - \frac{2 \log n}{n - 1} \approx 1$ .

We have that for any  $k \leq n - 2$ ,  $\text{Tr}A^k = 1 + (1 - \alpha)^k \sum_{i=0}^{n-2} \omega_i^k = 1$  since  $\sum_{i=0}^{n-2} \omega_i^k = 0$  for  $k \leq n - 2$ . For  $k = n - 1$ , we have

$$\begin{aligned} \text{Tr}A^{n-1} &= 1 + (1 - \alpha)^{n-1} \sum_{i=0}^{n-2} \omega_i^{n-1} \\ &= 1 + (n - 1)(1 - \alpha)^{n-1} \\ &\leq 1 + (n - 1) \exp(-2 \log n) \\ &\leq 1 + \frac{1}{n} \\ &\approx 1 \end{aligned}$$

which completes the proof. Note that such equations might help to construct matrices with  $\Gamma(n) \approx \frac{1}{\log n}$ , but will not help to obtain  $\Gamma(n) \in o(\frac{1}{\log n})$ .  $\square$

**8. (Jordan Form)** We now try and understand the Jordan form of Chet Matrices. The Jordan forms of Hessenberg matrices are well understood (see [Zem06] for instance) and are easy to derive using the resolvent  $(t \cdot I - A)^{-1}$ , and we only state the final forms here. Assume that  $A = VQV^{-1}$  is the Jordan decomposition of  $A$ , where  $Q$  contains two blocks, 1 block of length 1 for eigenvalue 1 and another of length  $n - 1$  for eigenvalue 0. Specifically,  $Q$  contains all zeros, except  $Q_{1,1} = 1$ , and  $Q_{i,i+1} = 1$  for  $i = 2$  to  $n - 1$ . The columns of  $V$  are the most interesting parts, and can be described as follows. Let  $A_{[1,j]}$  denote the submatrix of  $A$  consisting of all rows and columns with indices  $\{1, 2, \dots, j\}$ , with  $A_{[1,0]} = 1$ . Let the columns of  $V$  be  $V_i$  for  $1 \leq i \leq n$ . Note that since  $A$  is doubly stochastic, the first column  $V_1$  is just a multiple of the all ones vector. Consider the second column. The entries of the second column, for  $i = 1$  to  $n$ , are given by

$$V_2(i) = \left. \frac{\det(t \cdot I - A_{[1,i-1]})}{r^{i-1}} \right|_{t=0}$$

(Note  $I$  has dimension that of  $A_{[1,i-1]}$ , thus for  $i = 1$  the numerator is simply  $-1$ ). Similarly, the third column,  $V_3$ , can be described as follows,

$$V_3(i) = \left. \frac{1}{r^{i-1}} \cdot \frac{d}{dt} (\det(t \cdot I - A_{[1,i-1]})) \right|_{t=0}$$

and in general, for  $2 \leq j \leq n$ ,

$$V_j(i) = \left. \frac{1}{(j - 2)! \cdot r^{i-1}} \cdot \frac{d^{(j-2)}}{dt^{(j-2)}} (\det(t \cdot I - A_{[1,i-1]})) \right|_{t=0} .$$

Thus, note that even the Jordan form has Hessenberg structure! This follows simply because  $\det(t \cdot I - A_{[1,i-1]})$  has degree  $i - 1$  in  $t$ , and when it is differentiated more than  $i - 1$  times, the term becomes zero. We find this property beautiful, but do not know how to employ it to show nonnegativity of variables at present.

**9. (Generating functions)** We now express all the entries of the matrix in terms of generating functions, in order to link it to the combinatorics of the underlying chain, and obtain closed form expressions for some of the quantities. Since the matrix has all eigenvalues 0 except the trivial eigenvalue, let  $\chi_t(C_n)$  be the characteristic polynomial of  $C_n$ , then  $\chi_t(C_n) = t^{n-1} \cdot (t - 1)$ , and thus except the coefficient of  $t^n$  ( $= 1$ ) and  $t^{n-1}$  ( $= -1$ ), all the coefficients are 0. However, we know that  $\chi_t(C_n) = \det(t \cdot I - C_n)$ , and since  $t \cdot I - C_n$  also has the Hessenberg structure (see point (1)), letting  $C'_n$  denote  $C_n$  with the entries  $r$  replaced by  $-r$ , we get from point (2) that  $\text{perm}(t \cdot I - C'_n) = \det(t \cdot I - C_n)$ . Thus, we have that

$$\text{perm}(t \cdot I - C'_n) = t^{n-1} \cdot (t - 1). \quad (4.11.3)$$

The important thing about the permanent is that the underlying combinatorics is much more amenable to generating functions than the determinant. The permanent is the sum of weights of all the cycle covers of the matrix which is much simpler to deal with than the number of weighted cycles of length  $k$  (for all  $k$ ) as is the case with the determinant.

We are going to let  $Z_n = t \cdot I - C'_n$ , and count the cycle covers in  $Z$ . Let  $Z_{1,1} = Z_{n,n} = q_0 = t - b_0$ ,  $Z_{i,i} = a_0 = t - c_0$  for  $2 \leq i \leq n - 1$ , and we let  $q_i = -b_i$  and  $a_i = -c_i$  for  $i \geq 2$  for the corresponding entries in  $Z$ . Note that  $Z$  has  $r$  above the diagonal, since  $C'_n$  had  $-r$ . To count the cycle covers in  $Z_n$ , note that due to the structure of our matrix, starting at vertex  $i$ , if a cycle goes back  $k$  steps to vertex  $i - k$ , then one of the cycles must be the cycle  $\{i, i - k, i - k + 1, i - k + 2, \dots, i - 1, i\}$  of length  $k + 1$ , since this is the only manner in which the cycle can be a part the cover. Note that the weight of this cycle is  $c \cdot r^k$  where  $c$  denotes the weight of the edge from vertex  $i$  to vertex  $i - k$ . Thus, note that any particular cycle disconnects the graph into two parts, and thus, we can define the following two polynomials:

$$R(x) = \sum_{i \geq 0} a_i r^i x^{i+1}$$

$$G(x) = \sum_{i \geq 0} q_i r^i x^{i+1}$$

where assume that  $a_l = 0$  for  $l \geq n - 1$  and  $q_l = 0$  for  $l \geq n$ . Note that  $R$  and  $G$  do not have constant terms, and since the  $b_i$ 's were chosen to ensure the first column and last row of  $C_n$  sum to 1, we have that

$$\begin{aligned} c_i &= b_i - b_{i+1} \\ a_i &= q_i - q_{i+1} \\ R &= G - \frac{G - q_0x}{rx} \\ G - R &= \frac{G'}{rx} \end{aligned} \tag{4.11.4}$$

where  $G' = G - q_0x$ . This equation will be useful later.

The coefficients of  $x^{k+1}$  in the two polynomials for  $k \geq 1$  are

$$\begin{aligned} [x^k]R(x) &= a_k r^k \\ [x^k]G(x) &= q_k r^k. \end{aligned}$$

The first coefficient is exactly the length of a cycle of length  $k + 1$  starting at any vertex except the first and last vertex, and the second coefficient is the length of a cycle of length  $k + 1$  starting at the first or last vertex. Thus, since the permanent of  $Z$  is the sum of the weights of all cycle covers of length  $n$  in our graph, we get that

$$\begin{aligned} H(x) &= G(x)^2 \sum_{i \geq 0} R(x)^i + G(x) \\ &= \frac{G(x)^2}{1 - R(x)} + G(x) \end{aligned}$$

where the first term counts the weights of all cycle covers by fixing the cover, and considering the cycle in which the first vertex appears, the cycle in which the last vertex appears, and then the number of different ways in which to divide the remaining vertices into  $i$  cycles, and the second term counts the one cycle cover in which all vertices appear in a single cycle. Note that the coefficients of  $x^k$  in  $H(x)$  are polynomials in  $t$ . Thus we have

$$\begin{aligned} t^{n-1} \cdot (t - 1) &= \text{perm}(Z) = [x^n]H(x) \\ &= [x^n] \frac{G(x)^2}{1 - R(x)} - b_n r^{n-1} \end{aligned}$$

Thus, to compare coefficients on both sides of the above equation, we have the following  $n + 1$  equations:

$$\begin{aligned}
1 &= \frac{1}{n!} \cdot \frac{d^n}{dt^n} [x^n] \frac{G(x)^2}{1-R(x)} \Big|_{t=0} \\
-1 &= \frac{1}{(n-1)!} \cdot \frac{d^{n-1}}{dt^{n-1}} [x^n] \frac{G(x)^2}{1-R(x)} \Big|_{t=0} \\
0 &= \frac{1}{k!} \cdot \frac{d^k}{dt^k} [x^n] \frac{G(x)^2}{1-R(x)} \Big|_{t=0} \\
0 &= [x^n] \frac{G(x)^2}{1-R(x)} \Big|_{t=0} - b_n r^{n-1}
\end{aligned} \tag{4.11.5}$$

where the second last equation holds for  $1 \leq k \leq n-2$ . The last equation is redundant, since it represents  $0 = \det(t \cdot I - C_n)|_{t=0}$  which we know to be true based on the way we have set values of the  $c_i$ 's and  $b_i$ 's in  $C_n$ . To understand other equations, note that there is only one term/coefficient in  $G(x)$  that is dependent on  $t$ , namely  $q_0x = (t - b_0)x$  and similarly for  $R(x)$  the term  $a_0x = (t - c_0)x$ , and thus

$$\begin{aligned}
\frac{d}{dt} G(x)^2 &= 2G(x) \cdot x \\
\frac{d^2}{dt^2} G(x)^2 &= 2x^2 \\
\frac{d^i}{dt^i} G(x)^2 &= 0
\end{aligned}$$

for  $i \geq 3$ , and similarly we can write,

$$\begin{aligned}
\frac{d}{dt} (1 - R(x))^{-1} &= (1 - R(x))^{-2} x \\
\frac{d^i}{dt^i} (1 - R(x))^{-1} &= i! \cdot x^i \cdot (1 - R(x))^{-(i+1)}
\end{aligned}$$

for all  $i$ . Thus we get

$$\begin{aligned}
\frac{d^k}{dt^k} \frac{G(x)^2}{1-R(x)} &= \sum_{i=0}^k \binom{k}{i} \frac{d^i}{dt^i} (1-R)^{-1} \frac{d^{k-i}}{dt^{k-i}} G^2 \\
&= k! x^k (1-R)^{-k+1} G^2 + \\
&\quad k(k-1)! x^{k-1} (1-R)^{-k} \cdot 2 \cdot G \cdot x + \\
&\quad \binom{k}{2} (k-2)! x^{k-2} (1-R)^{-(k-1)} 2x^2 \\
&= k! \cdot x^k \cdot \left( G^2 (1-R)^{-(k+1)} + 2G(1-R)^{-k} + (1-R)^{-(k-1)} \right) \\
&= k! \cdot x^k \cdot (1-R)^{-(k+1)} \cdot (G+1-R)^2.
\end{aligned}$$

Thus, from equation 4.11.5, we have

$$\begin{aligned}
\frac{1}{k!} \cdot \frac{d^k}{dt^k} [x^n] \frac{G(x)^2}{1-R(x)} &= \frac{1}{k!} \cdot [x^n] \frac{d^k}{dt^k} \frac{G(x)^2}{1-R(x)} \\
&= [x^{n-k}] (1-R)^{-(k+1)} \cdot (G+1-R)^2 \\
&= \sum_{j=0}^{n-k} [x^j] (1-R)^{-(k+1)} \cdot [x^{n-k-j}] (G+1-R)^2. \quad (4.11.6)
\end{aligned}$$

To compute each of the terms in the above equation, we can write

$$\begin{aligned}
[x^j] (1-R)^{-(k+1)} &= [x^j] \left( \sum_{i=0}^{\infty} \binom{k+i}{k} R^i \right) \\
&= \sum_{i=0}^{\infty} \binom{k+i}{k} [x^j] R^i \\
&= \sum_{i=0}^j \binom{k+i}{i} [x^j] R^i \\
&\quad [\text{since } \deg_x(\mathbf{R}) \geq 1] \\
&= [x^j] \sum_{i=0}^j \binom{k+i}{i} R^i
\end{aligned}$$

Note that the first few terms look like the following:

$$\begin{aligned}
[x^0] (1-R)^{-(k+1)} &= 1 \\
[x^1] (1-R)^{-(k+1)} &= (k+1) \cdot a_0 \\
[x^2] (1-R)^{-(k+1)} &= \binom{k+1}{1} \cdot r a_1 + \binom{k+2}{2} \cdot a_0^2 \\
[x^3] (1-R)^{-(k+1)} &= \binom{k+1}{1} \cdot r^2 a_2 + \binom{k+2}{2} \cdot r \cdot 2a_0 a_1 + \binom{k+3}{3} \cdot a_0^3 \\
[x^4] (1-R)^{-(k+1)} &= \binom{k+1}{1} \cdot r^3 a_3 + \binom{k+2}{2} \cdot r^2 \cdot (2a_0 a_2 + a_1^2) \\
&\quad + \binom{k+3}{3} \cdot r \cdot (3a_1 a_0^2) + \binom{k+4}{4} \cdot a_0^4
\end{aligned}$$

Similarly, for the second term in 4.11.6, the coefficients are much easier to compute.

$$\begin{aligned}
[x^0] (G + 1 - R)^2 &= 1 \\
[x^{n-k-j}] (G + 1 - R)^2 &= [x^{n-k-j}] \left( \frac{G'}{rx} + 1 \right)^2 \\
&\text{[from 4.11.4]} \\
&= r^{n-k-j-2} \left( 2 \cdot q_{n-k-j} \cdot r + \sum_{i=1}^{n-k-j-1} q_i q_{n-k-j-i} \right)
\end{aligned}$$

As a consequence, our final expression for equation 4.11.5 becomes the following

$$\begin{aligned}
0 &= \frac{1}{k!} \cdot \frac{d^k}{dt^k} [x^n] \frac{G(x)^2}{1 - R(x)} \Bigg|_{t=0} \\
&= \sum_{j=0}^{n-k} [x^j] (1 - R)^{-(k+1)} \cdot [x^{n-k-j}] (G + 1 - R)^2 \\
&= \sum_{j=0}^{n-k} r^{n-k-j-2} \left( 2 \cdot q_{n-k-j} \cdot r + \sum_{i_1=1}^{n-k-j-1} q_{i_1} q_{n-k-j-i_1} \right) \cdot [x^j] \sum_{i_2=0}^j \binom{k+i_2}{i_2} R^{i_2}
\end{aligned}$$

This gives us a closed form expression for the coefficients of the characteristic polynomial 4.11.3, and can be used to infer the values of the  $c_i$ 's of Chet Matrices in construction 4.10, but at present we do not know how to use these equations to show the nonnegativity of the variables using these equations. We now formally state some of our conjectures for which these equations might be useful.

#### 4.12 Conjectures for proving nonnegativity of Chet Matrices

We state the main conjecture of this thesis in this section, and a sequence of related conjectures, each interesting in their own right.

**Conjecture 4.12.1.** (*Chet Conjecture*) Let  $C_n$  denote the  $n \times n$  Chet matrix, and let  $C = \{n : C_n \text{ is entry-wise nonnegative}\}$ . Then the following is true:

$$|C| = \infty.$$

More strongly,

$$C = \mathbb{N}.$$

The stronger conjecture might be easier to prove or disprove.

**Numerical Simulation.** We analytically simulated the Chet matrices  $C_n$  with exact precision up till  $n = 21$  in Maple, and all the matrices are nonnegative, and we numerically simulated the matrices up till  $n = 500$  with 100 digits of precision in Matlab, and not only are the matrices nonnegative, but the entries  $c_i$  are substantially far from 0, and they decay gracefully as  $i$  increases. For  $n = 500$ , the first nonzero digit appears 6 places after the decimal in the smallest matrix entry. The code we used is given in Appendix A.2, and the outputs for  $n = 100$  and  $n = 500$  are given in appendices A.3 and A.4 respectively. The primary reason for giving these numbers is to illuminate that the numbers behave very smoothly, and there are no sudden jumps or discontinuities in the values of the  $c_i$  or  $b_i$  as  $i$  increases, strongly supporting the (human) intuition that the Chet Conjecture is true.

We state some ideas, progress, and other conjectures that will help prove the Chet Conjecture.

**Trace conjectures.** We formulate some interesting conjectures which if true, would be helpful (although not by direct implication but by general understanding) in establishing the nonnegativity of Chet Matrices  $C_n$ . The conjectures are as follows.

**Conjecture 4.12.2.** (*Trace Conjecture*) *Let  $A$  be a nonnegative matrix that is substochastic, that is,  $\sum_i A_{i,j} \leq 1$  and  $\sum_j A_{i,j} \leq 1$  for all  $j$  and  $i$ . Assume the following: Above the diagonal,  $A$  has nonzero entries only for entries that are at a distance of 1 from the diagonal, and below the diagonal,  $A$  has nonzero entries only for entries that are at a distance at most  $k$  from the diagonal, where the diagonal has distance zero from the diagonal. Assume  $\text{Tr}A^l \leq 1$  for  $l \leq k + 1$ , then  $\text{Tr}A^l \leq 1$  for all  $l$ .*

It is easy to see that the Trace Conjecture 4.12.2 holds for symmetric matrices provided  $k \geq 1$ , since for a symmetric matrix, all eigenvalues are real, and

$$\text{Tr}A^2 = \sum_i \lambda_i^2 \leq 1$$

implies that  $|\lambda_i| \leq 1$ , and for any  $l$ ,

$$\text{Tr}A^l = \sum_i \lambda_i^l \leq \sum_i |\lambda_i|^l \leq \sum_i |\lambda_i|^2 \leq 1.$$

Note that if conjecture is true, it would mean that it is always possible to fill in nonnegative values in the entries at distance  $k + 1$  from the diagonal and ensure that



$\text{Tr}A^{k+2} = 1$ , and inductively, fill the matrix with nonnegative entries. The Trace conjecture does not directly imply the Chet conjecture due to the presence of the first row and last column in Chet matrices which are required to ensure that the matrices  $C_n$  remain doubly stochastic, and thus the entries  $C_n[k+1, 1]$  and  $C_n[n, n - (k+1)]$  are always  $\geq 0$  for any fixed  $k$ , while they are zero in the trace conjecture. In spite of this, we feel that attempts to prove the Trace conjecture will be helpful in proving the Chet conjecture.

The Trace Conjecture 4.12.2 is interesting in its own right, and since we do not know its proof, the following conjecture should be relatively easier to prove.

**Conjecture 4.12.3.** (*Toeplitz Trace Conjecture*) *Let  $A$  be a nonnegative matrix that is substochastic, that is,  $\sum_i A_{i,j} \leq 1$  and  $\sum_j A_{i,j} \leq 1$  for all  $j$  and  $i$ . Assume the following: Above the diagonal,  $A$  has nonzero entries only for entries that are at a distance of 1 from the diagonal, and below the diagonal,  $A$  has nonzero entries only for entries that are at a distance at most  $k$  from the diagonal, with entry  $c_l$  at distance  $l$  below the diagonal, where the diagonal has distance zero from the diagonal. Assume  $\text{Tr}A^l \leq 1$  for  $1 \leq l \leq k+1$ , then  $\text{Tr}A^l \leq 1$  for all  $l$ .*

The infinite version of the Toeplitz Trace Conjecture is also interesting, which also remains open as of this writing.

**Conjecture 4.12.4.** (*Infinite Toeplitz Trace Conjecture*) *Consider the following Markov Chain on  $\mathbb{N}$ . From every vertex  $i$ , there is an edge of weight  $r$  to  $i-1$ , and edges of weight  $c_l$  to vertices  $i+l$  for  $0 \leq l \leq k$ , and assume that  $r + \sum_{i=0}^k c_i \leq 1$ . Let  $p_l$  be the probability of starting at  $i$  and returning to  $i$  in exactly  $l$  steps, and let  $p_l \leq \alpha/k$  for  $1 \leq l \leq k+1$  for some constant  $\alpha$ . Then  $p_l \leq \alpha/k$  for all  $l$ .*

It is also interesting to understand the behavior of eigenvalues of Hessenberg or Hessenberg-Toeplitz matrices, which would provide further insights into the Trace Conjectures 4.12.2, 4.12.3 and 4.12.4, and it leads to the following conjecture.

**Conjecture 4.12.5.** (*Eigenvalues of Toeplitz-Hessenberg Matrices*) *Let  $A$  be a nonnegative matrix that is substochastic, that is,  $\sum_i A_{i,j} \leq 1$  and  $\sum_j A_{i,j} \leq 1$  for all  $j$  and  $i$ . Assume the following: Above the diagonal,  $A$  has nonzero entries only for entries that are at a distance of 1 from the diagonal, and below the diagonal,  $A$  has nonzero entries only for entries that are at a distance at most  $k$  from the diagonal, where the diagonal has distance zero from the diagonal. Then the eigenvalues of  $A$  are contained in the convex hull of the  $k+1$  roots of unity in the complex plane.*

It is possible to construct many similar conjectures, and insights into any would possibly be helpful to prove our original Chet Conjecture [4.12.1](#).

*Chapter 5*

## CONNECTIONS AND EXTENSIONS

But as more arts were invented, and some were directed to the necessities of life, others to recreation, the inventors of the latter were naturally always regarded as wiser than the inventors of the former, because their branches of knowledge did not aim at utility. Hence when all such inventions were already established, the sciences which do not aim at giving pleasure or at the necessities of life were discovered, and first in the places where men first began to have leisure. This is why the mathematical arts were founded in Egypt; for there the priestly caste was allowed to be at leisure.

~ Aristotle, *Metaphysics*

In this chapter, we study some other combinatorial quantities and relate them to the edge expansion and spectral gap. Many of these connections are also not well-studied for nonreversible chains (with some exceptions, notably Mihail's result connecting the mixing time and edge expansion), and our aim will be to derive new results or provide elementary proofs of known results. Further, another aim of this section is to provide a cohesive treatment of some topics that have appeared in different places in different communities, and fill-in the missing lemmas. We start by studying the most well-studied (implying we will have little to contribute) combinatorial quantity, the Mixing time.

### 5.1 Mixing time – Definitions and preliminary lemmas

To motivate the definition of mixing time for general nonnegative matrices, we first consider the mixing time of doubly stochastic matrices. The mixing time of a doubly stochastic matrix  $A$  (i.e., of the underlying Markov chain) is the worst-case number of steps required for a random walk starting at any vertex to reach a distribution approximately uniform over the vertices. To avoid complications of periodic chains, we assume that  $A$  is  $\frac{1}{2}$ -lazy, meaning that for every  $i$ ,  $A_{i,i} \geq \frac{1}{2}$ . Given any doubly stochastic matrix  $A$ , it can be easily converted to the lazy random walk  $\frac{1}{2}I + \frac{1}{2}A$ . This is still doubly stochastic and in the conversion both  $\phi(A)$  and the spectral gap are halved. The mixing time will be finite provided only that the chain is connected. Consider the indicator vector  $\mathbf{1}_{\{i\}}$  for any vertex  $i$ . We want to find the smallest  $\tau$  such that  $A^\tau \mathbf{1}_{\{i\}} \approx \frac{1}{n} \mathbf{1}$  or  $A^\tau \mathbf{1}_{\{i\}} - \frac{1}{n} \mathbf{1} \approx 0$ , which can further be written as  $\left(A^\tau - \frac{1}{n} \mathbf{1} \cdot \mathbf{1}^T\right) \mathbf{1}_{\{i\}} \approx 0$ . Concretely, for any  $\epsilon$ , we want to find  $\tau = \tau_\epsilon(A)$  such that for any  $i$ ,

$$\left\| \left( A^\tau - \frac{1}{n} \mathbf{1} \cdot \mathbf{1}^T \right) \mathbf{1}_{\{i\}} \right\|_1 \leq \epsilon.$$

Given such a value of  $\tau$ , for any vector  $x$  such that  $\|x\|_1 = 1$ , we get

$$\begin{aligned} \left\| \left( A^\tau - \frac{1}{n} \mathbf{1} \cdot \mathbf{1}^T \right) x \right\|_1 &= \left\| \sum_i \left( A^\tau - \frac{1}{n} \mathbf{1} \cdot \mathbf{1}^T \right) x_i \mathbf{1}_{\{i\}} \right\|_1 \\ &\leq \sum_i |x_i| \left\| \left( A^\tau - \frac{1}{n} \mathbf{1} \cdot \mathbf{1}^T \right) \mathbf{1}_{\{i\}} \right\|_1 \\ &\leq \sum_i |x_i| \cdot \epsilon \\ &= \epsilon. \end{aligned}$$

Thus, the mixing time  $\tau_\epsilon(A)$  is the number  $\tau$  for which  $\|(A^\tau - J) \cdot x\|_1 \leq \epsilon$  for any  $x$  such that  $\|x\|_1 = 1$ .

