UNIVERSITY OF CALIFORNIA, SAN DIEGO

Chip-Firing Games with Dirichlet Eigenvalues and Discrete Green's Functions

A dissertation submitted in partial satisfaction of the requirements for the degree Doctor of Philosophy in Mathematics

by

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Dedicated in memory of Rosa Q. Huang (1963-1995)

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The text of Chapter III is in part a reprint of the material as it appears in "A chip-firing game and Dirichlet eigenvalues," to appear this year in the special Kleitman issue of *Discrete Mathematics*. My thesis advisor Professor Fan Chung Graham and I contributed roughly equally to this co-authored paper. My contribution consists primarily of, but is not limited to, Sections 6 and 7 of the paper, which appear here as Sections III.D and III.E; the rest of the paper is included and expanded by a significant amount of new material, especially in Sections III.B and III.F. Permission to include the reprinted material was obtained from *Discrete Mathematics* and authorized by Dr. Richard Attiyeh, Dean of Graduate Studies. The text of Chapter II is in part a reprint of the material as it appears in "Discrete Green's functions for products of regular graphs," to be submitted for publication shortly. I am the sole author of this work, which was supervised by Prof. Graham. The material in Chapter IV was developed in response to a problem posed by Professor Andrew Kahng, and also benefitted from his constructive observations.

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PUBLICATIONS

F. R. K. Chung and R. B. Ellis, "A chip firing game and Dirichlet eigenvalues," *Discrete Mathematics*, special Kleitman issue, to appear.

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ABSTRACT OF THE DISSERTATION

Chip-Firing Games with Dirichlet Eigenvalues
and Discrete Green's Functions

by

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The combinatorial Laplacian of a graph is the adjacency matrix of the graph subtracted from the diagonal matrix of its vertex degrees. The Laplacian governs many diffusion-like problems on graphs such as electric potential, random walks, and chip-firing games or other balancing games. We survey properties of the eigensystems of Laplacians for graphs with and without boundary, concentrating on the smallest eigenvalue of the Dirichlet Laplacian for a graph with boundary. A method for extracting eigenvectors of the Dirichlet Laplacian from those of the Laplacian is given. We present methods for deriving discrete Green's functions, the inverses or pseudo-inverses of Laplacians, for products of regular graphs with or without boundary. Explicit formulas are derived for tori of fixed dimension. We define the Dirichlet chip-firing game, a discrete balancing process in which chips are removed from the game if they are fired into the boundary of the graph. We give bounds on the length of the game, and examine the relations among three equinumerous families, the set of spanning forests rooted in the boundary, a set of "critical" configurations of chips, and a coset group, called the sandpile group associated with the graph. An algorithm is given for computing the critical configuration determined uniquely by an arbitrary configuration. The Dirichlet game is applied to solve a problem in microchip manufacturing in which fill metal is added to balance surface metal density.

Chapter I

Introduction and Terminology

As the field of graph theory matured in the last half-century, it became popular to use linear algebra to study correlations between properties of graphs and properties of types of adjacency matrices associated with them. Graphs can be associated with matrices which record edge-vertex incidence or vertex-vertex adjacency. A natural extension of the so-called vertex-vertex *adjacency matrix* is the *combinatorial Laplacian*, which is constructed by subtracting the adjacency matrix from the diagonal matrix comprised of vertex degrees. *Spectral graph theory* is the study of the eigenvalues and eigenvectors of these matrices arising from graphs, and of information about the graphs which can be deduced therefrom; thus inverse problems are conspicuous in the field (as in x-ray crystallography). More recently, spectral graph theory has begun to include problems of a more geometric flavor, such as the construction of *expander graphs* with both a small number of edges and a small diameter, the determination of bottlenecks and other isoperimetric problems, and the behavior of processes on graphs such as electrical current, random walks, and a discrete load-balancing game called *chip-firing*. This thesis contributes to the corpus of spectral graph theory by characterizing properties of a certain chip-firing game in which chips are removed after crossing the boundary; by developing compact formulas for *discrete Green's functions*, or matrix inverses of Laplacians of products of regular graphs; and by applying both advances to computational problems in chip-firing games and random walks.

For an introduction to graph theory, see [119], and for a more advanced treatment, see [20]. Algebraic graph theory, which shares many linear algebraic techniques with spectral graph theory, is presented in [10, 12]. The authority on spectral graph theory, especially with respect to newer problems, is [29]; more traditional texts include [38, 41]. This document is divided into four chapters. Chapter I is a substantive introduction to Laplacians of graphs, including properties of the spectra of Laplacians and the primary examples and techniques that will be used in the subsequent chapters. Chapter II introduces discrete Green's functions, develops formulas for discrete Green's functions for products of regular graphs, demonstrates these formulas on tori, and discusses implications for computing hitting times and other quantities for random walks. In Chapter III, the Dirichlet chip-firing game is described and certain configurations of the game are shown to be equinumerous with a set of rooted spanning trees on the graph and the elements of the critical group, or sandpile group, associated with the graph. A bound on the length of the Dirichlet chip-firing game is obtained in terms of the smallest positive eigenvalue of a Laplacian of the underlying graph, and this result is combined with the discrete Green's function to allow fast computation of the configurations in question. Chapter IV concludes the document by presenting a major application of the Dirichlet chip-firing game to a microchip layer manufacturing process in which discrete units of fill metal are distributed across the surface of the chip in order to balance overall metal density.