We want to extend this definition to any nonnegative matrix  $R$  with PF eigenvalue 1 and corresponding positive left and right eigenvectors  $u$  and  $v$ . Fixing the largest eigenvalue to 1 was irrelevant while studying edge expansion and spectral gap since both the quantities are unchanged by scalar multiplications, but it will be relevant for studying mixing time to avoid the involvement of the largest eigenvalue in every equation. Note that if  $R$  is reducible, then the mixing time is infinite. Further, if  $R$  is periodic, then mixing time is again ill-defined. Thus, we again assume that  $R$  is irreducible and  $\frac{1}{2}$ -lazy, i.e.  $R_{i,i} \geq \frac{1}{2}$  for every  $i$ . Let  $x$  be any nonnegative vector for the sake of exposition, although our final definition will not require

nonnegativity and will hold for any  $x$ . We want to find  $\tau$  such that  $R^\tau x$  about the same as the component of  $x$  along the direction of  $v$ . Further, since we are right-multiplying and want convergence to the right eigenvector  $v$ , we will define the  $\ell_1$ -norm using the left eigenvector  $u$ . Thus, for the starting vector  $x$ , instead of requiring  $\|x\|_1 = 1$  as in the doubly stochastic case, we will require  $\|D_u x\|_1 = 1$ . Since  $x$  is nonnegative,  $\|D_u x\|_1 = \langle u, x \rangle = 1$ . Thus, we want to find  $\tau$  such that  $R^\tau x \approx v$ , or  $(R^\tau - v \cdot u^T) x \approx 0$ . Since we measured the norm of the starting vector  $x$  with respect to  $u$ , we will also measure the norm of the final vector  $(R^\tau - v \cdot u^T) x$  with respect to  $u$ . Thus we arrive at the following definition.

**Definition 5.1.1.** (Mixing time of general nonnegative matrices  $R$ ) Let  $R$  be a  $\frac{1}{2}$ -lazy, irreducible nonnegative matrix with PF eigenvalue 1 with  $u$  and  $v$  as the corresponding positive left and right eigenvectors, where  $u$  and  $v$  are normalized so that  $\langle u, v \rangle = \|D_u v\|_1 = 1$ . Then the mixing time  $\tau_\epsilon(R)$  is the smallest number  $\tau$  such that  $\|D_u (R^\tau - v \cdot u^T) x\|_1 \leq \epsilon$  for every vector  $x$  with  $\|D_u x\|_1 = 1$ .  $\diamond$

We remark that similar to the doubly stochastic case, using the triangle inequality, it is sufficient to find mixing time of standard basis vectors  $\mathbf{1}_{\{i\}}$ . We state it as an elementary lemma.

**Lemma 5.1.2.** Let  $R$  be as stated in Definition 5.1.1. Then the mixing time  $\tau_\epsilon(R)$  is the smallest number  $\tau$  such that  $\|D_u (R^\tau - v \cdot u^T) y\|_1 \leq \epsilon$  for every vector  $y = \frac{\mathbf{1}_{\{i\}}}{\|D_u \mathbf{1}_{\{i\}}\|_1}$  where  $\mathbf{1}_{\{i\}}$  represents the standard basis vectors.

*Proof.* Let  $y_i = \frac{\mathbf{1}_{\{i\}}}{\|D_u \mathbf{1}_{\{i\}}\|_1}$ , then  $y_i$  is nonnegative,  $\|D_u y_i\|_1 = \langle u, y_i \rangle = 1$ , then for any  $x$ , such that  $\|D_u x\|_1 = 1$ , we can write

$$x = \sum_i c_i \mathbf{1}_{\{i\}} = \sum_i c_i \|D_u \mathbf{1}_{\{i\}}\|_1 y_i$$

with

$$\|D_u x\|_1 = \left\| D_u \sum_i c_i \mathbf{1}_{\{i\}} \right\|_1 = \sum_i |c_i| \|D_u \mathbf{1}_{\{i\}}\|_1 = 1.$$

Thus, if for every  $i$ ,  $\|D_u (R^\tau - v \cdot u^T) y_i\|_1 \leq \epsilon$ , then

$$\begin{aligned} \left\| D_u (R^\tau - v \cdot u^T) x \right\|_1 &= \left\| D_u (R^\tau - v \cdot u^T) \sum_i c_i \|D_u \mathbf{1}_{\{i\}}\|_1 y_i \right\|_1 \\ &\leq \sum_i |c_i| \|D_u \mathbf{1}_{\{i\}}\|_1 \left\| D_u (R^\tau - v \cdot u^T) y_i \right\|_1 \\ &\leq \epsilon. \end{aligned}$$

Thus, it is sufficient to find mixing time for every nonnegative  $x$  with  $\|D_u x\|_1 = \langle u, x \rangle = 1$ , and it will hold for all  $x$ .

□

The next lemma is similar to 3.0.3, but connects the mixing times of  $R$  and  $A = D_u^{\frac{1}{2}} D_v^{-\frac{1}{2}} R D_u^{-\frac{1}{2}} D_v^{\frac{1}{2}}$  showing they are the same.

**Lemma 5.1.3.** *The mixing time of  $R$  and  $A = D_u^{\frac{1}{2}} D_v^{-\frac{1}{2}} R D_u^{-\frac{1}{2}} D_v^{\frac{1}{2}}$  are the same, where  $R$  is an irreducible  $\frac{1}{2}$ -lazy nonnegative matrix with largest eigenvalue 1 and corresponding positive eigenvectors  $u$  and  $v$  normalized so that  $\langle u, v \rangle = 1$ .*

*Proof.* We first show that the mixing time of  $R$  and  $A = D_u^{\frac{1}{2}} D_v^{-\frac{1}{2}} R D_u^{-\frac{1}{2}} D_v^{\frac{1}{2}}$  are the same. Note that if  $R$  is  $\frac{1}{2}$ -lazy, then  $A$  is also  $\frac{1}{2}$ -lazy, since if  $R = \frac{1}{2}I + \frac{1}{2}C$  where  $C$  is nonnegative, then

$$A = \frac{1}{2} D_u^{\frac{1}{2}} D_v^{-\frac{1}{2}} I D_u^{-\frac{1}{2}} D_v^{\frac{1}{2}} + D_u^{\frac{1}{2}} D_v^{-\frac{1}{2}} C D_u^{-\frac{1}{2}} D_v^{\frac{1}{2}} = \frac{1}{2} I + D_u^{\frac{1}{2}} D_v^{-\frac{1}{2}} C D_u^{-\frac{1}{2}} D_v^{\frac{1}{2}}.$$

Let  $w = D_u^{\frac{1}{2}} D_v^{\frac{1}{2}} \mathbf{1}$ , the left and right eigenvector of  $A$  for eigenvalue 1. We will show that for every  $x$  for which  $\|D_u x\|_1 = 1$ , there exists some  $y$  with  $\|D_w y\|_1 = 1$  such that

$$\|D_u(R^\tau - v \cdot u^T)x\|_1 = \|D_w(A^\tau - w \cdot w^T)y\|_1$$

which would imply that  $\tau_\epsilon(R) = \tau_\epsilon(A)$  by definition.

Let  $x$  be a vector with  $\|D_u x\|_1 = 1$  and let  $y = D_u^{\frac{1}{2}} D_v^{-\frac{1}{2}} x$ . Then since  $D_w = D_u^{\frac{1}{2}} D_v^{\frac{1}{2}}$ , we get  $\|D_w y\|_1 = \|D_u x\|_1 = 1$ . Let  $R = v \cdot u^T + B_R$  and  $A = w \cdot w^T + B_A$  where  $B_A = D_u^{\frac{1}{2}} D_v^{-\frac{1}{2}} B_R D_u^{-\frac{1}{2}} D_v^{\frac{1}{2}}$  and  $B_A^\tau = D_u^{\frac{1}{2}} D_v^{-\frac{1}{2}} B_R^\tau D_u^{-\frac{1}{2}} D_v^{\frac{1}{2}}$ . Then

$$\begin{aligned} D_u(R^\tau - v \cdot u^T)x &= D_u B_R^\tau x \\ &= D_u(D_u^{-\frac{1}{2}} D_v^{\frac{1}{2}} B_A^\tau D_u^{\frac{1}{2}} D_v^{-\frac{1}{2}})x \\ &= D_w B_A^\tau y \\ &= D_w(A^\tau - w \cdot w^T)y \end{aligned}$$

as required. □

We state a final simple lemma here, that shows the inequality between the eigenvalues of  $AA^T$  and  $\tilde{A}$  whenever  $A$  is lazy. This was shown by Fill [Fil91] (albeit for row-stochastic matrices), and can be obtained in multiple ways.

**Lemma 5.1.4.** (Fill [Fil91]) Let  $A$  be a  $\frac{1}{2}$ -lazy irreducible nonnegative matrix with largest eigenvalue 1 and the corresponding left and right eigenvector  $w$ . Then

$$\lambda_2(AA^T) \leq \lambda_2\left(\frac{A + A^T}{2}\right).$$

*Proof.* Since  $A$  is  $\frac{1}{2}$ -lazy, we have that  $2A - I$  is nonnegative, has PF eigenvalue 1, and has the same left and right eigenvector  $w$  for eigenvalue 1 implying that the PF eigenvalue is 1 by Perron-Frobenius (Theorem 2.0.1, part 2), and also that its largest singular value is 1 from Lemma 3.0.3. Further,  $\frac{1}{2}(A + A^T)$  also has the same properties. Thus, for any  $x$ ,

$$\begin{aligned} AA^T &= \frac{A + A^T}{2} + \frac{(2A - I)(2A^T - I)}{4} - \frac{I}{4} \\ \Rightarrow \langle x, AA^T x \rangle &\leq \langle x, \frac{A + A^T}{2} x \rangle + \|x\|_2 \frac{\|(2A - I)\|_2 \|(2A^T - I)\|_2}{4} \|x\|_2 - \frac{\|x\|_2^2}{4} \\ &\leq \langle x, \frac{A + A^T}{2} x \rangle \\ \Rightarrow \max_{x \perp w} \langle x, AA^T x \rangle &\leq \max_{x \perp w} \langle x, \frac{A + A^T}{2} x \rangle. \end{aligned}$$

where the last implication followed by the variational characterization of eigenvalues since  $AA^T$  and  $\frac{1}{2}(A + A^T)$  are symmetric, and thus

$$\lambda_2(AA^T) \leq \lambda_2\left(\frac{A + A^T}{2}\right)$$

□

We start by giving general bounds for nonnegative matrices, and will infer bounds for the reversible case from those equations.

## 5.2 Mixing time and singular values

We first show a simple lemma relating the mixing time of nonnegative matrices to the second singular value. This lemma is powerful enough to recover the bounds obtained by Fill [Fil91] and Mihail [Mih89] in an elementary way, and also give all the bounds for the mixing time of reversible chains that depend on the second eigenvalue or the edge expansion. Since the largest singular value of any general nonnegative matrix  $R$  with PF eigenvalue 1 could be much larger than 1, the relation between mixing time and second singular value makes sense only for nonnegative matrices with the same left and right eigenvector for eigenvalue 1, which have largest singular value 1 by Lemma 3.0.3.

**Lemma 5.2.1.** (*Mixing time and second singular value*) Let  $A$  be a nonnegative matrix (not necessarily lazy) with PF eigenvalue 1, such that  $Aw = w$  and  $A^T w = w$  for some  $w$  with  $\langle w, w \rangle = 1$ , and let  $\kappa = \min_i w_i^2$ . Then for every  $c > 0$ ,

$$\tau_\epsilon(A) \leq \frac{\ln\left(\sqrt{\frac{n}{\kappa}} \cdot \frac{1}{\epsilon}\right)}{\ln\left(\frac{1}{\sigma_2(A)}\right)} \leq \frac{c \cdot \ln\left(\frac{n}{\kappa \cdot \epsilon}\right)}{1 - \sigma_2^c(A)}.$$

*Proof.* Writing  $\tau$  as shorthand for  $\tau_\epsilon(A)$  and since  $A = w \cdot w^T + B$  with  $Bw = 0$  and  $B^T w = 0$ , we have that  $A^\tau = w \cdot w^T + B^\tau$ . Let  $x$  be a nonnegative vector such that  $\langle w, x \rangle = \|D_w x\|_1 = 1$ . As discussed after Definition 5.1.1, this is sufficient for bounding mixing time for all  $x$ . Then we have

$$\|D_w(A^\tau - w \cdot w^T)x\|_1 = \|D_w B^\tau x\|_1 = \|D_w B^\tau D_w^{-1} y\|_1 \leq \|D_w\|_1 \|B^\tau\|_1 \|D_w^{-1}\|_1 \|y\|_1$$

where  $y = D_w x$  and  $\|y\|_1 = 1$ . Further, since  $\|w\|_2 = 1$  and  $\kappa = \min_i w_i^2$ , we have  $\|D_w\|_1 \leq 1$  and  $\|D_w^{-1}\|_1 \leq \frac{1}{\sqrt{\kappa}}$ , and using these bounds to continue the inequalities above, we get

$$\|D_w(A^\tau - w \cdot w^T)x\|_1 \leq \frac{1}{\sqrt{\kappa}} \|B^\tau\|_1 \leq \frac{\sqrt{n}}{\sqrt{\kappa}} \|B^\tau\|_2 \leq \frac{\sqrt{n}}{\sqrt{\kappa}} \|B\|_2^\tau \leq \frac{\sqrt{n}}{\sqrt{\kappa}} (\sigma_2(A))^\tau \leq \epsilon$$

where the second inequality is Cauchy-Schwarz, the fourth inequality used  $\|B\|_2 \leq \sigma_2(A)$  since  $A$  has identical left and right PF eigenvector, and the last inequality was

obtained by setting  $\tau = \tau_\epsilon(A) = \frac{\ln\left(\frac{\sqrt{n}}{\sqrt{\kappa} \cdot \epsilon}\right)}{\ln\left(\frac{1}{\sigma_2(A)}\right)}$ , and the subsequent inequality follows

from  $1 - x \leq e^{-x}$ . □

For the case of  $c = 2$ , Lemma 5.2.1 was obtained by Fill [Fil91] in a different manner, but we find our proof much simpler.

### 5.3 Mixing time and edge expansion

We now relate the mixing time of general nonnegative matrices  $R$  to its edge expansion  $\phi(R)$ . The upper bound for row stochastic matrices  $R$  in terms of  $\phi(R)$  were obtained by Mihail [Mih89] and simplified by Fill [Fil91] using Lemma 5.2.1 for  $c = 2$ . Thus, the following lemma is not new, but we prove it here since our proof again is elementary and holds for any nonnegative matrix  $R$ .



**Lemma 5.3.1.** (Mixing time and edge expansion) Let  $\tau_\epsilon(R)$  be the mixing time of a  $\frac{1}{2}$ -lazy nonnegative matrix  $R$  with PF eigenvalue 1 and corresponding positive left and right eigenvectors  $u$  and  $v$ , and let  $\kappa = \min_i u_i \cdot v_i$ . Then

$$\frac{\frac{1}{2} - \epsilon}{\phi(R)} \leq \tau_\epsilon(R) \leq \frac{4 \cdot \ln\left(\frac{n}{\kappa \cdot \epsilon}\right)}{\phi^2(R)}.$$

*Proof.* From Lemma 5.1.3, we have that the mixing times of  $R$  and  $A = D_u^{\frac{1}{2}} D_v^{-\frac{1}{2}} R D_u^{-\frac{1}{2}} D_v^{\frac{1}{2}}$  are the same. Further, from Lemma 3.0.3, we have that  $\phi(R) = \phi(A)$ . Thus, we show the bound for  $\tau_\epsilon(A)$  and  $\phi(A)$ , and the bound for  $R$  will follow.

We first lower bound  $\tau_\epsilon(A)$  using  $\phi$ , showing the lower bound on mixing time in terms of the edge expansion. We will show the bound for nonnegative vectors  $x$ , and by Definition 5.1.1 and the discussion after, it will hold for all  $x$ . By definition of mixing time, we have that for any nonnegative  $x$  such that  $\|D_w x\|_1 = \langle w, x \rangle = 1$ , since  $A^\tau = w \cdot w^T + B^\tau$ ,

$$\|D_w(A^\tau - w \cdot w^T)x\|_1 = \|D_w B^\tau x\|_1 \leq \epsilon$$

and letting  $y = D_w x$ , we get that for any nonnegative  $y$  with  $\|y\|_1 = 1$ , we have

$$\|D_w B^\tau D_w^{-1} y\|_1 \leq \epsilon.$$

Plugging the standard basis vectors for  $i$ , we get that for every  $i$ ,

$$\sum_j \left| \frac{1}{w(i)} \cdot B^\tau(j, i) \cdot w(j) \right| = \frac{1}{w(i)} \cdot \sum_j |B^\tau(j, i)| \cdot w(j) \leq \epsilon.$$

Thus, for any set  $S$ ,

$$\sum_{i \in S} w(i)^2 \cdot \frac{1}{w(i)} \cdot \sum_j |B^\tau(j, i)| \cdot w(j) = \sum_{i \in S} \sum_j w(i) \cdot |B^\tau(j, i)| \cdot w(j) \leq \sum_{i \in S} w(i)^2 \cdot \epsilon. \quad (5.3.2)$$

Moreover, for any set  $S$  for which  $\sum_{i \in S} w_i^2 \leq \frac{1}{2}$ ,

$$\begin{aligned}
\phi_S(A^\tau) &= \frac{\langle \mathbf{1}_S, D_w A^\tau D_w \mathbf{1}_{\bar{S}} \rangle}{\langle \mathbf{1}_S, D_w^2 \mathbf{1} \rangle} = \frac{\langle \mathbf{1}_{\bar{S}}, D_w A^\tau D_w \mathbf{1}_S \rangle}{\langle \mathbf{1}_S, D_w^2 \mathbf{1} \rangle} \\
&= \frac{\sum_{i \in S} \sum_{j \in \bar{S}} A^\tau(j, i) \cdot w(i) \cdot w(j)}{\sum_{i \in S} w_i^2} \\
&= \frac{\sum_{i \in S} \sum_{j \in \bar{S}} w(j) \cdot w(i) \cdot w(i) \cdot w(j) + \sum_{i \in S} \sum_{j \in \bar{S}} B^\tau(j, i) \cdot w(i) \cdot w(j)}{\sum_{i \in S} w_i^2} \\
&\geq \sum_{j \in \bar{S}} w_j^2 - \frac{\sum_{i \in S} \sum_{j \in \bar{S}} |B^\tau(j, i)| \cdot w(i) \cdot w(j)}{\sum_{i \in S} w_i^2} \\
&\geq \sum_{j \in \bar{S}} w_j^2 - \frac{\sum_{i \in S} \sum_j |B^\tau(j, i)| \cdot w(i) \cdot w(j)}{\sum_{i \in S} w_i^2} \\
&\geq \frac{1}{2} - \epsilon \\
&\quad [\text{since } \sum_{i \in S} w_i^2 \leq \frac{1}{2} \text{ and } \sum_i w_i^2 = 1, \text{ and the second term follows from equation 5.3.2}]
\end{aligned}$$

and thus

$$\phi(A^\tau) \geq \frac{1}{2} - \epsilon,$$

and using Lemma 3.7.6, we obtain

$$\phi(A^\tau) \leq \tau \cdot \phi(A),$$

or

$$\frac{\frac{1}{2} - \epsilon}{\phi(A)} \leq \tau_\epsilon(A).$$

We now upper bound  $\tau_\epsilon(A)$  in terms of  $\phi(A)$ . From Lemma 5.2.1 for  $c = 2$ , we have that

$$\tau_\epsilon(A) \leq \frac{2 \cdot \ln\left(\frac{n}{k \cdot \epsilon}\right)}{1 - \sigma_2^2(A)} = \frac{2 \cdot \ln\left(\frac{n}{k \cdot \epsilon}\right)}{1 - \lambda_2(AA^T)}. \quad (5.3.3)$$

and replacing Lemma 5.1.4 in equation 5.3.3, gives

$$\tau_\epsilon(A) \leq \frac{2 \cdot \ln\left(\frac{n}{k \cdot \epsilon}\right)}{1 - \sigma_2^2(A)} = \frac{2 \cdot \ln\left(\frac{n}{k \cdot \epsilon}\right)}{1 - \lambda_2(AA^T)} \leq \frac{2 \cdot \ln\left(\frac{n}{k \cdot \epsilon}\right)}{1 - \lambda_2\left(\frac{A+A^T}{2}\right)} \leq \frac{4 \cdot \ln\left(\frac{n}{k \cdot \epsilon}\right)}{\phi^2\left(\frac{A+A^T}{2}\right)} = \frac{4 \cdot \ln\left(\frac{n}{k \cdot \epsilon}\right)}{\phi^2(A)}$$

where the second last inequality follows from Cheeger's inequality 3.0.1 for the symmetric matrix  $(A + A^T)/2$ .  $\square$

#### 5.4 Mixing time and spectral gap of Reversible Matrices

We derive the bounds between the mixing time and spectral gap of reversible nonnegative matrices. These bounds are well-known, we state them here to contrast them with the bounds for general matrices. Further, they are simple to derive given Lemma 5.2.1.

**Lemma 5.4.1.** (*Mixing time and spectral gap of reversible matrices*) Let  $\tau_\epsilon(R)$  be the mixing time of a  $\frac{1}{2}$ -lazy nonnegative reversible matrix  $R$  with PF eigenvalue 1 and corresponding positive left and right eigenvectors  $u$  and  $v$ , normalized so that  $\langle u, v \rangle = 1$ , and let  $\kappa = \min_i u_i v_i$ . Then for  $\epsilon < 1$ ,

$$\frac{1 - \epsilon}{2 \cdot \Delta(R)} \leq \frac{\ln\left(\frac{1}{\epsilon}\right)}{\ln\left(\frac{1}{\lambda_2(R)}\right)} \leq \tau_\epsilon(R) \leq \frac{\ln\left(\frac{n}{\kappa \epsilon}\right)}{\Delta(R)}.$$

*Proof.* Since  $R$  is reversible, all eigenvalues are real, and since it is lazy,  $\lambda_i(R) \geq 0$  for all  $i$ , and thus  $\sigma_2(R) = \lambda_2(R)$ . The upper bound thus follows from Lemma 5.2.1. We show the lower bound for  $A = D_u^{\frac{1}{2}} D_v^{-\frac{1}{2}} R D_u^{-\frac{1}{2}} D_v^{\frac{1}{2}}$  and it follows for  $R$  from 5.1.3. Let  $x$  be the eigenvector for eigenvalue  $\lambda_2(A)$ , then  $\langle x, w \rangle = 0$ , and let  $x$  be normalized so that  $\|D_w x\|_1 = 1$  as required in Definition 5.1.1, where  $w = D_u^{\frac{1}{2}} D_v^{\frac{1}{2}} \mathbf{1}$ . Thus,

$$\begin{aligned} \|D_w(A^\tau - w \cdot w^T)x\|_1 &= \|D_w(A^\tau x - w \cdot w^T x)\|_1 \\ &= \|D_w(\lambda_2^\tau(A)x - w \cdot \mathbf{0})\|_1 \\ &= \lambda_2^\tau(A) \|D_w x\|_1 \\ &[\text{since } A \text{ is } \frac{1}{2}\text{-lazy and thus } \lambda_2(A) \geq 0] \\ &= \lambda_2^\tau(A) \\ &= (1 - \Delta(A))^\tau \end{aligned}$$

which is greater than  $\epsilon$  unless  $\tau \geq \frac{\ln\left(\frac{1}{\epsilon}\right)}{\ln\left(\frac{1}{1 - \Delta(A)}\right)}$ . If  $\Delta(A) \leq \frac{1}{2}$ , then

$$\begin{aligned} 1 - \Delta(A) &\geq \exp(-2\Delta(A)), \\ 2\Delta(A) &\geq \ln\left(\frac{1}{1 - \Delta(A)}\right) \end{aligned}$$

and since  $\ln(\frac{1}{\epsilon}) \geq 1 - \epsilon$ , this would give

$$\tau \geq \frac{1 - \epsilon}{2\Delta(A)}.$$

Now assume  $\Delta(A) > \frac{1}{2}$  or  $\lambda_2(A) < \frac{1}{2}$ , then we know that the maximum mixing time will be for  $\lambda_2(A) = \frac{1}{2}$ , and thus be at least

$$\frac{\ln(\frac{1}{\epsilon})}{\ln 2} \geq \frac{1 - \epsilon}{\ln(2)} \geq \frac{1 - \epsilon}{2} \geq 1$$

which is always true since the mixing time at least 1, and we again get that

$$\tau \geq \frac{1 - \epsilon}{2\Delta(A)}$$

as required.  $\square$

## 5.5 Mixing time and spectral gap of Nonreversible Matrices

We obtain bounds for the mixing time of nonnegative matrices in terms of the spectral gap, using methods similar to the ones used to obtain the upper bound on  $\phi$  in Theorem 1.4.1.

**Lemma 5.5.1.** (*Mixing time and spectral gap*) Let  $\tau_\epsilon(R)$  be the mixing time of a  $\frac{1}{2}$ -lazy nonnegative matrix  $R$  with PF eigenvalue 1 and corresponding positive left and right eigenvectors  $u$  and  $v$ , and let  $\kappa = \min_i u_i \cdot v_i$ . Then

$$(1 - \Delta) \frac{1 - \epsilon}{\Delta} \leq \tau_\epsilon(R) \leq 20 \cdot \frac{n + \ln\left(\frac{1}{\kappa \cdot \epsilon}\right)}{\Delta(R)}.$$

*Proof.* Since the mixing time (as shown in the proof of Lemma 5.1.3), eigenvalues, edge expansion, and value of  $\kappa$  for  $R$  and  $A = D_u^{\frac{1}{2}} D_v^{-\frac{1}{2}} R D_u^{-\frac{1}{2}} D_v^{\frac{1}{2}}$  are the same, we provide the bounds for  $A$  and the bounds for  $R$  follow.

To obtain the lower bound, let  $y$  be eigenvector for the second eigenvalue  $\lambda_2$  of  $A$  normalized so that  $\|D_w y\| = 1$ . Note that since  $w$  is both the left and right eigenvector for eigenvalue 1 of  $A$ , we have that  $\langle w, y \rangle = 0$ . To consider the mixing time of  $y$ , note that

$$\|D_w(A^\tau - w \cdot w^T)y\|_1 = \|D_w(A^\tau - w \cdot w^T)y\|_1 = \|D_w \lambda_2^\tau y\|_1 = |\lambda_2|^\tau$$

which is less than  $\epsilon$  for

$$\tau_\epsilon(A) \geq \frac{\ln(\frac{1}{\epsilon})}{\ln(\frac{1}{|\lambda_2|})} \geq \frac{1-\epsilon}{1-|\lambda_2|} |\lambda_2| \geq (1-\Delta) \frac{1-\epsilon}{\Delta}$$

where the last inequality follows since  $1-x \leq \ln(1/x) \leq 1/x - 1$  and  $\operatorname{Re}\lambda_2 \leq |\lambda_2|$ .

For the upper bound on  $\tau_\epsilon(A)$ , we also restrict to nonnegative vectors, the bound for general vectors follows by the triangle inequality as discussed in Lemma 5.1.2.

Similar to the proof of Lemma 5.2.1, we have for any nonnegative vector  $x$  with  $\langle w, x \rangle = 1$ , for  $A = w \cdot w^T + B$ ,

$$\|D_w(A^\tau - w \cdot w^T)x\|_1 \leq \sqrt{\frac{n}{k}} \cdot \|B^\tau\|_2$$

and having

$$\|B^\tau\|_2 \leq \frac{\epsilon\sqrt{k}}{\sqrt{n}}$$

is sufficient. Let  $T$  be the triangular matrix in the Schur form of  $B$ , from the proof of Lemma 3.7.10, we have that for

$$k \geq \frac{3.51n + 1.385 \ln\left(\frac{n}{\delta}\right)}{1 - |\lambda_m(A)|},$$

the norm

$$\|B^k\|_2 \leq \delta,$$

and thus setting  $\delta = \frac{\epsilon\sqrt{k}}{\sqrt{n}}$ , we get that

$$\tau_\epsilon(A) \leq \frac{3.51n + 1.385 \ln\left(n \cdot \frac{\sqrt{n}}{\sqrt{k} \cdot \epsilon}\right)}{1 - |\lambda_m(A)|}.$$

Further, since  $A$  is  $\frac{1}{2}$ -lazy,  $2A - I$  is also nonnegative, with the same positive left and right eigenvector  $w$  for PF eigenvalue 1, thus having largest singular value 1, and thus every eigenvalue of  $2A - I$  has magnitude at most 1. Similar to the proof of Lemma 3.7.14, if  $\lambda_r = a + i \cdot b$  is any eigenvalue of  $A$ , the corresponding eigenvalue in  $2A - I$  is  $2a - 1 + i \cdot 2b$ , whose magnitude is at most 1, giving  $(2a - 1)^2 + 4b^2 \leq 1$  or  $a^2 + b^2 \leq a$ . It further gives that

$$1 - |\lambda_r| = 1 - \sqrt{a^2 + b^2} \geq 1 - \sqrt{1 - (1 - a)} \geq 1 - e^{\frac{1}{2}(1-a)} \geq \frac{1}{4}(1 - a)$$

or

$$1 - |\lambda_m| \geq \frac{1}{4}(1 - \operatorname{Re}\lambda_m) \geq \frac{1}{4}(1 - \operatorname{Re}\lambda_2),$$

which gives

$$\begin{aligned}\tau_\epsilon(A) &\leq 4 \cdot \frac{3.51n + 1.385 \ln\left(n \cdot \frac{\sqrt{n}}{\sqrt{\kappa \cdot \epsilon}}\right)}{1 - \operatorname{Re}\lambda_2(A)} \\ &\leq 20 \cdot \frac{n + \ln\left(\frac{1}{\kappa \cdot \epsilon}\right)}{1 - \operatorname{Re}\lambda_2(A)}\end{aligned}$$

completing the proof.  $\square$

We remark that there is only *additive* and not multiplicative dependence on  $\ln\left(\frac{n}{\kappa \cdot \epsilon}\right)$ . Further, our constructions in Sections 4.8 and 4.10 also show that the upper bound on  $\tau$  using  $\operatorname{Re}\lambda_2$  in Lemma 5.5.1 is also (almost) tight. For the construction of  $A_n$  in Theorem 4.8.3, letting the columns of  $U_n$  be  $u_1, \dots, u_n$ , for  $x = u_2$ ,  $(A_n^k - J)u_2 = (1 - (2 + \sqrt{n})^{-1})^k u_3$ , and so for  $k = O(\sqrt{n})$ , the triangular block of  $A^{O(\sqrt{n})}$  has norm about  $1/e$ , which further becomes less than  $\epsilon$  after about  $\ln\left(\frac{n}{\epsilon}\right)$  powers. Thus for the matrices  $A_n$ ,  $\tau_\epsilon(A_n) \in O\left(\sqrt{n} \cdot \ln\left(\frac{n}{\epsilon}\right)\right)$ . This shows Lemma 5.5.1 is also (almost) tight since  $\lambda_2(A_n) = 0$ .

## 5.6 Mixing time of a nonnegative matrix and its additive symmetrization

We can also bound the mixing time of a nonnegative matrix  $A$  with the same left and right eigenvector  $w$  for PF eigenvalue 1, with the mixing time of its *additive symmetrization*  $M = \frac{1}{2}(A + A^T)$ . Since  $\phi(A) = \phi(M)$ , we can bound  $\tau_\epsilon(A)$  and  $\tau_\epsilon(M)$  using the two sided bounds between edge expansion and mixing time in Lemma 5.3.1. For the lower bound, we get  $\gamma_1 \cdot \sqrt{\tau_\epsilon(M)} \leq \tau_\epsilon(A)$ , and for the upper bound, we get

$$\tau_\epsilon(A) \leq \gamma_2 \cdot \tau_\epsilon^2(M),$$

where  $\gamma_1$  and  $\gamma_2$  are some functions polylogarithmic in  $n, \kappa, \frac{1}{\epsilon}$ . However, by bounding the appropriate operator, we can show a tighter upper bound on  $\tau_\epsilon(A)$ , with only a *linear* instead of quadratic dependence on  $\tau_\epsilon(M)$ .

**Lemma 5.6.1.** *Let  $A$  be a  $\frac{1}{2}$ -lazy nonnegative matrix with positive left and right eigenvector  $w$  for PF eigenvalue 1, let  $M = \frac{1}{2}(A + A^T)$ , and  $\kappa = \min_i w_i^2$ . Then*

$$\frac{1 - 2\epsilon}{4 \cdot \ln^{\frac{1}{2}}\left(\frac{n}{\kappa \cdot \epsilon}\right)} \cdot \tau_\epsilon^{\frac{1}{2}}(M) \leq \tau_\epsilon(A) \leq \frac{2 \cdot \ln\left(\frac{n}{\kappa \cdot \epsilon}\right)}{\ln\left(\frac{1}{\epsilon}\right)} \cdot \tau_\epsilon(M).$$

*Proof.* Since  $\phi(A) = \phi(M)$  and each have the same left and right eigenvector  $w$  for PF eigenvalue 1, the lower bound on  $\tau_\epsilon(A)$  in terms of  $\tau_\epsilon(M)$  follows immediately

from Lemma 5.3.1, since

$$\sqrt{\tau_\epsilon(M)} \leq \ln^{\frac{1}{2}}\left(\frac{n}{\kappa \cdot \epsilon}\right) \cdot \frac{1}{\phi(M)} = \ln^{\frac{1}{2}}\left(\frac{n}{\kappa \cdot \epsilon}\right) \cdot \frac{1}{\phi(A)} \leq \ln^{\frac{1}{2}}\left(\frac{n}{\kappa \cdot \epsilon}\right) \cdot \frac{2\tau_\epsilon(A)}{1 - 2\epsilon}.$$

For the upper bound, we first define a new quantity for *positive semidefinite* nonnegative matrices  $M$  with PF eigenvalue 1 and  $w$  as the corresponding left and right eigenvector. Let  $T_\epsilon(M)$  be defined as the smallest number  $k$  for which

$$\|M^k - w \cdot w^T\|_2 = \epsilon.$$

Since  $M$  is symmetric, we can write  $M = w \cdot w^T + UDU^*$  where the first column of the unitary  $U$  is  $w$ , and the diagonal matrix  $D$  contains all eigenvalues of  $M$  except the eigenvalue 1 which is replaced by 0. Further, since  $M$  is positive semidefinite,  $\lambda_2(M)$  is the second largest eigenvalue of  $M$ , then for every  $i > 2$ ,  $0 \leq \lambda_i(M) \leq \lambda_2(M)$ . Thus we have

$$\|M^k - w \cdot w^T\|_2 = \|UD^kU^*\|_2 = \|D^k\|_2 = \lambda_2^k(M)$$

and

$$T_\epsilon(M) = \frac{\ln\left(\frac{1}{\epsilon}\right)}{\ln\left(\frac{1}{\lambda_2(M)}\right)}.$$

Further, for the eigenvector  $y$  of  $M$  corresponding to  $\lambda_2$ , we have for  $k = T_\epsilon(M)$ ,

$$(M^k - w \cdot w^T)y = \lambda_2^k \cdot y = \epsilon \cdot y.$$

Setting  $x = \frac{y}{\|D_w y\|_1}$ , we have  $\|D_w x\|_1 = 1$ , and we get

$$\|D_w(M^k - w \cdot w^T)x\|_1 = \left\| D_w \frac{\epsilon \cdot y}{\|D_w y\|_1} \right\|_1 = \epsilon,$$

which implies that

$$\tau_\epsilon(M) \geq k = T_\epsilon(M), \tag{5.6.2}$$

since there is some vector  $x$  with  $\|D_w x\|_1 = 1$  that has  $\|D_w(M^k - w \cdot w^T)x\|_1 = \epsilon$  and for every  $t < k$ , it is also the case that  $\|D_w(M^t - w \cdot w^T)x\|_1 > \epsilon$ .

Now we observe that since  $A$  is  $\frac{1}{2}$ -lazy with PF eigenvalue 1, and the same left and right eigenvector  $w$  for eigenvalue 1, we have that  $M = \frac{1}{2}(A + A^T)$  is positive semidefinite. From Lemma 5.2.1, we have

$$\tau_\epsilon(A) \leq \frac{2 \cdot \ln\left(\frac{\sqrt{n}}{\sqrt{\kappa \cdot \epsilon}}\right)}{\ln\left(\frac{1}{\sigma_2^2(A)}\right)}$$

and since  $A$  is  $\frac{1}{2}$ -lazy, as shown in the proof of Lemma 5.3.1,

$$\sigma_2^2(A) = \lambda_2(AA^T) \leq \lambda_2(M),$$

giving

$$\tau_\epsilon(A) \leq \frac{2 \cdot \ln\left(\frac{\sqrt{n}}{\sqrt{\kappa \cdot \epsilon}}\right)}{\ln\left(\frac{1}{\lambda_2(M)}\right)} = \frac{2 \cdot \ln\left(\frac{\sqrt{n}}{\sqrt{\kappa \cdot \epsilon}}\right)}{\ln\left(\frac{1}{\epsilon}\right)} \cdot \frac{\ln\left(\frac{1}{\epsilon}\right)}{\ln\left(\frac{1}{\lambda_2(M)}\right)} = \frac{2 \cdot \ln\left(\frac{\sqrt{n}}{\sqrt{\kappa \cdot \epsilon}}\right)}{\ln\left(\frac{1}{\epsilon}\right)} \cdot T_\epsilon(M) \leq \frac{2 \cdot \ln\left(\frac{\sqrt{n}}{\sqrt{\kappa \cdot \epsilon}}\right)}{\ln\left(\frac{1}{\epsilon}\right)} \cdot \tau_\epsilon(M)$$

where the last inequality followed from equation 5.6.2.  $\square$

One example application of Lemma 5.6.1 is the following: given any undirected graph  $G$  such that each vertex has degree  $d$ , any manner of orienting the edges of  $G$  to obtain a graph in which every vertex has in-degree and out-degree  $d/2$  cannot increase the mixing time of a random walk (up to a factor of  $\ln\left(\frac{n}{\kappa \cdot \epsilon}\right)$ ).

### 5.7 Mixing time of the continuous operator

Let  $R$  be a nonnegative matrix with PF eigenvalue 1 and associated positive left and right eigenvectors  $u$  and  $v$ . The continuous time operator associated with  $R$  is defined as  $\exp(t \cdot (R - I))$ , where for any matrix  $M$ , we formally define  $\exp(M) = \sum_{i=0}^{\infty} \frac{1}{i!} M^i$ . The reason this operator is considered continuous, is that starting with any vector  $x_0$ , the vector  $x_t$  at time  $t \in \mathbb{R}_{\geq 0}$  is defined as  $x_t = \exp(t \cdot (R - I))x_0$ . Since

$$\exp(t \cdot (R - I)) = \exp(t \cdot R) \cdot \exp(-t \cdot I) = e^{-t} \sum_{i=0}^{\infty} \frac{1}{i!} t^i R^i$$

where we split the operator into two terms since  $R$  and  $I$  commute, it follows that  $\exp(t \cdot (R - I))$  is nonnegative, and if  $\lambda$  is any eigenvalue of  $R$  for eigenvector  $y$ , then  $e^{t(\lambda-1)}$  is an eigenvalue of  $\exp(t \cdot (R - I))$  for the same eigenvector  $y$ . Thus, it further follows that  $u$  and  $v$  are the left and right eigenvectors for  $\exp(t \cdot (R - I))$  with PF eigenvalue 1. The mixing time of  $\exp(t \cdot (R - I))$ , is the value of  $t$  for which

$$\left\| D_u \left( \exp(t \cdot (R - I)) - v \cdot u^T \right) v_0 \right\|_1 \leq \epsilon$$

for every  $v_0$  such that  $\|D_u v_0\|_1 = 1$ , and thus, it is exactly same as considering the mixing time of  $\exp(R - I)$  in the sense of Definition 5.1.1.

**Lemma 5.7.1.** *Let  $R$  be a nonnegative matrix (not necessarily lazy) with positive left and right eigenvectors  $u$  and  $v$  for PF eigenvalue 1, normalized so that  $\langle u, v \rangle = 1$  and let  $\kappa = \min_i u_i \cdot v_i$ . Then the mixing time of  $\exp(t \cdot (R - I))$ , or  $\tau_\epsilon(\exp(R - I))$  is bounded as*

$$\frac{\frac{1}{2} - \epsilon}{\phi(R)} \leq \tau_\epsilon(\exp(R - I)) \leq \frac{100 \cdot \ln\left(\frac{n}{\kappa \cdot \epsilon}\right)}{\phi^2(R)}.$$



*Proof.* We will first find the mixing time of the operator  $\exp\left(\frac{R-I}{2}\right)$ , and the mixing time of the operator  $\exp(R-I)$  will simply be twice this number. By the series expansion of the exp function, it follows that  $\exp\left(\frac{R-I}{2}\right)$  has PF eigenvalue 1, and  $u$  and  $v$  as the corresponding left and right eigenvectors. Further,

$$\exp\left(\frac{R-I}{2}\right) = e^{-\frac{1}{2}} \left( I + \sum_{i \geq 1} \frac{1}{i!} \frac{R^i}{2^i} \right)$$

which is  $\frac{1}{2}$ -lazy due to the first term since  $e^{-\frac{1}{2}} \geq \frac{1}{2}$  and all the other terms are nonnegative. Further, for any set  $S$  for which  $\sum_{i \in S} u_i v_i \leq \frac{1}{2}$ , let  $\delta = \frac{1}{2}$ , then

$$\begin{aligned} \phi_S \left( \exp\left(\frac{R-I}{2}\right) \right) &= e^{-\delta} \cdot \frac{\langle \mathbf{1}_S, D_u \exp\left(\frac{R}{2}\right) D_v \mathbf{1}_{\bar{S}} \rangle}{\langle \mathbf{1}_S, D_u D_v \mathbf{1} \rangle} \\ &= e^{-\delta} \cdot \sum_{i \geq 1} \frac{\delta^i}{i!} \cdot \frac{\langle \mathbf{1}_S, D_u R^i D_v \mathbf{1}_{\bar{S}} \rangle}{\langle \mathbf{1}_S, D_u D_v \mathbf{1} \rangle} \\ &\quad [\text{since } \langle \mathbf{1}_S, D_u I D_v \mathbf{1}_{\bar{S}} \rangle = 0] \\ &= e^{-\delta} \cdot \sum_{i \geq 1} \frac{\delta^i}{i!} \cdot \phi_S(R^i) \\ &\quad [\text{since } R^i \text{ also has } u \text{ and } v \text{ as the left and right eigenvectors for eigenvalue 1}] \\ &\leq e^{-\delta} \cdot \sum_{i \geq 1} \frac{\delta^i}{i!} \cdot i \cdot \phi_S(R) \\ &\quad [\text{using Lemma 3.7.6}] \\ &= e^{-\delta} \cdot \delta \cdot \phi_S(R) \sum_{i \geq 1} \frac{\delta^{i-1}}{(i-1)!} \\ &= e^{-\delta} \cdot \delta \cdot \phi_S(R) \cdot e^{\delta} \\ &= \delta \cdot \phi_S(R) \end{aligned}$$

and thus,

$$\phi \left( \exp\left(\frac{R-I}{2}\right) \right) \leq \frac{1}{2} \phi(R). \quad (5.7.2)$$

Moreover, considering the first term in the series expansion, we get

$$\phi_S \left( \exp\left(\frac{R-I}{2}\right) \right) = e^{-\delta} \sum_{i \geq 1} \frac{\delta^i}{i!} \cdot \phi_S(R^i) \geq e^{-\delta} \cdot \delta \cdot \phi_S(R)$$

or

$$\phi \left( \exp\left(\frac{R-I}{2}\right) \right) \geq \frac{3}{10} \cdot \phi(R). \quad (5.7.3)$$

Since  $\exp\left(\frac{R-I}{2}\right)$  has left and right eigenvectors  $u$  and  $v$ , and is  $\frac{1}{2}$ -lazy, we get from Lemma 5.3.1 and equations 5.7.2 and 5.7.3 that

$$\frac{1}{2} \cdot \frac{\frac{1}{2} - \epsilon}{\frac{1}{2}\phi(R)} \leq \tau_\epsilon(\exp(R - I)) \leq 2 \cdot \frac{4 \cdot \ln\left(\frac{n}{\kappa \cdot \epsilon}\right)}{\left(\frac{3}{10}\right)^2 \phi^2(R)} \leq \frac{100 \cdot \ln\left(\frac{n}{\kappa \cdot \epsilon}\right)}{\phi^2(R)}$$

giving the result.  $\square$

## 5.8 Comparisons with the canonical paths method

For the case of symmetric nonnegative matrices  $M$  with PF eigenvalue 1, as shown in Lemma 5.4.1, since  $\tau$  varies inversely with  $1 - \lambda_2$  (up to a loss of a factor of  $\ln\left(\frac{n}{\kappa \cdot \epsilon}\right)$ ), it follows that any lower bound on the spectral gap can be used to upper bound  $\tau_\epsilon(M)$ . Further, since  $1 - \lambda_2$  can be written as a minimization problem for symmetric matrices (see Section 2), any relaxation of the optimization problem can be used to obtain a lower bound on  $1 - \lambda_2$ , and inequalities obtained thus are referred to as *Poincare inequalities*. One such method is to use *canonical paths* [Sin92] in the underlying weighted graph, which helps to bound mixing time in certain cases in which computing  $\lambda_2$  or  $\phi$  is infeasible. However, since it is possible to define canonical paths in many different ways, it leads to multiple relaxations to bound  $1 - \lambda_2$ , each useful in a different context. We remark one particular definition and lemma here, since it is relevant to our construction in Theorem 4.8.3, after suitably modifying it for the doubly stochastic case.

**Lemma 5.8.1.** [Sin92] *Let  $M$  represent a symmetric doubly stochastic matrix. Let  $W$  be a set of paths in  $M$ , one between every pair of vertices. For any path  $\gamma_{u,v} \in S$  between vertices  $(u, v)$  where  $\gamma_{u,v}$  is simply a set of edges between  $u$  and  $v$ , let the number of edges or the (unweighted) length of the path be  $|\gamma_{u,v}|$ . Let*

$$\rho_W(M) = \max_{e=(x,y)} \frac{\sum_{(u,v):e \in \gamma_{u,v}} |\gamma_{u,v}|}{n \cdot M_{x,y}}.$$

Then for any  $W$ ,

$$1 - \lambda_2(M) \geq \frac{1}{\rho_W(M)}$$

and thus,

$$\tau_\epsilon(M) \leq \rho_W(M) \cdot \ln\left(\frac{n}{\epsilon}\right).$$

**Corollary 5.8.2.** *Combining Lemma 3.5.1 and Lemma 5.8.1, it follows that for any doubly stochastic matrix  $A$ , and any set  $W$  of paths in the underlying graph of  $AA^T$ ,*

$$\tau_\epsilon(A) \leq \frac{2 \cdot \ln\left(\frac{n}{\epsilon}\right)}{1 - \sigma_2^2(A)} = \frac{2 \cdot \ln\left(\frac{n}{\epsilon}\right)}{1 - \lambda_2(AA^T)} \leq 2 \cdot \rho_W(AA^T) \cdot \ln\left(\frac{n}{\epsilon}\right).$$

Consider the example  $A_n$  in Theorem 4.8.3. It is not difficult to see that

$$\tau_\epsilon(A_n) \in O\left(\sqrt{n} \cdot \ln\left(\frac{n}{\epsilon}\right)\right). \quad (5.8.3)$$

This follows since the factor of  $\sqrt{n}$  ensures that the only non zero entries in the triangular matrix  $T_n$  in the Schur form of  $A^{\lceil\sqrt{n}\rceil}$  are about  $e^{-1}$ , and the factor of  $\ln\left(\frac{n}{\epsilon}\right)$  further converts these entries to have magnitude at most  $\frac{\epsilon}{n}$  in  $A^\tau$ . Thus, the operator norm becomes about  $\frac{\epsilon}{n}$ , and the  $\ell_1$  norm gets upper bounded by  $\epsilon$ . However, from Theorem 4.8.3, since  $\phi(A_n) \geq \frac{1}{6\sqrt{n}}$ , it follows from Lemma 5.3.1 that  $\tau_\epsilon(A_n) \in O\left(n \cdot \ln\left(\frac{n}{\epsilon}\right)\right)$ , about a quadratic factor off from the actual upper bound in equation 5.8.3. Further, from Theorem 4.8.3, the second eigenvalue of  $A_n$  is 0, and even employing Lemma 5.5.1 leads to a quadratic factor loss from the actual bound. However, Lemma 5.2.1 and Corollary 5.8.2 do give correct bounds. Since  $\sigma_2(A_n) = 1 - \frac{1}{\sqrt{n+2}}$  from Theorem 4.8.3, it follows from Lemma 5.2.1 for  $c = 1$  that  $\tau_\epsilon(A_n) \in O\left(\sqrt{n} \cdot \ln\left(\frac{n}{\epsilon}\right)\right)$ , matching the bound in equation 5.8.3. Now to see the bound given by canonical paths and corollary 5.8.2, consider the matrix  $M = A_n A_n^T$ . Every entry of  $M$  turns out to be positive, and the set  $W$  is thus chosen so that the path between any pair of vertices is simply the edge between the vertices. Further for  $r_n, \alpha_n, \beta_n$  defined in the proof of Theorem 4.8.3,  $M = J + r_n^2 B$ , where

$$B_{1,1} = \frac{n-2}{n}, \quad B_{n,n} = (n-2) \cdot \beta_n^2, \quad B_{i,i} = \alpha_n^2 + (n-3) \cdot \beta_n^2, \quad B_{1,n} = B_{n,1} = \frac{n-2}{\sqrt{n}} \cdot \beta_n,$$

$$B_{n,j} = B_{j,n} = \alpha_n \cdot \beta_n + (n-3) \cdot \beta_n^2, \quad B_{1,j} = B_{j,1} = \frac{1}{\sqrt{n}} \cdot (\alpha_n + (n-3) \cdot \beta_n), \quad B_{i,j} = 2 \cdot \alpha_n \cdot \beta_n + (n-4) \cdot \beta_n^2,$$

and  $2 \leq i, j \leq n-1$ . It follows that any entry of the matrix  $M$  is at least  $c \cdot n^{-\frac{3}{2}}$  (for some constant  $c$ ), and from Corollary 5.8.2, we get that  $\tau_\epsilon(A_n) \in O\left(\sqrt{n} \cdot \ln\left(\frac{n}{\epsilon}\right)\right)$ , matching the bound in equation 5.8.3.

## 5.9 Schur Complements

This is the first time we talk about Laplacians in this thesis. The reason for avoiding it so far was that it did not seem necessary to obtain any of our required bounds for nonnegative matrices, although it is implicitly present in all of them. Our assumptions will essentially be the same that have been so far.

Let  $R$  be an irreducible nonnegative matrix. We require the notion of irreducibility since we will deal with inverses of submatrices of  $R$ , which will not exist without this property. Further,  $R$  has positive  $u$  and  $v$  as left and right eigenvectors for eigenvalue 1, normalized so that  $\sum_i u_i v_i = 1$ .

**Definition 5.9.1.** (Laplacian of a nonnegative matrix) Let  $R$  be an irreducible nonnegative matrix with PF eigenvalue 1. Define the Laplacian of  $R$  as  $L = I - R$ .  $\diamond$

**Remark 5.9.2.** There are many different definitions for laplacians of nonnegative matrices  $R$  in literature. For simplicity, assume we want to understand the Laplacian of irreducible nonnegative matrices  $A$  with largest eigenvalue 1 and left and right positive eigenvector  $w$ , then two of the most prominent definitions of the laplacian of  $A$  are  $I - \frac{1}{2}(A + A^T)$  and  $I - A$ . The first definition has been widely used to derive results about irreducible matrices mostly since symmetric matrices are easier to deal with and the results are cleaner. However, the first definition loses all information about the eigenvalues of  $A$ , and the primary definition for us is the second one. This definition is much more difficult to deal with due to a lack of the variational characterization of eigenvalues as in the symmetric case and requires entirely new ideas and tools. This definition has also been used in many other contexts such as statistical physics (see [Tol79])  $\diamond$

**Notation.** Let  $L_{S,T}$  denote the submatrix of  $L$  indexed by rows in  $S$  and columns in  $T$ , where we will let  $L_S = L_{S,S}$  for brevity. Similarly, for some vector  $x \in \mathbb{R}^n$ , we will denote that  $x_S$  as the vector in  $\mathbb{R}^{|S|}$  containing the entries corresponding to indices in  $S$ . We remark that we will always write  $x_{\{i\}}$  for singletons.

The first simple lemma is the following.

**Lemma 5.9.3.** *Given a laplacian  $L = I - R$  of irreducible nonnegative  $R$  with positive (left and right) eigenvectors  $u$  and  $v$  for largest eigenvalue 1,  $L_{U,U}$  is invertible except when  $U = [n]$ .*

*Proof.* Assume not, then there is an eigenvalue 0 for  $L_{U,U}$  corresponding to eigenvector  $x_U \neq 0$ , and extend it to vector  $x$  which has 0 values outside  $U$ , implying  $Lx = 0$  or  $Rx = x$  which is a contradiction to the Perron-Frobenius Theorem 2.0.1 since  $v$  is the unique positive vector for eigenvalue 1 of  $R$ , and  $x$  has zeros outside  $U$  is thus not positive.  $\square$

**Definition 5.9.4.** (Inverse of Laplacians) A basic problem of linear algebra, is to solve for  $x$  in the equation  $Lx = b$  given  $b$  (where  $L = I - R$  and  $R$  is irreducible nonnegative with largest eigenvalue 1). Since the kernel of  $L$  has dimension 1, it implies that for  $b \neq 0$ , there is a unique solution for  $x$  with  $\langle x, v \rangle = 0$  where  $x = L^+b$ .  $\diamond$

To understand the solution  $x = L^+b$  more clearly, for some fixed set  $U \subset [n]$ , let matrix  $R = \begin{bmatrix} A & B \\ C & D \end{bmatrix}$  giving  $L = \begin{bmatrix} I - A & -B \\ -C & I - D \end{bmatrix} = \begin{bmatrix} A' & B' \\ C' & D' \end{bmatrix}$  and assume that the vertices that  $A$  is on is the set  $U$ , and write  $x_U = y$ ,  $x_{\bar{U}} = z$  for brevity and similarly for  $b$ , then from  $Lx = b$ , we get

$$A'y + B'z = b_1 \quad (5.9.5)$$

and

$$C'y + D'z = b_2 \quad (5.9.6)$$

and if  $D'$  is invertible which is the case if  $L$  is a laplacian from Lemma 5.9.3, then

$$z = b_2 - D'^{-1}C'y \quad (5.9.7)$$

and

$$(A' - B'D'^{-1}C')y = b_1 - B'b_2. \quad (5.9.8)$$

This brings us to the definition of Schur Complements.

**Definition 5.9.9.** (Schur Complement) The Schur complement of a Laplacian  $L = I - R$  ( $R = \begin{bmatrix} A & B \\ C & D \end{bmatrix}$  is irreducible nonnegative with largest eigenvalue 1) with respect to some set  $U \subset [n]$ , written as  $L|_U$  is defined as

$$L|_U = A' - B'D'^{-1}C' = (I - A) - B(I - D)^{-1}C = L_U - L_{U,\bar{U}}L_{\bar{U}}^{-1}L_{\bar{U},U}.$$

We allow the operator  $|$  to operate on nonnegative matrices  $R$  too, and define it as

$$R|_U = I_U - (I - R)|_U = I_U - L|_U = A + B(I - D)^{-1}C.$$

◇

## 5.10 Properties of Schur Complements

We now list some properties of Schur complements, or specifically the  $|$  operator as defined 5.9.9.

1. **Well-defined.** Schur complement is well-defined. This follows from Lemma 5.9.3 since  $I - D$  is invertible.

2. **Transitivity.** Let  $U$  and  $V$  be two subsets of indices with  $U \subseteq V$ . Then

$$(L|_V)|_U = L|_U$$

This can be easily seen from the equations 5.9.5, 5.9.6, 5.9.7, 5.9.8, since solving a subset of equations cannot change the final solution. It can also be seen by direct calculation from the definition but it is long and not insightful.

3. **Commutativity with the inverse.**  $(L^{-1})|_U = (L|_U)^{-1}$ . Follows again from equations 5.9.5, 5.9.6, 5.9.3, 5.9.8 or by direct calculation from the definition.

4. **Commutativity with the transpose.**  $L^T|_U = (L|_U)^T$ , again follows immediately by transposing the definition.

5. **Closure for Laplacians.**  $L|_U$  is the Laplacian of an irreducible nonnegative matrix  $R|_U$  with left and right eigenvectors  $u_U$  and  $v_U$  with eigenvalue 1. To see this, first note that

$$R|_U = A + B(I - D)^{-1}C = A + B \sum_{i=0}^{\infty} D^i C$$

is nonnegative, where the series expansion is well defined since  $I - D$  is invertible (Lemma 5.9.3) and  $\|D\| < 1$  since  $R$  is irreducible, and each of  $A$ ,  $B$ ,  $C$ ,  $D$  are nonnegative since  $R$  was nonnegative. Further, note that

$$R|_U v_U = v_U, \quad R^T|_U u_U = u_U.$$

We show for  $R|_U$  and the other equation follows directly from (4) above. To see this equation, note that  $Lv = 0$ , which gives  $A'v_1 + B'v_2 = 0$  and  $C'v_1 + D'v_2 = 0$ , or  $v_2 = -D'^{-1}C'v_1$  (since  $D'$  is invertible) and substituting in the first equation gives  $L|_U v_U = 0$  which gives  $(I - R|_U)v_U = 0$  as required.

6. **Closure for PSD Laplacians.** If  $L$  is positive semidefinite, then so is  $L|_U$ . To see this, note that since  $L$  is psd,  $\langle x_1, A'x_1 \rangle + \langle x, B'y \rangle + \langle y, B^*x \rangle + \langle y, Dy \rangle \geq 0$  for all  $x, y$ , and now set  $y = -D^{-1}B^*x$ , then since  $L$  is hermitian, so is  $D$  and  $BD^{-1}B^*$  (in fact also psd, considering vectors only supported on  $D$  shows  $D$  is psd, and so is  $D^{-1}$ , and so is  $BD^{-1}B^*$ ), thus, the above change in

$y$  gives  $\langle x, Ax \rangle - \langle x, BD^{-1}B^*x \rangle \geq 0$ , showing that the schur complement is psd.

7. **Eigenvalue-Eigenvector pairs.** Let  $Rx = \lambda x$ , then  $(\lambda, x|_U)$  is an eigenpair for  $(A + B(\lambda I - D)^{-1}C)$ . This easily follows again by using equations 5.9.5, 5.9.6, 5.9.7, 5.9.8 and part (5) above.

8. **Combinatorial interpretation.** The Schur complement of the Laplacian  $L$  on some set of vertices  $U$ , is *exactly* the operation of replacing the weight of every edge  $(i, j)$  in  $R$  with the sum of the weights of all paths of all length that go from  $i$  to  $\bar{U}$  to  $j$ , i.e. all intermediate vertices in the path from  $i$  to  $j$  come from  $\bar{U}$  (including the empty set). This follows directly by looking at  $R|_U$  :

$$I - L|_U = R|_U = A + B(I - D)^{-1}C = A + B \sum_{i=0}^{\infty} D^i C.$$

This provides a robust understanding of Schur complement of the Laplacian as a combinatorially meaningful operation. Essentially, it is arrived at by removing vertices from the graph, and adding the “effect” those vertices had on the rest of the graph with regards to different paths.

Given these properties, we move forward to the main problem of this section, and we will explore some more properties of schur complements as we uncover more lemmas.

### 5.11 Capacity and the Dirichlet Lemmas

In this section, we begin exploring a different combinatorial notion of expansion that has been studied at different points of time in different communities under different names. Our first aim will be exposition of a unified framework will will comprehensively cover all concepts and definitions, hopefully from multiple perspectives. Our next aim will be to derive many lemmas for the nonreversible versions of these quantities, that to the best of our knowledge, are not known as we state them.

We start by a second problem, very similar to the basic problem 5.9.4, is called the Dirichlet problem and will be defined next. We will assume  $R$  to be an irreducible nonnegative matrix with positive  $u$  and  $v$  as left and right eigenvectors for eigenvalue 1, normalized so that  $\sum_i u_i v_i = 1$ . Further, since  $R$  is irreducible, we have from

Lemma 5.9.3 that  $L = I - R$  contains only the space spanned by  $v$  in its right kernel, and the space spanned by  $u$  in its left kernel.

Note that in problem 5.9.4, we dealt with the case in which we were given  $b$ , and we wanted to find  $x$  such that  $Lx = b$ . Our problem now is modified to the case in which we have a *subset* of values in  $b$  and  $x$ , and we want to find the remaining values. This is called the Dirichlet problem.

**Definition 5.11.1.** (Dirichlet Problem) Let  $U$  be a subset of the vertices, then the Dirichlet problem given the boundary  $U$ , a vector  $a \in R^{|U|}$  and  $b \in R^{|\bar{U}|}$  is to find a vector  $q \in R^n$  (called the Dirichlet vector) such that  $q_U = a$  and  $(LD_v q)_{\bar{U}} = b$ . Typically,  $b = 0$ .  $\diamond$

Note that we “normalize” our vector  $q$  by multiplying (or “re-weighing”) it with  $D_v$  before considering the effect of  $L$  on it. This is similar to what we did for the definition of edge expansion 2.0.4. The direct solution of the Dirichlet problem follows directly by using equations similar to 5.9.5, 5.9.6, 5.9.7, 5.9.8. This brings us to the most important definition of this section.

**Definition 5.11.2.** (Capacity) Consider the setting of the Dirichlet problem above with  $b = 0$ , i.e. let  $q$  be some vector with  $q_U = a$  and  $(LD_v q)_{\bar{U}} = 0$ . Then we define the capacity of the set  $U$  with values  $a$  on the boundary as

$$\text{cap}_{U,a}(R) = \langle D_u q, L_R D_v q \rangle.$$

We will write  $\text{cap}_{U,a}(R) = \text{cap}(R)$  when  $U$  and  $a$  are clear from context.  $\diamond$

The immediate consequence of the definition is the following, similar to Lemma 3.0.3 and 5.1.3.

**Lemma 5.11.3.** Let  $A = D^{1/2} R D^{-1/2}$  where  $D = D_u D_v^{-1}$ , then for any  $U$  and any  $a$ ,

$$\text{cap}_{U,a}(A) = \text{cap}_R(U, a)$$

*Proof.* The proof is immediate from the definition, noting that  $u, v, w$  are positive vectors.  $\square$

Given Lemma 5.11.3, we will exclusively deal with  $A = D_u^{1/2} D_v^{-1/2} R D_v^{1/2} D_u^{-1/2}$  onwards, since it makes calculations simpler and intelligible due to it having the same principal left and right eigenvector.



**Remark 5.11.4.** (Alternate definition of Capacity) Another way to define capacity is as follows. Consider the setting of the Dirichlet problem above with  $b = 0$ , i.e. let  $q$  be some vector with  $q_U = a$  and  $(LD_v q)_{\bar{U}} = 0$ . Then we have defined the capacity of the set  $U$  with values  $a$  on the boundary as

$$\text{cap}_{U,a}(R) = \langle D_u q, L_R D_v q \rangle.$$

We note two modifications that will not change the inherent meaning of capacity.

First, the definition can be equivalently written with treating  $y = D_v q$  as a vector, and imposing the condition that  $y_S = D_v^{-1} a$ , but since the string  $a$  was arbitrary, we can even write  $y_S = a$ , where the  $\text{cap}_{U,a}(R)$  in Definition 5.11.2 will be  $\text{cap}_{U,D_v^{-1}a}(R)$  in the new definition. Thus we have

$$\text{cap}_{U,a}(R) = \langle D_u D_v^{-1} y, L_R y \rangle.$$

Second, the diagonal matrix  $D_u D_v^{-1}$  only redefines the inner product, since we can write the capacity as

$$\text{cap}_{U,a}(R) = \langle D_u^{1/2} D_v^{-1/2} y, D_u^{1/2} D_v^{-1/2} L_R y \rangle$$

which is only a rescaling of capacity, and thus even the diagonal multiplication is unnecessary. As a consequence, we can also simply define capacity as

$$\text{cap}_{U,a}(R) = \langle q, L_R q \rangle$$

with  $q_U = a$  and  $(L_R q)_{\bar{U}} = 0$ . However, we prefer Definition 5.11.2 to the above one, since it will become equivalent to a new type of expansion that we will define later.  $\diamond$

Based on the remark above, we can indeed define the capacity of a nonnegative  $A$  with identical left and right eigenvector  $w$  as follows.

**Lemma 5.11.5.** (Capacity simpler definition) Let  $L = I - A$  where  $A$  is an irreducible nonnegative matrix with largest eigenvalue 1 with  $w$  as the corresponding left and right eigenvector. Let  $U \subset [n]$  and  $a \in \mathbb{R}^{|U|}$ , and let  $q$  be such that  $q_U = (D_w)_{Ua}$ , and  $(Lq)_{\bar{U}} = 0$ . Then

$$\text{cap}_{U,a}(A) = \text{cap}(A) = \langle q, Lq \rangle.$$

Alternately, let  $q$  be a vector such that  $q_U = a$  and  $(Lq)_{\bar{U}} = 0$ , then for  $\bar{a} = (D_w^{-1})_{Ua}$

$$\text{cap}_{U,\bar{a}}(A) = \text{cap}(A) = \langle q, Lq \rangle$$

*Proof.* The proofs are immediate from the definition.  $\square$

These are the two definitions we will use henceforth in this section.

**Lemma 5.11.6.** (*Equivalent definitions of capacity*) *All the following are equivalent definitions of capacity. Let  $r = L_A D_w q$  or  $r = L_R D_v q$  (as will be clear from context) be the vector with  $r_{\bar{U}} = 0$ , and  $q_U = a$ . Then,*

$$\begin{aligned} \text{cap}_{U,a}(R) &= \langle D_u q, L_R D_v q \rangle \\ &= \langle (D_u)_{Ua}, L_R|_U (D_v)_{Ua} \rangle \\ &= \langle D_u D_v^{-1} L_R^+ r, r \rangle \\ &= \langle r_U, (L_R^+)_U r_U \rangle \end{aligned}$$

and

$$\begin{aligned} \text{cap}_{U,a}(A) &= \langle D_w q, L_A D_w q \rangle \\ &= \langle D_w a, L_A|_U D_w a \rangle \\ &= \langle r, L_A^+ r \rangle \\ &= \langle r_U, (L_A^+)_U r_U \rangle. \end{aligned}$$

*Proof.* The first equality is the definition, the second equality is obtained by noting that  $(L_A q)_{\bar{U}} = 0$  and using equations similar to 5.9.5, 5.9.6, 5.9.7, 5.9.8, the third equality follows by writing  $q = D_v^{-1} L_R^+ r$  or  $q = D_w^{-1} L_A^+ r$  in the definition, and the last equality follows from property 3 of Schur complements by noting that  $r_{\bar{U}} = 0$ .  $\square$

We now reach the first important lemma, albeit for reversible  $R$  or symmetric  $A$  (see Lemma 3.0.3).

**Lemma 5.11.7.** (*Dirichlet Lemma for symmetric A*) *Let  $L = I - A$  be psd, and for some fixed  $a$ , let  $q$  be such that  $q_U = a$  and  $(Lq)_{\bar{U}} = 0$ . Let  $x$  be any vector such that  $x_U = a$ . Then for  $\bar{a} = (D_w^{-1})_U a$ ,*

$$\text{cap}_{U,\bar{a}}(A) = \langle q, Lq \rangle \leq \langle x, Lx \rangle.$$

*Proof.* Since  $L$  is psd, we immediately get by Cauchy-Schwarz  $\langle y, Lz \rangle^2 \leq \langle y, Ly \rangle \langle z, Lz \rangle$  since  $L$  is psd and its square root always exists and thus  $\langle y, Lz \rangle^2 = \langle L^{1/2} y, L^{1/2} z \rangle^2 \leq \langle L^{1/2} y, L^{1/2} y \rangle \langle L^{1/2} z, L^{1/2} z \rangle$ . Let  $y = D_w x$  and  $z = D_w q$ , then since  $(Lz)_{\bar{U}} = 0$ , we get that  $\langle y, Lz \rangle = \langle z, Lz \rangle$  since  $y$  and  $z$  are equal in the indices in that are in  $U$ . Combining the two gives the lemma,  $\langle z, Lz \rangle^2 = \langle y, Lz \rangle^2 \leq \langle y, Ly \rangle \langle z, Lz \rangle$ .  $\square$

This lemma is important, since it is a basic step in a large number of other lemmas. It shows that  $q$  is in fact the minimizer of  $\langle x, Lx \rangle$  for all  $x$  with  $x_U = a$ . This gives us our first lemma for the capacity of nonreversible matrices.

**Lemma 5.11.8.** (*Lower bound on the capacity of nonreversible matrices*) For any  $U$  and  $a$ ,

$$\text{cap}_{U,a}(\tilde{A}) \leq \text{cap}_{U,a}(A),$$

where  $\tilde{A} = \frac{1}{2}(A + A^T)$ .

*Proof.* Note that  $L$  and  $\tilde{L} = \frac{1}{2}(L + L^T)$  have the same left and right eigenvector  $w$  for PF eigenvalue 1. Let  $q$  be the Dirichlet vector for  $L$  and  $g$  for  $\tilde{L}$  where  $q_U = a$  and  $g_U = a$ . Since  $\langle x, Lx \rangle = \langle x, \tilde{L}x \rangle$  for any real  $x$ , setting  $x = q$  in Lemma 5.11.7 gives

$$\langle g, \tilde{L}g \rangle \leq \langle q, \tilde{L}q \rangle = \langle q, Lq \rangle$$

which gives

$$\text{cap}_{U,\bar{a}}(\tilde{A}) \leq \text{cap}_{U,\bar{a}}(A)$$

as required, which holds for all  $a$  since  $w$  is positive and any vector can be obtained as  $\bar{a}$ .  $\square$

In fact, at this point, we can say something much stronger than Lemma 5.11.8. Before we proceed further, we need to understand the idea of clumping of vertices. These are essentially linear-algebraic modifications to ensure that the solutions to equations remain valid. Special cases of this idea have been used at many places without sufficient justification, and we provide complete clarification for its versatile use.

**Vertex Clumping.** The main idea is as follows. Let  $Q \in \mathbb{C}^{n \times n}$  be any matrix, and assume  $Q = \begin{bmatrix} A & B \\ C & D \end{bmatrix}$  without loss of generality, where neither  $A$  nor  $D$  have size 0. Let the vertices on which  $A$  is supported be  $U = \{1, \dots, r\}$ . For some vector  $x \in \mathbb{C}^n$ , if  $x \in \text{Ker}(Q)$ , then  $\langle x, Qx \rangle = 0$ . Assume that  $x \notin \text{Ker}(Q)$ . The primary aim of vertex clumping is to write

$$\langle x, Qx \rangle = \frac{1}{\langle y, Ty \rangle}$$

for some  $y$  that is independent of  $x$  and  $Q$ , and  $T$  that can be expressed as a function of  $Q$  and  $x$ . Our main result here is the following lemma.

**Lemma 5.11.9.** (*Vertex Clumping*) Let  $Q = \begin{bmatrix} A & B \\ C & D \end{bmatrix} \in \mathbb{C}^{n \times n}$  with  $A$  supported on vertices  $U \subset [n]$ , a given string  $a \in \mathbb{C}^{|U|}$  such that  $a \neq w_U$  for any  $w \in \text{Ker}(Q)$ ,

and the Dirichlet vector  $x$  such that  $x_U = a$  and  $(Qx)_{\bar{U}} = 0$ , then let  $x_{\bar{U}} = z$  and let  $y \in \mathbb{C}^{n-r+1}$  and  $T \in \mathbb{C}^{(n-r+1) \times (n-r+1)}$ , with

$$y = \begin{bmatrix} 1 \\ z \end{bmatrix} \text{ and } T = \begin{bmatrix} a^* A a & a^* B \\ C a & D \end{bmatrix}.$$

Then

$$\langle x, Qx \rangle = \langle y, Ty \rangle = \frac{1}{\langle e_1, T^+ e_1 \rangle}$$

where  $e_1$  is the standard basis vector.

*Proof.* Note that

$$\begin{aligned} \langle x, Qx \rangle &= \begin{bmatrix} a^* & z^* \end{bmatrix} \begin{bmatrix} A & B \\ C & D \end{bmatrix} \begin{bmatrix} a \\ z \end{bmatrix} \\ &= a^* A a + a^* B z + z^* C a + z^* D z \\ &= \begin{bmatrix} 1 & z^* \end{bmatrix} \begin{bmatrix} a^* A a & a^* B \\ C a & D \end{bmatrix} \begin{bmatrix} 1 \\ z \end{bmatrix} \\ &= \langle y, Ty \rangle. \end{aligned}$$

Thus, if  $b = Qx$  and  $c = Ty$  or  $y = T^+ c$ , letting  $c_{\{1\}} = r \neq 0$  (since  $x$  is not in the kernel of  $Q$ ), and since  $c_{\{2, \dots, n-r+1\}} = 0$ , we get

$$\begin{aligned} \langle a, Ba \rangle + \langle a, Bz \rangle &= c_{\{1\}} = r \\ b_{\{r+1, \dots, n\}} &= c_{\{2, \dots, n-r+1\}} = 0 \\ \langle x, Qx \rangle &= \langle y, Ty \rangle = \langle Q^+ b, b \rangle = \langle T^+ c, c \rangle = r \end{aligned}$$

What is essentially done here, is to clump the vertices  $U$  in  $Q$  with respect to  $x$ , by taking a weighted sum of all the edges in the cluster corresponding to  $U$ . Since  $Qx|_{\bar{U}} = 0$ , then  $\langle x, Qx \rangle = \langle y, Ty \rangle = \langle y, c \rangle = r$ , and also  $c = r \cdot e_1$  (where  $e_1$  is the standard basis vector), which gives

$$\langle T^+ c, c \rangle = r^2 \langle T^+ e_1, e_1 \rangle$$

which gives

$$\langle T^+ e_1, e_1 \rangle = \frac{1}{r} = \frac{1}{\langle x, Qx \rangle}.$$

□

As a consequence of vertex clumping, we get the following crucial lemma. Previous lemmas of this form have existed in folklore, but they had the following constraints.

1. They were always for symmetric laplacians
2. They always had the string  $a$  being a bit-string corresponding to vertices with potential 0 and 1
3. There were two clusters of vertices corresponding to where the current was entering and leaving the graph, and instead of  $e_1$  in lemma 5.11.9, they had vectors of the form  $e_i - e_j$  corresponding to currents.

In comparison, Lemma 5.11.9 holds for any laplacian (not necessarily symmetric), requires only one cluster of vertices, and does away altogether with the electrical point of view.

**Lemma 5.11.10.** *Let  $A$  be any nonnegative matrix with largest eigenvalue 1 for left and right eigenvector  $w$ , let  $L = I - A$ , then for any set  $U \subset [n]$  and  $\bar{a} = (D_w^{-1})_U a$ , with*

$$L = \begin{bmatrix} A & B \\ C & D \end{bmatrix}, \text{ and } T = \begin{bmatrix} a^* A a & a^* B \\ C a & D \end{bmatrix},$$

we get

$$\text{cap}_{U, \bar{a}}(A) = \frac{1}{\langle e_1, T^+ e_1 \rangle}$$

where  $e_1$  is the standard basis vector.

*Proof.* The proof is immediate from the vertex clumping in Lemma 5.11.9.  $\square$

As a consequence of this, we can now present one of our main lemmas.

**Lemma 5.11.11.** *Let  $R \in \mathbb{C}^{n \times n}$  be any matrix such that  $\tilde{R} = \frac{1}{2}(R + R^*)$  is positive definite. Then the following hold:*

1.  $R$  is invertible
2.  $\frac{1}{2}(R^{-1} + (R^*)^{-1})$  is positive definite.

3.

$$\left( \frac{R + R^*}{2} \right)^{-1} \succcurlyeq \frac{R^{-1} + (R^*)^{-1}}{2}$$

4.

$$\frac{R + R^*}{2} \succcurlyeq \frac{R^* R^{-1} R^* + R (R^*)^{-1} R}{2}$$

5. Let  $\tilde{R} = \frac{1}{2}(R + R^*)$  and  $\bar{R} = \frac{1}{2}(R - R^*)$ . Let  $W_\alpha = \tilde{R} + \alpha\bar{R}$  for  $-1 \leq \alpha \leq 1$ . Then for any  $\alpha, \beta$  such that  $|\alpha| \leq |\beta|$ ,

$$\frac{W_\alpha^{-1} + (W_\alpha^*)^{-1}}{2} \geq \frac{W_\beta^{-1} + (W_\beta^*)^{-1}}{2}.$$

*Proof.* For (1), let  $(\lambda, v)$  be some eigenvalue-eigenvector pair for  $R$  where  $v$  is nonzero, then

$$\operatorname{Re}\lambda = \operatorname{Re}\langle v, Rv \rangle = \frac{1}{2}(\langle v, Rv \rangle + \overline{\langle v, Rv \rangle}) = \frac{1}{2}(\langle v, Rv \rangle + \langle Rv, v \rangle) = \langle v, \frac{R + R^*}{2}v \rangle > 0$$

and thus  $R$  has no 0 eigenvalues and is invertible.

For (2), note that for any  $u \in \mathbb{C}^n$  such that  $u$  is nonzero,

$$\begin{aligned} \left\langle u, \frac{R^{-1} + (R^*)^{-1}}{2}u \right\rangle &= \left\langle u, R^{-1} \cdot \frac{R + R^*}{2} \cdot (R^*)^{-1}u \right\rangle \\ &= \left\langle (R^*)^{-1}u, \frac{R + R^*}{2} \cdot (R^*)^{-1}u \right\rangle \\ &= \left\langle v, \frac{R + R^*}{2} \cdot v \right\rangle \\ &> 0 \end{aligned}$$

where the last inequality follows since  $u \neq 0$ , and  $(R^*)^{-1}u$  is also nonzero since  $R^*$  (from (1)) and thus  $(R^*)^{-1}$  is invertible, and thus full rank, implying its kernel is trivial.

For (3), let  $L = \tilde{R} = \frac{1}{2}(R + R^*)$  and  $Q = \bar{R} = \frac{1}{2}(R - R^*)$  (we define these new symbols for ease of readability of the proof). Note that  $L = L^*$ , and since  $L$  is positive definite,  $L^{-1}$  exists and is well-defined. Further,  $Q$  is skew-hermitian, i.e.  $Q^* = -Q$ . We can also rewrite  $R = L + Q$  and  $R^* = L - Q$ . We then have that

$$\begin{aligned}
\left\langle u, \left( \frac{R + R^*}{2} \right)^{-1} u \right\rangle - \left\langle u, \frac{R^{-1} + (R^*)^{-1}}{2} u \right\rangle &= \langle u, L^{-1}u \rangle - \langle u, R^{-1} \cdot L \cdot (R^*)^{-1}u \rangle \\
&= \langle u, L^{-1}u \rangle - \langle (R^*)^{-1}u, L \cdot (R^*)^{-1}u \rangle \\
&= \langle R^*v, L^{-1}R^*v \rangle - \langle v, Lv \rangle \\
&\quad [\text{setting } u = R^*v] \\
&= \langle (L - Q)^*v, L^{-1}(L - Q)^*v \rangle - \langle v, Lv \rangle \\
&= \langle v, (L - Q)L^{-1}(L - Q)^*v \rangle - \langle v, Lv \rangle \\
&= \langle v, (L - Q)L^{-1}(L + Q)v \rangle - \langle v, Lv \rangle \\
&\quad [\text{since } (L - Q)^* = L^* - Q^* = L + Q] \\
&= \langle v, (L - Q + Q - QL^{-1}Q)v \rangle - \langle v, Lv \rangle \\
&= \langle v, -QL^{-1}Qv \rangle \\
&= \langle v, Q^*L^{-1}Qv \rangle \\
&\quad [\text{since } Q^* = -Q] \\
&= \langle Qv, L^{-1}Qv \rangle \\
&\geq 0 \\
&\quad [\text{since } L^{-1} \text{ is positive definite}]
\end{aligned}$$

For (4), starting with (3), we have

$$\begin{aligned}
& \frac{1}{2} \left( \left( \frac{R+R^*}{2} \right)^{-1} + \left( \frac{R+R^*}{2} \right)^{-1} \right) \geq \frac{R^{-1} + (R^*)^{-1}}{2} \\
\Leftrightarrow & \left( \frac{R+R^*}{2} \right)^{-1} L \left( \frac{R+R^*}{2} \right)^{-1} \geq R^{-1} L (R^*)^{-1} \\
\Leftrightarrow & L \geq L R^{-1} L (R^*)^{-1} L \\
\Leftrightarrow & L \geq \left( \frac{R+R^*}{2} \right) R^{-1} \left( \frac{R+R^*}{2} \right) (R^*)^{-1} \left( \frac{R+R^*}{2} \right) \\
\Leftrightarrow & L \geq \frac{1}{8} (I + R^* R^{-1}) (R+R^*) \left( (R^*)^{-1} R + I \right) \\
\Leftrightarrow & L \geq \frac{1}{8} (R+R^* + R^* + R^* R^{-1} R^*) \left( (R^*)^{-1} R + I \right) \\
\Leftrightarrow & L \geq \frac{1}{8} (R+R^* + R^* + R^* R^{-1} R^* + R(R^*)^{-1} R + R + R + R^*) \\
\Leftrightarrow & L \geq \frac{3}{4} L + \frac{1}{4} \cdot \frac{R^* R^{-1} R^* + R(R^*)^{-1} R}{2} \\
\Leftrightarrow & \frac{R+R^*}{2} \geq \frac{R^* R^{-1} R^* + R(R^*)^{-1} R}{2}
\end{aligned}$$

as required.

For (5), note that  $W_\alpha^* = W_{-\alpha}$ . In (3) above, we showed that

$$W_0^{-1} \geq \frac{W_1^{-1} + W_{-1}^{-1}}{2}.$$

We now want to extend this inequality. First note that for every  $\alpha$ ,  $\frac{1}{2}(W_\alpha + W_\alpha^*) = L$  and thus from (1),  $W_\alpha$  is invertible for every  $\alpha$ . To show the inequality, let  $K = W_\beta$ , then

$$W_\alpha = \frac{K + K^*}{2} + \frac{\alpha K - K^*}{\beta} = \frac{1}{2} \left( 1 + \frac{\alpha}{\beta} \right) K + \frac{1}{2} \left( 1 - \frac{\alpha}{\beta} \right) K^* = cK + (1-c)K^*$$

for

$$0 \leq c = \frac{1}{2} \left( 1 + \frac{\alpha}{\beta} \right) \leq 1.$$



Then we have that

$$\begin{aligned}
& \frac{W_\alpha^{-1} + (W_\alpha^*)^{-1}}{2} \succcurlyeq \frac{W_\beta^{-1} + (W_\beta^*)^{-1}}{2} \\
\Leftrightarrow & W_\alpha^{-1} \frac{W_\alpha + W_\alpha^*}{2} (W_\alpha^*)^{-1} \succcurlyeq K^{-1} \frac{K + K^*}{2} (K^*)^{-1} \\
\Leftrightarrow & L \succcurlyeq W_\alpha K^{-1} L (K^*)^{-1} W_\alpha^* \\
\Leftrightarrow & L \succcurlyeq (cK + (1-c)K^*) K^{-1} L (K^*)^{-1} (cK^* + (1-c)K) \\
\Leftrightarrow & L \succcurlyeq \left( cI + (1-c)K^* K^{-1} \right) L \left( cI + (1-c)(K^*)^{-1} K \right) \\
\Leftrightarrow & L \succcurlyeq \left( cI + (1-c)K^* K^{-1} \right) L \left( cI + (1-c)(K^*)^{-1} K \right) \\
\Leftrightarrow & L \succcurlyeq \left( c^2 L + (1-c)^2 K^* K^{-1} L (K^*)^{-1} K + c(1-c)L (K^*)^{-1} K + c(1-c)K^* K^{-1} L \right) \\
\Leftrightarrow & L \succcurlyeq \left( c^2 + (1-c)^2 \right) L + c(1-c) \left( L (K^*)^{-1} K + K^* K^{-1} L \right) \\
& \quad \text{[since } K^* K^{-1} L (K^*)^{-1} K = L \text{]} \\
\Leftrightarrow & L \succcurlyeq \left( c^2 + (1-c)^2 \right) L + c(1-c)L + c(1-c) \left( K (K^*)^{-1} K + K^* K^{-1} K^* \right) \\
& \quad \text{[on expanding } L = \frac{1}{2}(K + K^*) \text{]} \\
\Leftrightarrow & (c + (1-c))^2 L \succcurlyeq \left( c^2 + (1-c)^2 \right) L + c(1-c)L + c(1-c) \left( K (K^*)^{-1} K + K^* K^{-1} K^* \right) \\
\Leftrightarrow & L \succcurlyeq K (K^*)^{-1} K + K^* K^{-1} K^* \\
& \quad \text{[since } 0 \leq c \leq 1 \text{]} \\
\Leftrightarrow & \frac{K + K^*}{2} \succcurlyeq K (K^*)^{-1} K + K^* K^{-1} K^*
\end{aligned}$$

which is true by (4) since  $\frac{1}{2}(K + K^*) = L$  which is positive definite.  $\square$

As a consequence of these lemmas, we get the second primary contribution of this thesis.

**Theorem 5.11.12.** (*Monotonicity of Capacity*) *Let  $A$  be any nonnegative matrix with largest eigenvalue 1 for left and right eigenvector  $w$ , let  $L = I - A$ , and let  $L_\alpha = \tilde{L} + \alpha \bar{L}$  for some  $-1 \leq \alpha \leq 1$  where  $\tilde{L} = \frac{1}{2}(L + L^T)$  and  $\bar{L} = \frac{1}{2}(L - L^T)$ , and similarly define  $A_\alpha$ ,  $\tilde{A}$  and  $\bar{A}$ . Then for  $|\alpha| \leq |\beta|$ , we have*

$$\text{cap}_{U,a}(A_\alpha) \leq \text{cap}_{U,a}(A_\beta).$$

*Proof.* Let  $\alpha$  and  $\beta$  be as stated. Let

$$L = \begin{bmatrix} A & B \\ C & D \end{bmatrix}, \text{ and } H = \begin{bmatrix} a^* A a & a^* B \\ C a & D \end{bmatrix},$$

with  $\tilde{H} = \frac{1}{2}(H + H^T)$  and  $\bar{H} = \frac{1}{2}(H - H^T)$  defined similar to  $\tilde{L}$  and  $\bar{L}$ . Note

$$L_\alpha = \begin{bmatrix} \frac{1+\alpha}{2}A + \frac{1-\alpha}{2}A^T & \frac{1+\alpha}{2}B + \frac{1-\alpha}{2}C^T \\ \frac{1+\alpha}{2}C + \frac{1-\alpha}{2}B^T & \frac{1+\alpha}{2}D + \frac{1-\alpha}{2}D^T \end{bmatrix},$$

and let

$$\begin{aligned} H_\alpha &= \begin{bmatrix} a^*(\frac{1+\alpha}{2}A + \frac{1-\alpha}{2}A^T)a & a^*(\frac{1+\alpha}{2}B + \frac{1-\alpha}{2}C^T) \\ (\frac{1+\alpha}{2}C + \frac{1-\alpha}{2}B^T)a & \frac{1+\alpha}{2}D + \frac{1-\alpha}{2}D^T \end{bmatrix} \\ &= \frac{1+\alpha}{2} \begin{bmatrix} a^*Aa & a^*B \\ Ca & D \end{bmatrix} + \frac{1-\alpha}{2} \begin{bmatrix} a^*A^T a & a^*C^T \\ B^T a & D^T \end{bmatrix} \\ &= \tilde{H} + \alpha\bar{H}. \end{aligned}$$

Since  $a \neq w_U$  where  $w$  is the unique vector in the kernel of  $L_A$ , for any vector  $x$  that is not in the span of  $w$ ,  $H_\alpha$  is invertible for any  $\alpha$ . Thus, from part (5) of Lemma 5.11.11, we get that

$$\frac{H_\alpha^{-1} + (H_\alpha^*)^{-1}}{2} \geq \frac{H_\beta^{-1} + (H_\beta^*)^{-1}}{2},$$

and since  $H_\alpha$  is real, we have

$$\langle e_1, H_\alpha^{-1} e_1 \rangle = \langle e_1, (H_\alpha^*)^{-1} e_1 \rangle$$

and thus

$$\langle e_1, H_\alpha^{-1} e_1 \rangle \geq \langle e_1, H_\beta^{-1} e_1 \rangle$$

and since

$$\text{cap}_{U, \bar{a}}(A_\alpha) = \frac{1}{\langle e_1, H_\alpha^{-1} e_1 \rangle}$$

from Lemma 5.11.10 (note that we are operating in the space outside the kernel, so  $H_\alpha^{-1} = H_\alpha^+$ ), thus we get the theorem since the string  $\bar{a}$  is arbitrary since  $w$  is positive.  $\square$

This provides a sufficiently fine-tuned understanding of the capacity of non-symmetric nonnegative matrices, since it tells us that the capacity strictly increases as we move away from symmetry, and even for two non-symmetric matrices, the one farther from symmetry (in the sense of Theorem 5.11.12) strictly has higher capacity.

We would also like to remark that since Theorem 5.11.12 compares two inner products both for non-symmetric matrices, it is highly nontrivial, as all the tools for symmetric matrices are no longer usable.

Our next aim is to show a Dirichlet lemma similar to 5.11.7, but for non-symmetric nonnegative matrices. This is shown in part by Slowik [Slo12] relatively recently, however, the results there express the capacity as the infimums and supremums of different expressions, and the explicit solutions are not presented. We do that here, by showing the explicit expressions for the lemmas. <sup>1</sup>

**Lemma 5.11.13. (Dirichlet Lemma for non-symmetric matrices)** *Let  $L = I - A$  for some irreducible nonnegative  $A$  with largest eigenvalue 1 and the corresponding left and right eigenvector  $w$ . Let  $q$  be such that  $q_U = a \neq w_U$  and  $(Lq)_{\bar{U}} = 0$ . Let  $x$  be a vector such that  $x_U = a$ . Then*

$$\text{cap}_{U,\bar{a}}(A) = \langle q, Lq \rangle \leq \langle x, L\tilde{L}^+L^T x \rangle,$$

and the inequality is tight when  $U = \{s, t\}$  with  $a_s = 1$  and  $a_t = 0$ .

*Proof.* Note  $\langle x, Lq \rangle = \langle q, Lq \rangle$  since  $(Lq)_{\bar{U}} = 0$ , and  $\langle q, Lq \rangle = \langle q, \tilde{L}q \rangle$  since everything is real. By Cauchy-Schwarz inequality, for  $z = \tilde{L}^+L^T x$ , we have

$$\langle q, \tilde{L}z \rangle^2 \leq \langle q, \tilde{L}q \rangle \langle z, \tilde{L}z \rangle$$

or

$$\langle q, L^T x \rangle^2 \leq \langle q, \tilde{L}q \rangle \langle x, L\tilde{L}^+L^T x \rangle$$

which gives the lemma.

Let  $x = (L^T)^+ \tilde{L}q$ , then note that

$$\langle (L^T)^+ \tilde{L}q, L\tilde{L}^+L^T (L^T)^+ \tilde{L}q \rangle = \langle q, \tilde{L}L^+L\tilde{L}^+L^T (L^T)^+ \tilde{L}q \rangle = \langle q, \tilde{L}q \rangle = \langle q, Lq \rangle = \text{cap}_{U,\bar{a}}(A).$$

Note that the only difficulty is in verifying that  $x_U = a$ . To do this, we first assume that the set  $U = \{s, t\}$  and  $a_s = 1$  and  $a_t = 0$ . Then note that if  $q$  is the Dirichlet vector for this particular  $U$  and  $a$ , then since  $(Lq)_{\bar{U}} = 0$  and  $L^T w = 0$ , letting  $Lq = b$ , we have that  $w_s b_s + w_t b_t = 0$ . Similarly, letting  $p$  be the Dirichlet vector for  $L^T$  and since  $(L^T p)_{\bar{U}} = 0$  and  $Lw = 0$ , letting  $L^T p = c$ , we would similarly have  $w_s c_s + w_t c_t = 0$ . But since  $\langle q, Lq \rangle = \langle p, L^T p \rangle$  since the capacity for  $L$  and  $L^T$  are the same (use 5.11.6 or property (4)), we have that  $b_s = c_s$ , giving  $b_t = c_t$ , and thus

<sup>1</sup>There is a remark regarding explicit expressions in Slowik [Slo12] but it is incorrect.

$b = c$ . With this observation, note that our  $x$  becomes the following.

$$\begin{aligned}
 x &= (L^T)^+ \tilde{L}q \\
 &= (L^T)^+ \cdot \frac{1}{2}(L + L^T)q \\
 &= \frac{1}{2}q + \frac{1}{2}(L^T)^+Lq \\
 &= \frac{1}{2}q + \frac{1}{2}(L^T)^+b \\
 &= \frac{1}{2}q + \frac{1}{2}(L^T)^+c \\
 &= \frac{1}{2}q + \frac{1}{2}p
 \end{aligned}$$

and since  $p$  and  $q$  agree on  $U$ , so does  $x$ , and we get that the lemma is tight.  $\square$

We remark that Lemma 5.11.13 is a generalization of Lemma 5.11.7, and the latter follows as a corollary of the former if  $L$  was symmetric. A remarkable thing about Lemma 5.11.13 is that we can write the capacity of any matrix  $L$ , by using the matrix  $H = L\tilde{L}^+L^T$ . We believe this matrix is interesting enough to deserve study on its own right. We show one lemma to demonstrate its usefulness.

**Lemma 5.11.14.** *(Strengthening of Lemma 5.11.8) Let  $L = I - A$  for some irreducible nonnegative  $A$  with largest eigenvalue 1 and the corresponding left and right eigenvector  $w$ . Let  $U = \{s, t\}$  with  $a_s = 1$  and  $a_t = 0$ , and let  $q$  be such that  $q_U = a \neq w_U$  and  $(Lq)_{\bar{U}} = 0$ , and similarly let  $p$  be the Dirichlet vector for  $L^T$ . Let  $\bar{a} = (D_w^{-1})_U a$  and  $H = L\tilde{L}^+L^T$ . Then*

$$\langle p, Hp \rangle = \frac{(\text{cap}_{U, \bar{a}}(A))^2}{\text{cap}_{U, \bar{a}}(\tilde{A})}.$$

*Proof.* We first note the following. First, let  $\text{cap}_{U, \bar{a}}(A) = c$  and  $\text{cap}_{U, \bar{a}}(\tilde{A}) = \tilde{c}$ . Similar to the proof of tightness in Lemma 5.11.13, let  $p$  be the Dirichlet vector for  $L^T$ , then we know that  $Lq = L^T p = b$ , and we know that  $b_s = \text{cap}(A) = c$  and  $b_t = -c \cdot w_s/w_t$ . Thus, similar to the vertex clumping lemma, let  $\mu$  be the vector with  $\mu_s = 1$ ,  $\mu_t = -w_s/w_t$ , and  $\mu_i = 0$  otherwise. Then we have

$$\begin{aligned}
 c &= \langle q, Lq \rangle = \langle b, L^+b \rangle = c^2 \langle \mu, L^+\mu \rangle \\
 \frac{1}{c} &= \langle \mu, L^+\mu \rangle
 \end{aligned}$$

and similarly, we have

$$\langle \mu, \tilde{L}^+ \mu \rangle = \frac{1}{\tilde{c}}.$$

Now consider

$$\begin{aligned} \langle p, L\tilde{L}^+L^T p \rangle &= \langle b, \tilde{L}^+ b \rangle \\ &= c^2 \langle \mu, \tilde{L}^+ \mu \rangle \\ &= \frac{c^2}{\tilde{c}} \end{aligned}$$

as claimed.  $\square$

### 5.12 Normalized Capacity and Effective Conductance

We shall now consider the special case where  $U = S \cup T$  with disjoint  $S$  and  $T$ , and  $a_S = 1$  and  $a_T = 0$ . In this case, we refer  $\text{cap}_{U, \bar{a}}(A) = \text{cap}_{S, T}(A)$ , which we can call the *effective conductance* between the sets  $S$  and  $T$ , and  $1/\text{cap}(S, T)$  is generally referred to as the *effective resistance* between  $S$  and  $T$ . In fact, we can normalize the capacity, and we get the definition of normalized capacity.

**Definition 5.12.1. (Normalized capacity)** Let  $A$  be an irreducible nonnegative matrix with largest eigenvalue 1 and corresponding left and right eigenvector  $w$ , and  $L = I - A$  the corresponding Laplacian. The following quantity is referred to as the normalized capacity.

$$\sigma_A = \min_{\langle 1_S, D_w^2 1_S \rangle \leq \langle 1_T, D_w^2 1_T \rangle} \frac{\text{cap}_{S, T}(A)}{\langle 1_S, D_w^2 1_S \rangle}.$$

For exposition, note that for doubly stochastic  $A$ ,

$$\sigma_A = \min_{|S| \leq |T|} \frac{\text{cap}_{S, T}(A)}{|S|}$$

$\diamond$

Another completely different manner of understanding this definition is through the combinatorial lens discussed in property (8) of Schur complements. This will provide a beautiful perspective on understanding Normalized Capacity.

**Lemma 5.12.2.** *Let  $A$  be an irreducible nonnegative matrix with largest eigenvalue 1 and corresponding left and right eigenvector  $w$ , and  $L = I - A$  the corresponding Laplacian. Then*

$$\sigma_A = \min_{\langle 1_S, D_w^2 1_S \rangle \leq \langle 1_T, D_w^2 1_T \rangle} \frac{\text{cap}_{S, T}(A)}{\langle 1_S, D_w^2 1_S \rangle} = \min_U \phi(A|_U)$$

*Proof.* Note from Lemma 5.11.6,

$$\begin{aligned}
\text{cap}_{S,T}(A) &= \langle a, (D_w)_U L|_U (D_w)_U a \rangle \\
&= \langle 1_S, (D_w)_U (I - A|_U) (D_w)_U 1_S \rangle \\
&= \langle 1_S, (D_w^2)_U 1_S \rangle - \langle 1_S, (D_w)_U A|_U (D_w)_U 1_S \rangle \\
&= \langle 1, (D_w^2)_U 1_S \rangle - \langle 1_S, (D_w)_U A|_U (D_w)_U 1_S \rangle \\
&= \langle 1, (D_w)_U A|_U (D_w)_U 1_S \rangle - \langle 1_S, (D_w)_U A|_U (D_w)_U 1_S \rangle \\
&\quad [\text{since } A_u^T w_U = w_U \text{ from properties (5) and (7) of Schur Complements}] \\
&= \langle 1_{\bar{S}}, (D_w)_U A|_U (D_w)_U 1_S \rangle
\end{aligned}$$

and thus

$$\frac{\text{cap}_{S,T}(A)}{\langle 1_S, D_w^2 1_S \rangle} = \frac{\langle 1_{\bar{S}}, (D_w)_U A|_U (D_w)_U 1_S \rangle}{\langle 1_S, D_w^2 1_S \rangle} = \phi_S(A|_U)$$

and first minimizing over  $S$  and then  $U$  gives the result.  $\square$

The Lemma 5.12.2 now helps us obtain a combinatorial understanding of the notion of (normalized) capacity similar to property (8) of Schur complements, since it is *exactly* the edge expansion after some vertices of the graph are removed. We will first show a simple lemma and then give 2 different interpretations.

**Lemma 5.12.3.** (*Maximum principle*) Let  $L = I - A$  where  $A$  is an irreducible nonnegative matrix with largest eigenvalue 1 and corresponding left and right eigenvector  $w$ . Let  $a \in \{0, 1\}^{|U|}$  with  $U = S \cup T$  and  $a_S = 1$  and  $a_T = 0$ . Let  $q$  be a vector such that  $q_U = (D_w)_U a$  and  $(Lq)_{\bar{U}} = 0$ . Then for every entry of  $q$ ,

$$0 \leq q_i \leq w_i.$$

Further, for all  $i \in S$  and  $j \in T$ ,

$$(Lq)_i \geq 0, (Lq)_j \leq 0.$$

*Proof.* The statement is true for entries  $i \in S \cup T$ , we need to show it for entries  $i \in \bar{U}$ . Letting  $A = \begin{bmatrix} P & Q \\ R & W \end{bmatrix}$  be irreducible nonnegative, and let  $L = I - A$ , then from

$(Lq)_{\bar{U}} = 0$ , we have

$$\begin{aligned} -Rq_{\bar{U}} + (I - W)q_U &= 0 \\ q_{\bar{U}} &= (I - W)^{-1}Rq_U \\ &= \sum_{i \geq 0} W^i Rq_U \\ &= \sum_{i \geq 0} W^i R(D_w)_U a \end{aligned}$$

where  $I - S$  is invertible due to Lemma 5.9.3. Thus from the equation above, since  $W$ ,  $R$ ,  $w$  and  $a$  are all nonnegative, we get  $q_i \geq 0$  for all  $i \in \bar{U}$ . To note the upper bound, first note that the entries of  $q_{\bar{U}}$  cannot decrease with increasing the number of ones in  $a$ , again because all the matrices involved are nonnegative. Thus, the maximum entries in  $q_{\bar{U}}$  are achieved when  $a$  is the all ones vector. But in that case, note that  $q_U = w_U$ , and the vector  $q$  for which  $(Lq)_{\bar{U}} = 0$  is exactly  $w$ , which would imply  $q_{\bar{U}} = w_{\bar{U}}$ , thus showing that for any  $i \in \bar{U}$ ,  $q_i \leq w_i$ .

To see  $(Lq)_i \geq 0$  for  $i \in S$ , first let  $b = (Lq)_U$ , then

$$b = ((I - P) - Q(I - W)^{-1}R)(D_w)_U a.$$

However, from property (5) of Schur complements, we know that taking the Schur complement creates the Laplacian of another nonnegative matrix, specifically  $A' = P + Q(I - W)^{-1}R$  with  $w_U$  as the left and right PF eigenvector for eigenvalue 1, and thus we have

$$b = (I - A')(D_w)_U a.$$

Now we know that of  $a$  is the all ones vector,  $b = 0$ . Thus, assume  $a$  has ones in the first  $|S|$  entries, then for  $i \in S$ ,

$$b_i = (1 - A'_{i,i})w_i - \sum_{j \in S, j \neq i} A'_{i,j}w_j,$$

and since  $A'$  is nonnegative  $b_i = 0$  exactly when the entire row of  $A'_{i,j}$  is summed, we get that  $b_i \geq 0$ . Similarly, for  $i \in T$ , we can write

$$b_i = - \sum_{j \in T} A_{i,j}w_j \leq 0$$

as required. □

Similar to the combinatorial interpretation in Lemma 5.12.2 and property (8) of Schur complements, we can now give a similar explanation for  $\text{cap}(S, T)$ . However,

to truly understand capacity intuitively, we will write the interpretation for doubly stochastic matrices  $A$ , for which there is no rescaling by  $D_w$  since it has a uniform PF eigenvector and the diagonal matrix becomes identity. It is possible to write the interpretation for a completely general matrix, but it will be uninformative. For doubly stochastic matrices, the interpretation is immediately intuitive.

**Lemma 5.12.4.** (*Interpretation of capacity in terms of probabilities*) Let  $A$  be a doubly stochastic matrix with Laplacian  $I - A$ . Let  $S$  and  $T$  be two sets with  $U = S \cup T$ , and let  $q$  be the (Dirichlet) vector such that  $q_i = 1$ ,  $q_j = 0$  for  $i \in S$ ,  $j \in T$ , and  $(Lq)_{\overline{S \cup T}} = 0$ . Let  $\Pr_{S,T}(i)$  denote the probability that a random walk on  $A$  starting at  $i$  hits the set  $S$  before hitting the set  $T$ . Let  $v$  be a vector such that  $v_i = \Pr_{S,T}(i)$ . Then  $v = q$ .

*Proof.* The proof is immediate from the following. For  $i \in S$ ,  $v_i = 1$  and for  $j \in T$ ,  $v_j = 0$ , thus we need to compute  $v_i$  for  $i \in \overline{U}$ . Let  $A = \begin{bmatrix} P & Q \\ R & W \end{bmatrix}$  where we consider entries according to right multiplication by a vector, that is  $A_{j,i}$  represents the probability of going from vertex  $i$  to  $j$ . Then note that the probability of hitting the set  $S$  in exactly  $t$  steps before hitting the set  $T$  from vertex  $i \in U$  is exactly

$$(W^t R q_U)_i.$$

Thus the total probability of hitting the set  $S$  before  $T$  is

$$\sum_{t \geq 0} (W^t R q_U)_i$$

which is exactly  $q_{\overline{U}}$ . □

Before giving the second interpretation we note that we can again clump the vertices in  $S$  and  $T$  to single vertices  $s'$  and  $t'$  and adding all the corresponding edges similar to Lemma 5.11.9. Note however that Lemma 5.11.9 is cleaner and more general since it clumps everything into one super-vertex, and does not require values 1 and 0.

**Lemma 5.12.5.** Consider the setting of Lemma 5.11.9. Let  $L'$  be the matrix in which all the rows and columns corresponding to  $S$  have been summed to a single row/column, and similarly for  $T$ , creating new vertices  $s'$  and  $t'$  in the underlying graph (which is not doubly stochastic now). Then

$$\text{cap}_{S,T}(A) = \text{cap}_{s',t'}(A)$$



*Proof.* The rows can be summed up since it is just summing linear equations, and the columns can be summed up since  $v$  has the same value 1 at every vertex in  $S$ , and similarly has the same value 0 for every vertex in  $T$ . Since the linear equations do not change, the solution does not change.  $\square$

With this, we can now give an interpretation in terms of expectation, for the specific case where  $|S| = |T|$ .

**Lemma 5.12.6.** (*Interpretation of capacity in terms of expectations*) Let  $L = I - A$  with irreducible doubly stochastic  $A$  be such that  $|S| = |T| = 1$ , and we call the vertices  $s$  and  $t$ . Let  $q$  be the unique vector such that  $(Lq)_s = 1$ ,  $(Lq)_t = -1$  and  $Lq$  is zero everywhere else, and  $q_t = 0$ . Then

$$q_s = \frac{1}{\text{cap}_{s,t}(A)},$$

and

$$q_i = E_{s,t}(i),$$

where  $E_{s,t}(i)$  is the expected number of times vertex  $i$  is visited in a random walk starting from  $s$  before it hits  $t$ .

*Proof.* We provide a detailed proof for completeness. Let  $s$  and  $t$  be fixed. Let  $X_u$  be the number of times  $u$  is visited in a random walk that starts at  $s$  and stops on reaching  $t$ , and similarly  $Y_{i,j}$  for any edge  $i \rightarrow j$  be the number of times the edge is visited in a random walk that starts at  $s$  and ends at  $t$ . Then  $X_u = \sum_i Y_{i,u}$ . Now fix some vertex  $k$  and consider  $Y_{k,u}$ . Let the distribution of  $X_k$  be given by  $r_j$ , for any  $j \in \mathbb{N}$ . Thus  $\sum_j r_j = 1$ . Now fix some  $j$ , and let  $X_k$  be visited exactly  $j$  times. Let  $Z_1, \dots, Z_j$  be random variables, such that the  $Z_t = 1$  iff on the  $t$ 'th step, the walk went from vertex  $k$  to vertex  $u$ , and thus  $\mathbb{E}(Z_t) = p_{k,u}$ . Then given that  $X_k = j$ , we

have  $Y_{k,u} = \sum_{t=1}^{t-j} Z_t$ . Thus,  $\mathbb{E}(Y_{k,u}) = j \cdot p_{k,u}$ . Thus we can write

$$\begin{aligned} \mathbb{E}(Y_{k,u}) &= \sum_j \mathbb{E}(Y_{k,u} | X_k = j) \cdot \Pr[X_k = j] \\ &= \sum_{j=1}^{\infty} \mathbb{E} \left( \sum_{t=1}^j Z_t^{(j)} \right) \cdot r_j \\ &= \sum_{j=1}^{\infty} \sum_{t=1}^j \mathbb{E} Z_t^{(j)} \cdot r_j \\ &= \sum_{j=1}^{\infty} j \cdot p_{k,u} \cdot r_j \\ &= p_{k,u} \cdot \mathbb{E}(X_k) \end{aligned}$$

and thus

$$\begin{aligned} \mathbb{E}(X_u) &= \sum_i \mathbb{E}(Y_{i,u}) \\ &= \sum_i p_{i,u} \mathbb{E}(X_i) \end{aligned}$$

for every  $u$  except  $s$  and  $t$ . Since we never visit  $t$ , and always visit  $s$  at least once, we have

$$\begin{aligned} \mathbb{E}(X_t) &= 0 \\ \mathbb{E}(X_s) &= 1 + \sum_i \mathbb{E}(X_i) \cdot p_{i,s} \end{aligned}$$

Note that the equations for all vertices except  $t$  completely determine the equation for  $t$ , which turns out to be

$$\mathbb{E}(X_t) = -1 + \sum_i \mathbb{E}(X_i) \cdot p_{i,s}.$$

Note that these are exactly the equations  $(Lq)_s = 1$ ,  $(Lq)_t = -1$ ,  $(Lq)_i = 0$  for  $i \neq s, t$ , and  $q_t = 0$ . Since  $A$  is irreducible and the kernel has dimension 1, setting  $q_t = 0$ , we get a unique vector satisfying the equation. Thus,

$$q_u = \mathbb{E}(X_u)$$

as required. We now proceed to solve the equations. With  $L = I - A$ , with  $\chi_{s,t} = 1_s - 1_t$ , we get

$$Lq = \chi_{s,t},$$

with the solution

$$q = L^+ \chi_{s,t} + c \cdot \mathbf{1}$$

and with the constraint  $v_t = 0$ , it gives

$$q = L^+ \chi_{s,t} - \langle \mathbf{1}_t, L^+ \chi_{s,t} \rangle \cdot \mathbf{1}.$$

Note that

$$q_s = q_s - q_t = \langle \chi_{s,t}, q \rangle = \langle \chi_{s,t}, L^+ \chi_{s,t} \rangle = \frac{1}{\text{cap}_{s,t}(A)}.$$

where the last equality follows since taking the vector  $v = q/q_s$ , we have  $v_s = 1$ ,  $v_t = 0$ , and  $(Lv)_i = 0$  for  $i \neq s, t$ , and thus

$$\text{cap}_{s,t}(A) = \langle v, Lv \rangle = \frac{1}{q_s^2} \langle q, Lq \rangle = \frac{1}{q_s^2} \langle \chi_{s,t}, L\chi_{s,t} \rangle = \frac{1}{q_s^2} q_s = \frac{1}{q_s}.$$

□

In fact, for symmetric matrices  $A$ , the probability interpretation in Lemma 5.12.4 can be written in terms of voltages, and the expectation interpretation in Lemma 5.12.6 can be written in terms of currents, but we prefer the mathematical interpretations to avoid making assumptions about reality.

Our aim now is to further explore the notion of normalized capacity or  $\sigma_A$ . Towards this, note that we immediately get the following lemma as a corollary of Theorem 5.11.12.

**Lemma 5.12.7.** (*Monotonicity of Normalized Capacity*) *Let  $A$  be any nonnegative matrix with largest eigenvalue 1 for left and right eigenvector  $w$ , let  $L = I - A$ , and let  $A_\alpha = \tilde{A} + \alpha \bar{A}$  for some  $-1 \leq \alpha \leq 1$  where  $\tilde{A} = \frac{1}{2}(A + A^T)$  and  $\bar{A} = \frac{1}{2}(A - A^T)$ . Then for  $|\alpha| \leq |\beta|$ , we have*

$$\sigma_{A_\alpha} \leq \sigma_{A_\beta}.$$

*Proof.* Identical to the proof of Lemma 5.11.12. □

With this understanding of  $\sigma_A$ , an interesting question is to connect  $\sigma_A$  to the spectral gap of  $A$ . It turns out, that normalized capacity is equivalent to the spectral gap, up to constants, as shown by Schild [Sch18] and Miller et. al. [MWW18]. We present the proof for completeness mostly following [MWW18], with some changes to make it shorter and more streamlined, and then discuss possible versions for the non-symmetric case.

Before we proceed, we show a sequence of Lemmas.

**Lemma 5.12.8.**  $\forall x \in \mathbb{R}^n$ ,  $(x_i - x_j)^2 \leq \sum_{k=i}^{j-1} \frac{1}{p_k} (x_k - x_{k+1})^2$  for  $\sum p_k \leq 1$ .

*Proof.* Using the Cauchy-Schwarz inequality,

$$(x_i - x_j)^2 = \left( \sum_k \sqrt{p_k} \frac{(x_k - x_{k+1})}{\sqrt{p_k}} \right)^2 \leq \sum_{k=i}^{j-1} \frac{1}{p_k} (x_k - x_{k+1})^2.$$

□

**Lemma 5.12.9.** Let  $w_1, \dots, w_{n-1}$  be any nonnegative weights, and  $f_w(x) = \sum_{k=1}^{n-1} w_k (x_k - x_{k+1})^2$ . Then for any  $(i, j)$  with  $i < j$ , there exists an  $x$  with  $x_k = 1$  for  $k \leq i$ ,  $x_k = 0$  with  $k \geq j$ , and  $f_w(x) = \left( \sum_{k=i}^{j-1} \frac{1}{w_k} \right)^{-1}$ .

*Proof.* Let  $x$  be 1 on entries  $\leq i$  and 0 on entries  $\geq j$ , and for  $i \leq k \leq j$ , let

$$x_k = \frac{\sum_{r=k}^{j-1} \frac{1}{w_r}}{\sum_{r=i}^{j-1} \frac{1}{w_r}}. \text{ Then}$$

$$f_w(x) = \sum w_k (x_k - x_{k+1})^2 = \sum_{k=i}^{j-1} w_k (x_k - x_{k+1})^2 = \sum_{k=i}^{j-1} w_k \frac{\frac{1}{w_k^2}}{\left( \sum_{r=i}^{j-1} \frac{1}{w_r} \right)^2} = \left( \sum_{k=i}^{j-1} \frac{1}{w_k} \right)^{-1}$$

as required. □

We can now present the main lemma in [MWW18; Sch18]. We show it for doubly stochastic matrices for simplicity.

**Lemma 5.12.10.** (Normalized Capacity and Spectral Gap [MWW18; Sch18]) Let  $A$  be a symmetric irreducible doubly stochastic matrix with largest eigenvalue 1 and corresponding left and right eigenvector  $\mathbf{1}$ . Then the normalized capacity of  $A$  is equivalent to the spectral gap of  $A$ , up to constants. Quantitatively,

$$\frac{1}{2} \cdot \Delta(A) \leq \sigma_A \leq 4 \cdot \Delta(A).$$

*Proof.* We start by showing the lower bound, which is straightforward. It is sufficient to show that  $\lambda_2(L) \leq \lambda_2(L|_U)$  for any  $U$ , and the inequality will follow from the Cheeger-Buser inequality and the equivalence 5.12.2.

Let  $z = [x, y]^T$ , where  $(Lz)(j) = 0$  for  $j \in \overline{M}$ . Let  $x \perp 1$  be the vector such that  $\lambda_2(L|M) = \frac{\langle x, L|Mx \rangle}{\langle x, x \rangle}$ . Thus, there is a  $y$  such that for  $z = [x, y]^T$ ,  $\langle z, Lz \rangle = \langle x, L|Mx \rangle$  where  $Lz$  at any vertex in  $\overline{M}$  is 0. Let  $c_0 = \langle z, 1 \rangle / n$ , and  $z' = z - c_0 1$ , then  $z' \perp 1$  and  $\langle z, Lz \rangle = \langle z', Lz' \rangle$ , and

$$\begin{aligned} \langle z', z' \rangle &= \langle z, z \rangle - nc_0^2 \\ &= \langle x, x \rangle + \langle y, y \rangle - \frac{\langle y, 1 \rangle^2}{n} \\ &\quad [\text{since } x \perp 1] \\ &\geq \langle x, x \rangle \end{aligned}$$

since letting  $m = |\overline{M}| \leq n$ , and writing  $y = d_0 1 + \mu$  with  $\mu \perp 1$  and  $d_0 = \langle y, 1 \rangle / m$ , we get

$$\langle y, y \rangle - \frac{\langle y, 1 \rangle^2}{n} = md_0^2 + \langle \mu, \mu \rangle - m \cdot \frac{m}{n} d_0^2 \geq 0.$$

We now proceed to show the upper bound. Let  $x$  be a nonnegative vector such that  $x_i \geq x_{i+1}$  and let  $r \leq n/2$  be such that  $x_k = 0$  for  $k > r$ , which exists from Lemma 3.2.1.

Define weights  $w_1^{i,j}, \dots, w_r^{i,j}$ , with  $w_k^{i,j} = \frac{x_i - x_j}{x_k - x_{k+1}}$  where it is understood that  $w_k^{i,j}$  holds only for  $i \leq k < j$ , and  $\sum_{k=i}^{j-1} \frac{1}{w_k^{i,j}} = 1$ . Then note that  $(x_i - x_j)^2 = \sum_{k=i}^{j-1} w_k^{i,j} (x_k - x_{k+1})^2$ . Define  $w_k = \sum_{i,j} w_k^{i,j}$ . Then we get that  $\langle x, Lx \rangle = f_w(x)$  (defined in Lemma 5.12.9), and for all  $y$ , we get  $\langle y, Ly \rangle \leq f_w(y)$  by applying Lemma 5.12.8 to every edge.

Let  $R_i = \sum_{j=i}^r \frac{1}{w_j}$ , and let the vectors  $v_i$  be such that they have first  $i$  entries 1, last  $n/2$  entries 0, remaining entries such  $f_w(v_i) = R_i^{-1}$  (these exist by Lemma 5.12.9), then combining the definition of  $\sigma$  5.12.1, the Dirichlet Lemma 5.11.7, and the observation above, we get

$$\sigma \leq \frac{\langle v_i, Lv_i \rangle}{i} \leq \frac{f_w(v_i)}{i} \leq \frac{1}{i \cdot R_i}.$$

Note that  $\frac{1}{w_j} = R_j - R_{j+1}$ , and using  $\frac{a^2 - b^2}{a} \leq 2(a - b)$ ,

$$\begin{aligned}
\sum_i x_i^2 &= \sum_i \left( \sum_{j=i}^r x_j - x_{j+1} \right)^2 = \sum_i \left( \sum_{j=i}^r (x_j - x_{j+1}) w_j^{1/2} R_j^{1/4} \frac{1}{w_j^{1/2} R_j^{1/4}} \right)^2 \\
&\leq \sum_i \sum_{j=i}^r (x_j - x_{j+1})^2 w_j R_j^{1/2} \sum_{j=i}^r \frac{1}{w_j R_j^{1/2}} \\
&= \sum_i \sum_{j=i}^r (x_j - x_{j+1})^2 w_j R_j^{1/2} \sum_{j=i}^r \frac{R_j - R_{j+1}}{R_j^{1/2}} \\
&\leq 2 \sum_i \sum_{j=i}^r (x_j - x_{j+1})^2 w_j R_j^{1/2} R_i^{1/2} \\
&\leq \frac{2}{\sigma} \sum_{i=1}^r \sum_{j \geq i}^r (x_j - x_{j+1})^2 w_j \frac{1}{\sqrt{j}} \frac{1}{\sqrt{i}} \\
&= \frac{2}{\sigma} \sum_{j=1}^r (x_j - x_{j+1})^2 w_j \frac{1}{\sqrt{j}} \sum_{i=1}^j \frac{1}{\sqrt{i}} \\
&\leq \frac{4}{\sigma} \sum_{j=1}^r (x_j - x_{j+1})^2 w_j \\
&= \frac{4}{\sigma} f_w(x) \\
&= \frac{4}{\sigma} \langle x, Lx \rangle \\
\frac{\sigma}{4} &\leq \frac{\langle x, Lx \rangle}{\langle x, x \rangle}
\end{aligned}$$

as required.  $\square$

This raises the first interesting question. Since we know that  $\rho_{\tilde{L}} \leq \rho_L$  and  $\tau(\tilde{A}) \leq \tau(A)$ , does a relationship similar to Lemma 5.12.10 hold for nonreversible chains, i.e., is it possible that  $\sigma(A) \leq c \cdot \Delta(A)$  for some constant  $c$ ? This would be appealing as an equivalence, and also would imply better bounds for the mixing time since there is a linear dependence on  $\sigma$  instead of quadratic as was the case with  $\phi$  in Theorem 1.4.1. Unfortunately however, we show that this relation cannot hold.

**Lemma 5.12.11.** *It is not true that  $\sigma_A \in O(\Delta(A))$ . Specifically, let  $A$  be the directed cycle. Then*

$$\sigma_A \approx \sqrt{\Delta(A)}.$$

*Thus, the gap between  $\sigma_A$  and  $\sigma_{\tilde{A}}$  could be quadratic, since if  $A$  is the directed cycle, then  $\tilde{A}$  is the undirected cycle, and*

$$\sigma_{\tilde{A}} \leq \Delta(\tilde{A}) \leq \Delta(A).$$

*Proof.* Let  $A$  be the directed cycle. Then note that for any set  $S$  and  $T$  where  $|S| = |T| = n/4$ , and the vertices are on the opposite sides of the square, we get that the Dirichlet vector is 1 on half the vertices, and 0 on the other half, and  $A|_{S \cup T}$  is again a cycle, leaving the spectrum unchanged, except that the spectral gap now increases since the second eigenvalue will become the  $n/2$ 'th root of unity with real part closest to 1, instead of the  $n$ 'th root of unity with real part closest to 1. Thus  $\sigma(A) = \phi(A)$ , and the lemma follows.  $\square$

Thus, the gap between  $\sigma_A$  and  $\sigma_{\bar{A}}$  could be quadratic. In spite of this, it would be interesting to use the matrix  $H$  obtained in Lemma 5.11.13 to obtain a lemma similar to 5.12.10 for nonreversible chains.

### 5.13 Relation with log-Sobolev constants

We state the relation between log-Sobolev constant and the spectral gap, from [DS96], for the sake of comparison with other quantities. See [DS96] for related definitions. Let  $A$  be a symmetric matrix with largest eigenvalue 1 and corresponding left and right eigenvectors  $w$ . Let  $w$  be normalized so that  $\sum w_i^2 = 1$ , and let  $w_0 = \min_i w_i$ . Define the log-Sobolev constant for  $A$  as follows. Let  $\alpha$  be the log-Sobolev constant (for symmetric  $A$ ,  $\lambda = 1 - \lambda_2(A)$ ), then

$$\frac{\lambda}{1 + \frac{1}{2} \log(1/\pi_0)} \leq \alpha \leq \lambda$$

where the lower bound is achieved for the clique, and the upper bound for the hypercube. Thus,

$$\frac{c_1 \cdot \rho}{2 + \log(1/\pi_0)} \leq \alpha \leq c_2 \cdot \rho.$$

### 5.14 A different notion of expansion

So far, we have seen two primary definitions of expansion. The first definition was the standard Definition 2.0.4 expressed as the edge expansion  $\phi$ , and the second definition arose from normalized capacity 5.12.1 expressed as  $\sigma$ . In this subsection, we propose a new definition that will be expressed as  $\mu$ . We arrived at this definition by trying to understand the expansion of high dimensional expanders in [Baf+20]. As we have done throughout, to conceptually grasp the definition, we restrict to doubly stochastic matrices.

**Definition 5.14.1.** Let  $A$  be an irreducible doubly stochastic matrix. Let  $\mathbf{1}_S$  be the vector with ones on the set  $S$  and zeros elsewhere, and let  $\mathbf{1}'_S = \mathbf{1}_S/|S|$ . Define

$$\mu_S(A) = \frac{1}{2} \|A\mathbf{1}'_S - A\mathbf{1}'_{\bar{S}}\|_1$$

and let

$$\mu(A) = \max_{S: |S| \leq n/2} \mu_S(A).$$

◇

To understand the definition, observe that  $\mu$  should behave approximately like  $1 - \phi$ . Consider  $A = J = \frac{1}{n} \mathbf{1} \cdot \mathbf{1}^T$ . Then it is clear that  $\mu(J) = 0$ . Consider a graph  $A$  with two almost disconnected components corresponding to  $S$  and  $\bar{S}$ . Then  $\mu(A) \approx 1$ . However,  $\mu$  also has behavior different from  $1 - \phi$  in certain graphs. Consider a bipartite graph  $A$  with two components. Then for the set  $S$  supported on one component, we get  $\mu(A) = 1$ , and we also have that  $\phi(A) \approx \frac{1}{2}$ , showing that both  $\mu$  and  $\phi$  are constants.

**Lemma 5.14.2.** *Let  $A$  be an irreducible doubly stochastic matrix. Then*

$$\mu(A) \geq 1 - 2 \cdot \phi(A).$$

*Proof.* For any set  $|S| = k \leq n/2$ , let  $k' = n - k$ , and let  $v$  be the vector of sums of columns of  $A$  in  $\bar{S}$ . By the definition of  $\phi_S(A)$ , we have that

$$\phi_S(A) = \frac{1}{k} \sum_{i=1}^k v_i.$$

Further, since  $A$  is  $\frac{1}{2}$ -lazy, we have that  $v_i \leq 1/2$  for  $i \leq k$ . Thus we have



$$\begin{aligned}
\mu_S(A) &= \frac{1}{2} \|A1'_S - A1'_S\|_1 \\
&= \frac{1}{2} \sum_i \left| \frac{1-v_i}{k} - \frac{v_i}{k'} \right| \\
&= \frac{1}{2} \sum_i \left| \frac{1}{k} - \frac{n \cdot v_i}{k \cdot k'} \right| \\
&= \frac{1}{2} \frac{n}{k \cdot k'} \sum_i \left| \frac{k'}{n} - v_i \right| \\
&\geq \frac{1}{2} \frac{n}{k \cdot k'} \sum_{i=1}^k \left( \frac{k'}{n} - v_i \right) \\
&\quad \text{[since } A \text{ is } 1/2\text{-lazy]} \\
&= \frac{1}{2} \left( 1 - \frac{n}{k'} \phi_S(A) \right) \\
&\geq \frac{1}{2} - \phi_S(A)
\end{aligned}$$

as required. For general  $A$ , note that  $\sum_i v_i = k'$ , and thus,

$$\sum_{i>k} v_i = k' - k \cdot \phi_S(A).$$

Thus we get,

$$\begin{aligned}
\mu_S(A) &= \frac{1}{2} \|A1'_S - A1'_S\|_1 \\
&= \frac{1}{2} \frac{n}{k \cdot k'} \sum_i \left| \frac{k'}{n} - v_i \right| \\
&= \frac{1}{2} \frac{n}{k \cdot k'} \sum_i \left( \frac{k'}{n} - v_i \right) + 2 \cdot \frac{1}{2} \frac{n}{k \cdot k'} \sum_{i:v_i \geq k'/n} \left( v_i - \frac{k'}{n} \right) \\
&= 0 + \frac{n}{k \cdot k'} \sum_{i:v_i \geq k'/n} \left( v_i - \frac{k'}{n} \right) \\
&\geq \frac{n}{k \cdot k'} \sum_{i>k:v_i \geq k'/n} \left( v_i - \frac{k'}{n} \right)
\end{aligned}$$

To understand the minimum value that the sum can take, let there be  $r$  indices  $i > k$  such that  $v_i = k'/n$ , and the rest are greater than  $k'/n$ . Thus we have

$$\sum_{i>k+r} v_i = k' \left( 1 - \frac{r}{n} \right) - k \cdot \phi_S(A),$$

and continuing the summation above, we have

$$\begin{aligned}
\mu_S(A) &\geq \frac{n}{k \cdot k'} \sum_{i>k: v_i \geq k'/n} \left(v_i - \frac{k'}{n}\right) \\
&= \frac{n}{k \cdot k'} \sum_{i>k+r} \left(v_i - \frac{k'}{n}\right) \\
&= \frac{n}{k \cdot k'} \left(k' \left(1 - \frac{r}{n}\right) - k \cdot \phi_S(A) - \frac{k'}{n}(k' - r)\right) \\
&= \frac{n}{k \cdot k'} \left(k' \left(1 - \frac{k'}{n}\right) - k \cdot \phi_S(A)\right) \\
&= \frac{n}{k} \left(1 - \frac{k'}{n}\right) - \frac{n}{k'} \cdot \phi_S(A) \\
&= 1 - \frac{n}{k'} \cdot \phi_S(A) \\
&\geq 1 - 2 \cdot \phi_S(A)
\end{aligned}$$

as required. □

The second lemma we show is nicer, since it is similar to Lemma 3.7.1, except the binary function is minimum instead of addition. From Lemma 3.7.1, we have that for doubly stochastic  $A$  and  $B$ ,

$$\phi_S(AB) \leq \phi_S(A) + \phi_S(B).$$

The equivalent lemma for  $\mu$  is as follows.

**Lemma 5.14.3.** *Let  $\mu$  be as defined in 5.14.2, and let  $A$  and  $B$  be two doubly stochastic matrices. Then*

$$\mu_S(AB) \leq \min\{\mu_S(A), \mu_S(B)\}$$

and thus

$$\mu(AB) \leq \min\{\mu(A), \mu(B)\}.$$

*Proof.* Fix any set  $S$ . As the first step, note that

$$\mu_S(AB) = \frac{1}{2} \|AB1'_S - AB1'_{\bar{S}}\|_1 \leq \|A\|_1 \frac{1}{2} \|B1'_S - B1'_{\bar{S}}\|_1 \leq \mu_S(B).$$

Our aim is to now show that  $\mu_S(AB) \leq \mu_S(A)$ . Let the columns of  $B$  be  $B = (b_1, \dots, b_n)$ , let  $S$  contain the first  $k$  vertices with  $k' = n - k$ , let  $u = b_1 + \dots + b_k$ , then  $B1'_S = \frac{1}{k}u$ , and  $B1'_{\bar{S}} = \frac{1}{k'}(1 - u)$ , and

$$B1'_S - B1'_S = \frac{1}{k}u - \frac{1}{k'}(1-u) = \frac{n}{k \cdot k'}u - \frac{1}{k'}1 = \frac{n}{k'} \left( \frac{u}{k} - \frac{1}{n} \mathbf{1} \right)$$

where  $0 \leq u_i \leq 1$  and  $\sum_i u_i = k$  since  $B$  is doubly stochastic.

Let  $v$  be a vector with 1 in the first  $k$  entries and 0's otherwise, then  $u \leq v$  (or  $u$  is majorized by  $v$ ), and thus  $u = Rv$  where  $R$  is doubly stochastic. By the Birkhoff-von Neumann theorem (see 2),  $R$  can be written as  $R = \sum \alpha_i P_i$  with  $P_i$  being permutations, and  $\alpha_i \geq 0$ ,  $\sum \alpha_i = 1$ . Thus

$$u = \sum_i \alpha_i W_i$$

where  $W_i$  is a vector which has  $k$  entries that are 1 and 0's everywhere else. Now we know that for any set  $S$ ,

$$\begin{aligned} \mu_S(A) &\geq \frac{1}{2} \|A1'_S - A1'_S\|_1 \\ &= \frac{1}{2} \left\| \frac{1}{k}A1_S - \frac{1}{k'}A1_S \right\|_1 \\ &= \frac{1}{2} \left\| \frac{1}{k}A1_S - \frac{1}{k'}(1 - A1_S) \right\|_1 \\ &= \frac{1}{2} \frac{n}{k'} \left\| \frac{1}{k}A1_S - \frac{1}{n}1 \right\|_1 \end{aligned}$$

and particularly for all  $|S| = k$ . Thus for any set  $S$  with  $|S| = k$ , we have

$$\begin{aligned} \mu_S(AB) &= \frac{1}{2} \|AB1'_S - AB1'_S\|_1 \\ &= \frac{1}{2} \frac{n}{k'} \left\| \frac{1}{k}Au - \frac{1}{n}1 \right\|_1 \\ &= \frac{1}{2} \frac{n}{k'} \left\| \sum \alpha_i \left( \frac{1}{k}AW_i - \frac{1}{n}1 \right) \right\|_1 \\ &\leq \frac{1}{2} \frac{n}{k'} \sum \alpha_i \left\| \frac{1}{k}AW_i - \frac{1}{n}1 \right\|_1 \\ &\leq \mu_S(A) \end{aligned}$$

as required. □

## 5.15 Tensors and Beyond

Finally, we try to understand the expansion and mixing of systems that are no longer linear. Our operator will now be a  $k$ -tensor on  $n$  dimensions, written as  $T$ , such that  $T_{i_1, i_2, \dots, i_k}$  are some constant entries, and the dimension will be  $n$  in each index. We will throughout use the 3-tensor for exposition. There has been an upsurge of results

related to tensors due to its application in quantum information and machine learning, but relatively few and very specific results are known with regards to random walks and their convergence. Surprisingly, there are many versions of the Perron-Frobenius theorem which can be instantiated and interpreted in multiple ways for tensors (see [CPZ08; FGH13]). In fact, for the most natural definition of eigenvalue of a tensors (see [CQZ13]), it is possible for a  $k$ -tensor to have  $n(k-1)^{n-1}$  eigenvalues, which is exponential when  $k > 2$ . Our focus in this section will be on some very specific things that we think are very basic and important but unresolved.

The first question is to define a walk based on  $T$ . This is relatively simple, and there are two equivalent and mathematically pleasing ways to define the walk. Assume we have a distribution  $p \in \mathbb{R}^n$ , and for simplicity assume  $T$  is a nonnegative 3-tensor. Then we can define one step of the walk as follows:

$$p_t(i) = \sum_{j=1, k=1}^n T_{i,j,k} p_{t-1}(j) \cdot p_{t-1}(k).$$

Thus, our output distribution is quadratic in the input distribution. Note that we are using the first index as the output, although any index can be used, which is akin to taking the transpose as in the matrix case. Another way to define the walk is to consider the last two states, and evolve to the new state from the last two states. We can thus write

$$p_t(i) = \sum_{j=1, k=1}^n T_{i,j,k} p_{t-1}(j) \cdot p_{t-2}(k).$$

Both are interesting in their own right, and for the questions that we are interested in, it will not matter which definition is used. As the first step, to ensure that we are restricted to the simplex of probability distributions, we require that  $T$  is 1-line stochastic, i.e. for every fixed  $j, k$ ,

$$\sum_{i=1}^n T_{i,j,k} = 1.$$

As a consequence, note that if  $p_{t-1}$  and  $p_{t-2}$  are probability distributions, so is  $p_t$  since  $p_t(i) \geq 0$  since  $T$  is nonnegative, and

$$\sum_{i=1}^n p_t(i) = \sum_{j=1, k=1}^n p_{t-1}(j) \cdot p_{t-2}(k) \sum_{i=1}^n T_{i,j,k} = \sum_{j=1}^n p_{t-1}(j) \cdot \sum_{k=1}^n p_{t-2}(k) = 1.$$

Formally thus, we can define the tensor walk as follows.

**Definition 5.15.1.** Let  $T$  be a nonnegative  $k$ -tensor with dimension  $n$ . Let  $T$  be 1-line stochastic, i.e., for every fixed  $j_1, j_2, \dots, j_{k-1}$ ,

$$\sum_{i=1}^n T_{i,j_1,j_2,\dots,j_{k-1}} = 1.$$

Then  $p_t$  is a sequence of probability distributions due to the tensor walk defined as follows.

$$p_t(i) = \sum_{j_1,j_2,\dots,j_{k-1}=1}^n T_{i,j_1,j_2,\dots,j_{k-1}} p_{t-1}(j_1) p_{t-2}(j_2) \dots p_{t-k+1}(j_{k-1})$$

Succinctly, we write

$$p_t = T(p_{t-1}, p_{t-2}, \dots, p_{t-k}).$$

◇

We remark that it is possible to consider any number of inputs and outputs, where we have considered only 1 output and  $k - 1$  inputs in Definition 5.15.1. For evolution of probability distributions, this is indeed the most meaningful way. We then define the fixed point of the evolution  $T$  as a probability distribution that is preserved by  $T$ .

**Definition 5.15.2.** (Fixed point of tensor evolution) Let  $T$  be a  $k$ -tensor in  $n$  dimensions that is 1 line stochastic, with the evolution due to  $T$  defined as in 5.15.1. We say that a distribution  $p$  is a fixed point of  $T$ , if

$$p = T(p, p, \dots, p)$$

$$p(i) = \sum_{j_1,j_2,\dots,j_{k-1}=1}^n T_{i,j_1,j_2,\dots,j_{k-1}} p(j_1) p(j_2) \dots p(j_{k-1}).$$

◇

Given this definition, the first question is the following.

*If  $T$  is entry-wise positive, does  $T$  have a unique fixed point?*

Note that this is the first question to understand since positivity implied a unique fixed point in the case of matrices due to the Perron-Frobenius theorem. It intuitively does seem so, however, it turns out that  $T$  could have multiple fixed points. The following is an example constructed in [CZ13].

**Lemma 5.15.3.** [CZ13] Let  $T$  be a positive 4-tensor in 2 dimensions, defined as

$$T_{1,1,1,1} = 0.872, T_{1,1,1,2} = 2.416/3, T_{1,1,2,1} = 2.416/3, T_{1,1,2,2} = 0.616/3,$$

$$T_{1,2,1,1} = 2.416/3, T_{1,2,1,2} = 0.616/3, T_{1,2,2,1} = 0.616/3, T_{1,2,2,2} = 0.072,$$

$$T_{2,1,1,1} = 0.128, T_{2,1,1,2} = 0.584/3, T_{2,1,2,1} = 0.584/3, T_{2,1,2,2} = 2.384/3,$$

$$T_{2,2,1,1} = 0.584/3, T_{2,2,1,2} = 2.384/3, T_{2,2,2,1} = 2.384/3, T_{2,2,2,2} = 0.928,$$

Note that  $T$  is 1-line stochastic. Then the following are the 2 distinct positive fixed points of  $T$ :

$$p_1 = 0.2, p_2 = 0.8$$

and

$$q_1 = 0.6, q_2 = 0.4.$$

The proof can be checked by direct computation. In light of this, it would seem that even the most basic requirement is not satisfied by tensors. Almost every simple definition for matrices has multiple avenues for explication when considered for tensors. In fact, even the most intuitive way of defining the eigenvalues leads to  $2^n$  eigenvalues even for a 3-tensor. In spite of all this, we can actually show the existence of a unique fixed point in the case of 2-line stochastic tensors.

**Definition 5.15.4.** Let  $T$  be a nonnegative  $k$ -tensor in  $n$  dimensions. We say that  $T$  is 2-line stochastic, if apart from the output index, there is also an input index along which the tensor is stochastic. Formally, we say that  $T$  is 2-line stochastic, if there are some fixed input index  $j$  and the input index  $i$ , such that for every fixed  $l_1, \dots, l_{k-2}$ , we have that

$$\sum_{i=1}^n T_{i,j,l_1,\dots,l_{k-2}} = 1$$

and

$$\sum_{j=1}^n T_{i,j,l_1,\dots,l_{k-2}} = 1.$$

◇

Given a 2-line stochastic tensor, we can indeed show that the uniform distribution is a unique fixed point! This is our main theorem in this section.

**Theorem 5.15.5.** Let  $T$  be a positive 2-line stochastic tensor. Then for the tensor walk as defined in 5.15.1, the uniform distribution is the unique fixed point.

*Proof.* We first note two crucial things before delving into the proof.

1. The fact that  $T$  is line stochastic in the output index  $i$  will ensure that the walk remains within the probability simplex.
2. The fact that  $T$  is line stochastic in the input index  $j$  will ensure that there is a unique fixed point.

First we note that the uniform distribution is a fixed point for  $T$ , by noting that

$$\begin{aligned}
 p_t(i) &= \sum_{j, l_1, \dots, l_{k-2}=1}^n T_{i, j, l_1, \dots, l_{k-2}} \left(\frac{1}{n}\right)^{k-1} \\
 &= \left(\frac{1}{n}\right)^{k-1} \sum_{l_1, \dots, l_{k-2}=1}^n \sum_{j=1}^n T_{i, j, l_1, \dots, l_{k-2}} \\
 &= \left(\frac{1}{n}\right)^{k-1} n^{k-2} \\
 &= \frac{1}{n}.
 \end{aligned}$$

The next thing we show is that each  $p_t$  for  $t \geq k$  is a positive vector. To see this, let  $p_1$  to  $p_{k-1}$  be the  $k-1$  non-zero initial distributions provided to us. Note  $p_i$ 's for  $1 \leq i \leq k-1$  could have zero entries, but do not have all zero entries. Let  $x_1, \dots, x_{k-1} \in [n]$  be the indices corresponding to the non-zero entries in the  $p_i$ 's respectively. Thus we have

$$\begin{aligned}
 p_k(i) &= \sum_{j_1, j_2, \dots, j_{k-1}=1}^n T_{i, j_1, j_2, \dots, j_{k-1}} p_{k-1}(j_1) p_{k-2}(j_2) \dots p_1(j_{k-1}) \\
 &\geq T_{i, x_1, x_2, \dots, x_{k-1}} p_{k-1}(x_1) p_{k-2}(x_2) \dots p_1(x_{k-1}) \\
 &> 0
 \end{aligned}$$

since  $T$  is positive, and further, the result holds for all  $p_t$  inductively. Thus, it is not possible to have some starting probability vectors  $p_1 = p_2 = \dots = p_{k-1} = q$  that are not positive but the fixed point, since  $p = T(q, \dots, q)$  will be positive, and thus  $p \neq q$ . This establishes that the fixed point must be positive. Now we show that it must be unique.

Our next step is to define a doubly stochastic matrix  $A_t$  using  $T$  and  $p_t$  as follows.

$$A_t(i, j) = \sum_{l_1, \dots, l_{k-2}=1}^n T_{i, j, l_1, \dots, l_{k-2}} p_{t-2}(l_1) \dots p_{t-k+1}(l_{k-2}).$$

We note that  $A_t$  is doubly stochastic due to the 2-line stochastic condition that can be checked by direct calculation. Further, note that

$$p_{t+1} = A_t p_t.$$

Now assume there is a positive fixed point  $q$  for  $T$  that is not uniform. Let

$$A_q(i, j) = \sum_{l_1, \dots, l_{k-2}=1}^n T_{i,j,l_1, \dots, l_{k-2}} q_{l_1} \cdots q_{l_{k-2}}.$$

Note that  $A_q$  is doubly stochastic. Further, since  $q$  is positive,  $A_q$  is also positive and thus irreducible. Since  $q$  is a fixed point of  $T$ , we have that

$$q = A_q q.$$

However, this is a contradiction since  $A_q$  is irreducible and doubly stochastic and only has the uniform distribution as stationary distribution. Thus the tensor has a unique fixed point.  $\square$

The next interesting question is to understand how fast the tensor converges to the fixed point, starting from any fixed distribution. One way to achieve this is to use Mihail's proof showing that the convergence of a nonnegative matrix will be inversely proportional to the square of the expansion 5.3.1. The nice thing about Mihail's proof, unlike our simpler proof in Lemma 5.3.1 is that it is combinatorial, and does not depend on the spectra of the underlying object. However, it is not possible to extend it directly, since every matrix  $A_t$  in Lemma 5.15.5, although doubly stochastic, is a *different* doubly stochastic matrix, and we thus leave the problem of the speed of convergence to the fixed point as the most important next step to Theorem 5.15.5 for future work.



## SUMMARY OF RESULTS AND QUESTIONS

We collect the main results of this thesis and some important questions here. We restate some of our main theorems first.

**Theorem 5.15.6.** (*Spectral Gap and Edge Expansion*) Let  $R$  be an  $n \times n$  nonnegative matrix, with edge expansion  $\phi(R)$  defined as 2.0.4 and 2.0.6, and the spectral  $\Delta(R)$  defined as 2.0.2 and 2.0.6. Then

$$\frac{1}{15} \cdot \frac{\Delta(R)}{n} \leq \phi(R) \leq \sqrt{2 \cdot \Delta(R)}.$$

**Theorem 5.15.7.** (*Mixing Time, Singular Values, Edge Expansion, and Spectral Gap*). Let  $R$  and  $A$  be irreducible and  $\frac{1}{2}$ -lazy nonnegative matrices with largest eigenvalue 1, where  $A$  has the same corresponding left and right eigenvector. Let the mixing time be as defined in 5.1.1, then

$$\tau_\epsilon(A) \leq \frac{\ln\left(\sqrt{\frac{n}{\kappa}} \cdot \frac{1}{\epsilon}\right)}{\ln\left(\frac{1}{\sigma_2(A)}\right)},$$

$$\frac{\frac{1}{2} - \epsilon}{\phi(R)} \leq \tau_\epsilon(R) \leq \frac{4 \cdot \ln\left(\frac{n}{\kappa \cdot \epsilon}\right)}{\phi^2(R)},$$

$$(1 - \Delta) \frac{1 - \epsilon}{\Delta} \leq \tau_\epsilon(R) \leq 20 \cdot \frac{n + \ln\left(\frac{1}{\kappa \cdot \epsilon}\right)}{\Delta(R)}.$$

**Theorem 5.15.8.** (*Rootn Matrices 4.8*) There is a doubly stochastic matrix  $A_n$  for every  $n$ , such that

$$\phi(A_n) \leq \frac{\Delta(A_n)}{\sqrt{n}}.$$

**Theorem 5.15.9.** (*Chet Matrices 4.10*) There is a matrix  $C_n$  for every  $n$ , such that  $\sum_i C_{i,j} = 1$  and  $\sum_j C_{i,j} = 1$  for all  $i, j$ , and with  $\phi(C_n)$  defined similar to that for doubly stochastic matrices in 2.0.3, it holds that

$$\phi(C_n) \leq 2 \cdot \frac{\Delta(C_n)}{n}.$$

**Theorem 5.15.10.** (*Monotonicity of Capacity*) Let  $A$  be an irreducible nonnegative matrix with largest eigenvalue 1 and corresponding left and right eigenvector  $w$ . Let

$A_\alpha = \tilde{A} + \alpha \bar{A}$  where  $\tilde{A} = \frac{1}{2}(A + A^T)$ ,  $\bar{A} = \frac{1}{2}(A - A^T)$ , and  $-1 \leq \alpha \leq 1$ . Then for  $|\alpha| \leq |\beta|$ , and every  $U \subseteq [n]$  and  $a \in \mathbb{R}^{|U|}$ , we have that

$$\text{cap}_{U,a}(A_\alpha) \leq \text{cap}_{U,a}(A_\beta).$$

**Theorem 5.15.11.** (*Unique fixed point for tensors*) Let  $T$  be a  $k$ -tensor in  $n$  dimensions which is entry-wise positive. Let  $T$  be 2-line stochastic, such that for the output index  $i$  and some input index  $j$ , it holds that for any  $i, j, l_1, \dots, l_{k-2}$

$$\sum_i T_{i,j,l_1,\dots,l_{k-2}} = 1$$

and

$$\sum_j T_{i,j,l_1,\dots,l_{k-2}} = 1.$$

The  $T$  act on every probability distribution as 5.15.1. Then the uniform distribution is the unique fixed point for  $T$ .

We collect some of our main conjectures and open problems here.

**Conjecture 5.15.12.** (*Chet Conjecture*) Let  $C_n$  denote the  $n \times n$  Chet matrix defined in 4.10, and let  $C = \{n : C_n \text{ is entry-wise nonnegative}\}$ . Then the following is true:

$$|C| = \infty.$$

More strongly,

$$C = \mathbb{N}.$$

**Conjecture 5.15.13.** (*Trace Conjectures*) Let  $A$  be a nonnegative matrix that is substochastic, that is,  $\sum_i A_{i,j} \leq 1$  and  $\sum_j A_{i,j} \leq 1$  for all  $j$  and  $i$ . Assume the following: Above the diagonal,  $A$  has nonzero entries only for entries that are at a distance of 1 from the diagonal, and below the diagonal,  $A$  has nonzero entries only for entries that are at a distance at most  $k$  from the diagonal, where the diagonal has distance zero from the diagonal. Assume  $\text{Tr}A^l \leq 1$  for  $l \leq k + 1$ . Then for all  $l$ ,

$$\text{Tr}A^l \leq 1.$$

The first relaxation is to show it for the Toeplitz case where every diagonal has the same entry, and the second relaxation is to show it for the infinite case where the condition  $\text{Tr}A^l \leq 1$  is replaced by

$$p_l \leq c \cdot \frac{1}{l}$$

for some constant  $c$ , where  $p_l$  is the probability of returning back to the starting vertex after exactly  $l$  steps.

It is indeed possible to construct a large number of open problems from every Section, for eg., Is it possible to use the matrix  $H$  in Lemma 5.11.13 to obtain a bound more exact between capacities than Theorem 5.11.12, similar to the manner in which Lemma 5.11.14 is an exact version of Lemma 5.11.13? Is there a modified notion of normalized capacity, such that it is equivalent to the spectral gap of a general nonnegative  $R$  up to constants, similar to Lemma 5.12.10? For the higher order notion of expansion as defined in [LOT14], what is its relation with the spectral gap of a general nonnegative  $R$ ? And so on. However, the most important open problem from our own sense is the following, which we believe would only be the second step into a large and undiscovered area.

**Open Problem 5.15.14.** *Is there a notion of expansion  $\phi(T)$  for 2-line stochastic tensors  $T$ , such that the tensor walk converges to the uniform distribution in about  $1/\phi^2(T)$  steps similar to lemma 5.3.1?*

We hope these theorems, conjectures and questions get used, resolved or explored in the future.

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*Appendix A*

**CHET MATRICES – EXACT AND NUMERICAL  
COMPUTATIONS**

We present some Chet Matrices computed exactly and numerically. The exact computations were done in Maple, and the numerical ones in Matlab.

**A.1 Chet Matrix for  $n = 16$  computed exactly**

The equations for  $C_{16}$  where the matrices are defined in construction 4.10, are as follows.

$$r = \left(\frac{1}{16}\right)^{\frac{1}{15}}$$

$$14 \cdot c_0 = 2 * r - 1$$

$$13r \cdot c_1 = (8/7) * r^2 - 15/28$$

$$12r^2 \cdot c_2 = (528/637) * r^3 + (45/637) * r - 20/49$$

$$11r^3 \cdot c_3 = (38980/57967) * r^4 + (7095/231868) * r^2 + (110/1029) * r - 334605/927472$$

$$10r^4 \cdot c_4 = (5019075/35707672) * r + (15675/811538) * r^3 + (3650/93639) * r^2 \\ = - 21653/62426 + (2622960/4463459) * r^5$$

$$9r^5 \cdot c_5 = (194877/1092455) * r + (23279535/1624699076) * r^4 + (4980/218491) * r^3 \\ + (135515025/3249398152) * r^2 + (221814104/406174769) * r^6 \\ - 4578373505/12997592608$$

$$\begin{aligned}
8r^6 \cdot c_6 &= (22891867525/102356041788) * r + (10590760/656128473) * r^4 \\
&\quad + (63909555/2843223383) * r^3 + (4070764/99413405) * r^2 \\
&\quad + (33490290/2843223383) * r^5 + (96435386896/179123073129) * r^7 \\
&\quad - 569210253/1530966437 \\
7r^7 \cdot c_7 &= (1707630759/6123865748) * r + (98852689755/6505295100304) * r^4 \\
&\quad + (2013729/99413405) * r^3 + (389161747925/10645028345952) * r^2 \\
&\quad + (8450450/656128473) * r^5 + (4659561625/443542847748) * r^6 \\
&\quad + (14468197830722/25614599457447) * r^8 - 42029290110657/104084721604864 \\
6r^8 \cdot c_8 &= (126087870331971/364296525617024) * r + (12646467661976/19922466244681) * r^9 \\
&\quad + (74507973/5686446766) * r^4 + (68675602575/4139733245648) * r^3 \\
&\quad + (15368676831/557271783068) * r^2 \\
&\quad + (268437195855/22768532851064) * r^5 + (2018448010/179123073129) * r^6 \\
&\quad + (36526797305/3622266589942) * r^7 - 53944771607543/120370705142688 \\
5r^9 \cdot c_9 &= (269723858037715/631946201999112) * r \\
&\quad - 293344384450753313/580142217045110720 \\
&\quad + (42922251609375/4143872978893648) * r^4 + (11384205060/975225620369) * r^3 \\
&\quad + (210146450553285/16575491915574592) * r^2 \\
&\quad + (4192421772289592/5438833284797913) * r^{10} \\
&\quad + (197518666/19902563681) * r^5 + (10494908689675/1035968244723412) * r^6 \\
&\quad + (280853043700/26331091749963) * r^7 \\
&\quad + (225785202013625/21755333139191652) * r^8
\end{aligned}$$

$$\begin{aligned}
4r^{10} \cdot c_{10} = & (2640099460056779817/5076244399144718800) * r \\
& + (583988144046138064/571077494903780865) * r^{11} \\
& + (433842562719595/38071832993585391) * r^9 \\
& + (7074714234537/976200845989369) * r^4 \\
& + (42029290110657/7251777713063884) * r^3 \\
& - (269723858037715/28753552190959596) * r^2 \\
& - 487051361453894455/843437530934814816 \\
& + (504083501274005/65265999417574956) * r^5 \\
& + (136555337396/16300199654739) * r^6 \\
& + (239093054413515/25381221995723594) * r^7 \\
& + (284474332622540/26357422841712963) * r^8 \\
3r^{11} \cdot c_{11} = & (2435256807269472275/3936041811029135808) * r \\
& + (704066732737790/61500653297330247) * r^9 \\
& + (948306872766753891/232288943704862332288) * r^4 \\
& - (53944771607543/134183243557811448) * r^3 \\
& - (71282685421533055059/1847752961288677643200) * r^2 \\
& + (74092391002251/13666811843851166) * r^5 \\
& + (60910874936948457/4619382403221694108) * r^{10} \\
& + (454789092312238525/71270471363991851952) * r^6 \\
& + (10063658054264/1331182971803685) * r^7 \\
& + (2582373218800886646164/1714945717196053937595) * r^{12} \\
& + (1873806347700790155/203252825741754540752) * r^8 \\
& - 250148541000967840970441/376308088801876978306560
\end{aligned}$$

$$\begin{aligned}
2r^{12}c_{12} = & (250148541000967840970441/359203175674518933838080) * r \\
& + (251191067356462921/16167838411275929378) * r^{11} \\
& + (52904039025561315/5879213967736701592) * r^9 \\
& + (1059097700970891719/805904560808215556688) * r^4 \\
& - (36081359287442657499/6467135364510371751200) * r^3 \\
& - (75492961025353640525/1074539414410954075584) * r^2 \\
& - 611028831268072088101/795955121785891907840 \\
& + (204277892726612218/16789678350171157431) * r^{10} \\
& + (237927811316429277/73910118451547105728) * r^5 \\
& + (5335710693495901/1243679877790456106) * r^6 \\
& + (3520738115297033525/654797455656675139809) * r^7 \\
& + (8292429130967703269984/3273987278283375699045) * r^{13} \\
& + (54680493901861873/7995084928652932110) * r^8 \\
1r^{13}c_{13} = & (1833086493804216264303/2785842926250621677440) * r \\
& + (4397770296526056/395716324751508761) * r^{11} \\
& + (145628182696554137/27982797250285262385) * r^9 \\
& - (984757098601178871741/2589440999949952849180480) * r^4 \\
& - (2435256807269472275/341898904585303569504) * r^3 \\
& - (250148541000967840970441/2971589907852838452660480) * r^2 \\
& + (43699381559221754727/5885093181704438293592) * r^{10} \\
& + (1255133000992702981/940221987609584816136) * r^5 \\
& + (43750487609031995683/20177462337272359863744) * r^6 \\
& + (2167687960275208704611884/417105979253302064058333) * r^{14} \\
& + (16063263041956539/5540028546521122654) * r^7 \\
& - 41502574124308301104426128989/46982817503091944495530629120 \\
& + (14252777333017827436531/873936337483109086598412) * r^{12} \\
& + (80226936993830858719175/20974472099594618078361888) * r^8
\end{aligned}$$

## A.2 Matlab code to numerically compute the Chet Matrix $C_n$

```

digits(100);
n = 500;

```

```

chet(n);
function chet(n)
    A=zeros(n);
    r = (1/n)^(1/(n-1));
    for i=1:n-1
        A(i+1, i) = r;
    end

    ss=1-r;
    A(1,1)=ss; A(n,n)=ss;

    for j=1:n-2
        tempvar=(1-trace(A^j))/(j*(n-j-1)*(r^(j-1)));
        for i=2:n-j
            A(i, i+j-1) = tempvar;
        end
        ss=ss-tempvar;
        A(1,1+j)=ss; A(n-j,n)=ss;
    end

    A(1,n)=1;
    for k=1:n-1
        A(1,n)=A(1,n)-A(1,k);
    end
    disp("Second row of A");
    for j=2:n-1
        disp(vpa(A(2,j)));
    end
    disp("First row of A");
    for j=1:n
        disp(vpa(A(1,j)));
    end
end
end

```

### A.3 Chet Matrix for $n = 100$ computed numerically

The values of the entries  $c_i$  for  $i = 0$  to  $i = 97$  in sequence are as follows, computer to 70 decimal places.

0.00927649911554763451082550318460562266409397125244140625  
 0.00458635239881075192081016922429625992663204669952392578125  
 0.0030183677508908656438035844615797032020054757595062255859375  
 0.0022355644535450368108608909523127294960431754589080810546875  
 0.00176718760833881154137525726355306687764823436737060546875  
 0.001455962533911280519516306952709783217869699001312255859375  
 0.001234440142572338326709679989789947285316884517669677734375  
 0.00106889892853081537073267615056693102815188467502593994140625  
 0.000940614643884963024141054876992029676330275833606719970703125  
 0.00083836180743799941506022577186740818433463573455810546875  
 0.00075500402718139589773593822741304393275640904903411865234375  
 0.000685789053878697635498185025682005289127118885517120361328125  
 0.000627430873269885333760875756325958718662150204181671142578125  
 0.000577585350020265952085407601401811916730366647243499755859375  
 0.00053453574898018238990837769364361520274542272090911865234375  
 0.00049699628825328016901163863394685904495418071746826171875  
 0.000463985101801967121659675541422984679229557514190673828125  
 0.0004347396029322115489947064848053059904486872255802154541015625  
 0.0004086586154717751647423573668760354848927818238735198974609375  
 0.00038526189538680834061057378647774385171942412853240966796875  
 0.00036416123982717374385487119070603512227535247802734375  
 0.0003450394921882088644475572447589684088598005473613739013671875  
 0.00032763503675871190855273251685275681666098535060882568359375

0.0003117301793949118202987913495149996379041112959384918212890625  
0.00029714232432357843248504902788909021182917058467864990234375  
0.0002837171929111295697913119884248089874745346605777740478515625  
0.0002713235539701151321882732769807944350759498775005340576171875  
0.0002598490869311905295847842101153446492389775812625885009765625  
0.0002491971038234116662089812077596207018359564244747161865234375  
0.0002392839292024259603523794748269892807002179324626922607421875  
0.0002300367890884215892575992423729758229455910623073577880859375  
0.00022139209727659619922172928863091101447935216128826141357421875  
0.0002132940544976439137779544719109026118530891835689544677734375  
0.000205693495833029755918974768036378009128384292125701904296875  
0.000198546936585297022041796122238110910984687507152557373046875  
0.00019181577789447587707206965834672018900164403021335601806640625  
0.0001854656417805042832591677637310567661188542842864990234375  
0.00017946581168970437221606151201314105492201633751392364501953125  
0.00017378875954287265862170663854868735143099911510944366455078125  
0.00016840974409268810664704052459939020991441793739795684814453125  
0.0001633064683704545604590874230410690870485268533229827880859375  
0.00015845878633620921987872065539448840354452840983867645263671875  
0.00015384845069080918468669427756623235836741514503955841064453125  
0.00014945889527489948059475743935564651110325939953327178955078125  
0.0001452750466522170227044730150822715586400590837001800537109375  
0.00014128316041706764590903111500352906659827567636966705322265625  
0.00013747067852759768473956680789882511817268095910549163818359375  
0.0001338261045847499611065323232850232670898549258708953857421875  
0.00013033889448148155737645936813606795112718828022480010986328125



0.0001269993602602959687462857996109732994227670133113861083984375  
0.00012379858535742862169111433434665059394319541752338409423828125  
0.000120728349693369557617435294805119383454439230263233184814453125  
0.000117781063302744559424632686539524684121715836226940155029296875  
0.0001149497073909188315198048879750558626255951821804046630859375  
0.000112227781867207772261048337458788637377438135445117950439453125  
0.00010960925854074985807788678027208106868783943355083465576171875  
0.000107088539279988410771009277322463049131329171359539031982421875  
0.000104660418533254634420627537938486284474493004381656646728515625  
0.00010232004969022411304709063717410799654317088425159454345703125  
0.000100062914833618153112766713253023453944479115307331085205078125  
0.000097884797489730082827030788195088462089188396930694580078125  
0.0000957817580373360503119550823925010263337753713130950927734375  
0.000093750111477750115089417615177325160402688197791576385498046875  
0.0000917864073062732953312004013923797174356877803802490234375  
0.00008988741125727622827655538539914914508699439465999603271484375  
0.000088050088723021726244861995258617071158369071781635284423828125  
0.00008627158967016245838359267406048047632793895900249481201171875  
0.0000845492348988450648054893132865572624723426997661590576171875  
0.00008288050350720488931681451116872949569369666278362274169921875  
0.000081263021440117230265003100964094073788146488368511199951171875  
0.0000796945510142810231712928725755773484706878662109375  
0.00007817298132436461947404604533318206449621357023715972900390625  
0.00007669631944506240142471475973451333629782311618328094482421875  
0.00007526268235308626445602409038571067867451347410678863525390625  
0.000073870289501653195983477129260563742718659341335296630859375

0.00007251745598681541495229840865732739985105581581592559814453125  
0.00007120258625146517962763159648176269911346025764942169189453125  
0.000069924168278427396676366623040621561813168227672576904296875  
0.00006868076822896611831337221332205444923602044582366943359375  
0.00006747102548735893251703743533909118923475034534931182861328125  
0.0000662936480765519337877977879003310590633191168308258056640625  
0.0000651474084121149367605785318602329425630159676074981689453125  
0.00006403113936717818211082076107487637273152358829975128173828125  
0.00006294373062035610939986274292579082612064667046070098876953125  
0.00006188412526525913595100425457218307201401330530643463134765625  
0.0000608513166580003012399134598719996347426786087453365325927734375  
0.000059844345485455394052960731432477814450976438820362091064453125  
0.0000588622970348412897947758259942219183358247391879558563232421875  
0.0000579042986496464625353723654210824633992160670459270477294921875  
0.000056969517357141464630569671623305794128100387752056121826171875  
0.000056057157654134588437196129451223214346100576221942901611328125  
0.00005516645943811468899738159610279808475752361118793487548828125  
0.0000542966960742285876108208231283214217910426668822765350341796875  
0.0000534471725871295903743073141267672099274932406842708587646484375  
0.000052617223966913077674856236143341448041610419750213623046875  
0.00005180621358547815948937531604912010152474977076053619384765625  
0.0000510135317130936129475897444773835331943701021373271942138671875  
0.000050238594163273773431609148243381923748529516160488128662109375

The values of the entries  $b_i$  for  $i = 0$  to  $i = 99$  in sequence are as follows, computer to 70 decimal places.

0.045451543338165922847338151768781244754791259765625  
0.03617504422261828833651264858417562209069728851318359375  
0.03158869182380753815042595533668645657598972320556640625  
0.028570324072916673807664977857712074182927608489990234375  
0.02633475961937163656312321791119757108390331268310546875  
0.024567572011032823287024484670837409794330596923828125  
0.0231116094771215419001464397297240793704986572265625  
0.021877169334549202706075021751530584879219532012939453125  
0.0208082704060183858174593041212574462406337261199951171875  
0.0198676557621334237691002044812194071710109710693359375  
0.01902929395469542261931650273254490457475185394287109375  
0.0182742899275140265047401300080309738405048847198486328125  
0.0175885008736353272429386862540923175401985645294189453125  
0.0169610700003654420175980277463168022222816944122314453125  
0.016383484650345177258135009878969867713749408721923828125  
0.0158489489013649946513861976882253657095134258270263671875  
0.01535195261311171448237455905427850666455924510955810546875  
0.0148879675113097464933531455244519747793674468994140625  
0.0144532279083775354322494166581236640922725200653076171875  
0.01404456929290576021329695066697240690700709819793701171875  
0.01365930739751895252320768037179732345975935459136962890625  
0.01329514615769177877935280918109128833748400211334228515625  
0.01295010666550357007753557780915798502974212169647216796875  
0.012622471628744857952142410795204341411590576171875  
0.01231074144934994618605372806996456347405910491943359375  
0.0120135991250263675367282445449745864607393741607666015625

0.01172988193211523845482791017502677277661859989166259765625  
0.0114585583781451234852699627708716434426605701446533203125  
0.0111987092912139325762144181908297468908131122589111328125  
0.010949512187390521289476197352996678091585636138916015625  
0.0107102282581880946243924057625918067060410976409912109375  
0.01048019146909967384828643588434715638868510723114013671875  
0.010258799371823078272480955774881294928491115570068359375  
0.01004550531732543473817376167289694421924650669097900390625  
0.0098398118214924057411963076447136700153350830078125  
0.009641264884907109478096032262328662909567356109619140625  
0.00944944910701263351970879966756911017000675201416015625  
0.00926398346523212880276876290963627980090677738189697265625  
0.00908451765354242359029601772135720239020884037017822265625  
0.0089107288939995511756197998920470126904547214508056640625  
0.00874231914990686309607781367958523333072662353515625  
0.00857901268153640934877035562067248974926769733428955078125  
0.0084205538952001994512652771618377300910651683807373046875  
0.0082667054445093902936836371964091085828840732574462890625  
0.00811724654923449105703436856629195972345769405364990234375  
0.00797197150258227398011978692693446646444499492645263671875  
0.00783068834216520646973602737261899164877831935882568359375  
0.0076932176636376088663116235011329990811645984649658203125  
0.007559391559052859067835417050673640915192663669586181640625  
0.00742905266457137732072357749757429701276123523712158203125  
0.007302053304311081731448052067889875615946948528289794921875  
0.007178254718953652920021557548579949070699512958526611328125

0.00705752636926028353858697528266930021345615386962890625  
0.006939745305957538586139055070134418201632797718048095703125  
0.00682479559856661970040914155788414063863456249237060546875  
0.006712567816699412104330946249319822527468204498291015625  
0.00660295855815866243598843965401101741008460521697998046875  
0.0064958700188786737406143600992436404339969158172607421875  
0.00639120960034541933658669421447484637610614299774169921875  
0.006288889550655194816963788895236575626768171787261962890625  
0.006188826635821576514773223465226692496798932552337646484375  
0.006090941838331846540366409925582047435455024242401123046875  
0.005995160080294510869525215213116098311729729175567626953125  
0.00590140996881676101193381356324607622809708118438720703125  
0.0058096235615104872829217441676519229076802730560302734375  
0.005719736150253211352800786215766493114642798900604248046875  
0.00563168606153018926063769100665012956596910953521728515625  
0.00554541447186002699198947851755292504094541072845458984375  
0.0054608652369611820898143150770920328795909881591796875  
0.0053779847334539769565520117566848057322204113006591796875  
0.00529672171201386009220524186957845813594758510589599609375  
0.00521702716099957906903394899700288078747689723968505859375  
0.005138854179675214801925609009458639775402843952178955078125  
0.0050621578602301521565554054404856287874281406402587890625  
0.004986895177877066244465087407888859161175787448883056640625  
0.0049130248883754133737422620242796256206929683685302734375  
0.004840507432388597985895017927759909071028232574462890625  
0.00476930484613713283337244064341575722210109233856201171875

0.004699380677858705328275856771824692259542644023895263671875  
0.004630699909629738993122050061401751008816063404083251953125  
0.004563228884142379870869632441099383868277072906494140625  
0.004496935236065827991291943277474274509586393833160400390625  
0.004431787827653713325581907866990150068886578083038330078125  
0.004367756688286534953735706920951997744850814342498779296875  
0.00430481295766617887144089849016381776891648769378662109375  
0.004242928832400919871015165796279688947834074497222900390625  
0.004182077515742919915364694816162227652966976165771484375  
0.004122233170257464697494587113624220364727079868316650390625  
0.004063370873222623726184199455246925936080515384674072265625  
0.00400546657457297693161191176614011055789887905120849609375  
0.003948497057215835832899575308374551241286098957061767578125  
0.003892439899561701312225014959267355152405798435211181640625  
0.003837273440123586433492253178201281116344034671783447265625  
0.0037829767440493576764748429042128918808884918689727783203125  
0.003729529571462227889588891827088446007110178470611572265625  
0.0036769123474953147034938183423946611583232879638671875  
0.003625106133909836679529714587033595307730138301849365234375  
0.00357409260219674305980586126452180906198918819427490234375  
0.0035238540080334691644015077116591783124022185802459716796875  
0.00690000660105437486901980292941516381688416004180908203125

#### **A.4 Chet Matrix for $n = 500$ computed numerically**

The values of the entries  $c_i$  for  $i = 0$  to  $i = 497$  in sequence are as follows, computer to 100 decimal places in Matlab.

0.001958325731775443535875869116580361151136457920074462890625  
0.0009744604963271090956877795719037749222479760646820068359375  
0.000646424359494959127094004802671634024591185152530670166015625  
0.0004825194782553630934440747068947530351579189300537109375  
0.0003842721184705963528849270716136743430979549884796142578125  
0.000318845535005767878600213549589170725084841251373291015625  
0.0002721662296516986546436600580278764027752913534641265869140625  
0.00023719828353077406922662373478516428804141469299793243408203125  
0.000210033684311804256898692511157378248753957450389862060546875  
0.0001883282678841950545656214188738886150531470775604248046875  
0.00017059076651722713722190982732485053929849527776241302490234375  
0.00015582734787566377885302537631417862939997576177120208740234375  
0.00014335022976914193310570000416959146605222485959529876708984375  
0.00013266833047788240281493477024099547634250484406948089599609375  
0.00012342166865425956167635901383761165561736561357975006103515625  
0.0001153403701699478255647546287576687973341904580593109130859375  
0.000108218148043479411922300481574410468965652398765087127685546875  
0.000101894625903682883687195737110187110374681651592254638671875  
0.00009624324605580665006020202323355761109269224107265472412109375  
0.000091162806984470558767374992470422512269578874111175537109375  
0.000086571420087329839488342331232928472672938369214534759521484375  
0.00008240211560177918156087917278540544430143199861049652099609375  
0.000078599595591595828605012419298958548097289167344570159912109375  
0.000075117799284187751311658853836661364766769111156463623046875  
0.000071918053188966074248424098502852075398550368845462799072265625  
0.000068967648472342628872266967476889476529322564601898193359375

0.000066238734756000208574698573382733002290478907525539398193359375  
0.000063707451184388317450522920548650063210516236722469329833984375  
0.0000613532374523595804872988512812526096240617334842681884765625  
0.0000591582827733469048740559681487383159037563018500804901123046875  
0.000057107081617524147886151564268431002346915192902088165283203125  
0.0000551860728461235186038426336896378643359639681875705718994140625  
0.000053383344537563586309526775242062512916163541376590728759765625  
0.00005168839096917306262339575351205667175236158072948455810546875  
0.0000500919113142148041107303002572592731667100451886653900146484375  
0.000048585641935410220251627400056548822249169461429119110107421875  
0.0000471622159127936730650676455667280606576241552829742431640625  
0.000045815044784048927100673920254081394887180067598819732666015625  
0.000044538218506346330502650154858912401323323138058185577392578125  
0.000043326420447503810194807283284745835771900601685047149658203125  
0.0000421748548376638845015633438872981741951662115752696990966796875  
0.0000410791846023243775276427569576043197230319492518901824951171875  
0.0000400354778847797612077556717036230793382856063544750213623046875  
0.00003904016187383907280673833728457111647003330290317535400390625  
0.0000380899827990605183126136823457130731185316108167171478271484375  
0.0000371819711537280889819719054134594671268132515251636505126953125  
0.00003631341136594654485196531634727534765261225402355194091796875  
0.00003548181526828966705737478104509818876977078616619110107421875  
0.000034684898822593808963808681422591462251148186624050140380859375  
0.000033920561643514723286323142570353184055420570075511932373046875  
0.0000331868689361517076497239131516181487313588149845600128173828125  
0.000032482035522262450548403034389366439427249133586883544921875



0.0000318044116788212841650217155287094783489010296761989593505859375  
0.00003115247055357925841899413565982968066236935555934906005859375  
0.000030524796956631758599633175155219078078516758978366851806640625  
0.00002992007735568226573191590034195286307294736616313457489013671875  
0.00002933709092694703978961880130871264782399521209299564361572265625  
0.000028774701534079559083097177296650670541566796600818634033203125  
0.0000282318505247945833436760965096112840910791419446468353271484375  
0.0000277075502496670019229006720618002646006061695516109466552734375  
0.00002720087822003305978225441708051590694594779051840305328369140625  
0.0000267109718327488915106358857709523135781637392938137054443359375  
0.000026237023598668198832474518500390558983781374990940093994140625  
0.00002577827681966678437610641927424381947275833226740360260009765625  
0.00002533402166578841419844643489955871018537436611950397491455078125  
0.000024903591610023545553469215274589032560470513999462127685546875  
0.0000244863601832463899962526177045418762645567767322063446044921875  
0.0000240817380163164439037769282148104821317247115075588226318359375  
0.00002368917014011676414639122334460097363262320868670940399169921875  
0.00002330813351772713205660968183163817002423456870019435882568359375  
0.000022938134785744119397733753462631511865765787661075592041015625  
0.0000225787081844194519454453728979359539152937941253185272216796875  
0.0000222294136584283525347703613928018739898107014596462249755859375  
0.00002188983511212697313612352001399585788021795451641082763671875  
0.00002155957880481291445077911272942827736187609843909740447998046875  
0.00002123827187310362553059918389042337594219134189188480377197265625  
0.0000209255609688028634579777531588007377649773843586444854736328125  
0.00002062111100191814835858560017722851398502825759351253509521484375

0.00002032460397943584197856352335787022411750513128936290740966796875  
0.00002003573793150512379166068577251991200682823546230792999267578125  
0.00001975422591741851855297144868739422918224590830504894256591796875  
0.00001947979510458813421323875925139645914896391332149505615234375  
0.000019212185914323153218367934425003795695374719798564910888671875  
0.00001895115122885018775207403851634779812229680828750133514404296875  
0.00001869645565450380494780524553988243496860377490520477294921875  
0.0000184478748365002947150713408230870982151827774941921234130859375  
0.00001820519482115785935721387345243016397944302298128604888916015625  
0.00001796821146174221192170876448823690907374839298427104949951171875  
0.00001773672986454179431614099071712331578964949585497379302978515625  
0.00001751056387197735957918752480733104448518133722245693206787109375  
0.0000172895355799611145333934125734032249965821392834186553955078125  
0.000017073474886818349707980069229762420945917256176471710205078125  
0.0000168622190714432323662731738611597620547399856150150299072265625  
0.00001665561239848803212738014012384013540213345550000667572021484375  
0.0000164535057485725580493467201659285592540982179343700408935546875  
0.00001625575627171368597802432465204702793926117010414600372314453125  
0.0000160622270622634037901856063346173186801024712622165679931640625  
0.00001587278685384899419683231436284387427804176695644855499267578125  
0.00001568730973285858041016242736542807278965483419597148895263671875  
0.00001550567486919664361298860921767328591158729977905750274658203125  
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The values of the entries  $b_i$  for  $i = 0$  to  $i = 499$  in sequence are as follows, computer to 100 decimal places in Matlab.

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