Before presenting a more detailed summary of the contents of this chapter, we mention some important contributions to the field of spectral graph theory. An early fundamental problem in the study of the spectra of graphs was the question of whether a graph is completely determined by its spectrum. This question was quickly resolved in the negative, and graphs with the same spectra, or *isospectral graphs*, were investigated [25, 41, 48, 72, 95]. Other early papers, such as [5], considered bounds for eigenvalues of the Laplacian, taking motivation from the study of eigenvalues of Laplacians of compact Riemannian manifolds (e.g., [24]). More recent work includes characterizations of general properties of spectra [43, 78, 92, 96, 97] and of eigenspaces [39, 40]. The second-smallest eigenvalue, also known as the *algebraic connectivity* of a graph [58, 59, 60], has been scrutinized repeatedly due to its connections with graph diameter [33], expansion properties [3], isoperimetric number [98], mixing times for random walks [86, 87], and with applications such as bandwidth and minimum-sum problems in graph layout [76]. Articles which survey properties of the second-smallest eigenvalue include [93, 94, 99, 100, 101]. A more careful treatment of the spectrum of a Laplacian yields improved results on mixing times of random walks from Sobolev inequalities [30, 47]. The heat kernel of a Laplacian employs the entire spectrum and can be used, for example, in counting spanning trees [31]. The reader is referred to [29] for additional applications.

The remainder of this chapter is divided as follows. Section I.A defines the combinatorial Laplacian and normalized Laplacian, gives a list of basic properties in Lemma I.1, and presents general eigenvalues and eigenvectors in Theorem I.3. Examples of Laplacians and their eigensystems are given in Section I.B for three families of graphs: complete graphs, complete bipartite graphs, and hypercubes. Section I.C defines the Dirichlet versions of the Laplacians introduced in Section I.A, which arise from specifying a set of boundary vertices. Basic properties of Dirichlet eigenvalues are given by I.5, and general properties of Dirichlet eigensystems are obtained by inspecting the corresponding non-Dirichlet eigensystems (Theorem I.7), and by techniques of the Courant-Fischer Theorem (Theorem I.8). An important lower bound on the first positive eigenvalue of various Laplacians in terms of diameter is obtained from a more general bound in Section I.D. In Section I.E, the eigensystem of the Laplacian of the cycle is derived from the theory of circulants, and then used with Theorem I.7 to derive the Dirichlet eigensystem of the path. The cycle and path with boundary form the basis for the major examples in Chapters II-IV. Section I.F defines Cartesian products of graphs, gives a formula for the eigensystems of their Laplacians in terms of the factor graphs, and applies the formula to cycles and paths with boundary to obtain the eigensystems of tori and grids with boundary, respectively.

I.A Laplacians and their spectra

The basic definitions of spectral graph theory follow those of [29]. A more deliberate introduction may be found in [41]. Let $\Gamma = (V, E)$ be a simple graph (with neither loops nor multiple edges). Let $x, y \in V$ be arbitrary vertices; $x \sim y$ iff $\{x, y\} \in E$ is an edge. Unless otherwise noted, the matrices defined are square matrices indexed in the rows and columns by the vertices of Γ. The *adjacency matrix* A is defined by

$A(x,y) = \chi(x \sim y)$, where $\chi(X)$ is the indicator function of the event X. The diagonal *degree matrix* T is defined by $T(x,y) = \chi(x = y) \cdot d_x$, where d_x is the degree of x in Γ. We define $d_{\max}(\Gamma)$, or $d_{\max}$ when the context is apparent, to be the *maximum degree* over all $x \in V$. The *volume* of a vertex subset $S \subseteq V$ is $vol(S) = \sum_{v \in S} d_v$, and $vol(\Gamma) = vol(V)$. The *combinatorial Laplacian*, $L = T - A$, of Γ is

$$L(x,y) = \begin{cases} d_x, & \text{if } x = y \\ -1, & \text{if } x \sim y \\ 0, & \text{otherwise.} \end{cases}$$

The *normalized Laplacian*, $\mathcal{L} = T^{-1/2} L T^{-1/2}$, is

$$\mathcal{L}(x,y) = \begin{cases} 1, & \text{if } x = y \\ -1/\sqrt{d_x d_y}, & \text{if } x \sim y \\ 0, & \text{otherwise.} \end{cases}$$

The *discrete Laplace* operator Δ is

$$\Delta(x,y) = \begin{cases} 1, & \text{if } x = y \\ -1/d_x, & \text{if } x \sim y \\ 0, & \text{otherwise.} \end{cases}$$

We refer to L, $\mathcal{L}$ and Δ as the Laplacian, normalized Laplacian and Laplace operator, respectively. In general, the following relations hold between L, $\mathcal{L}$, and Δ, provided that Γ has no isolated vertices:

$$\begin{aligned} L &= T^{1/2} \mathcal{L} T^{1/2} = T\Delta \\ \mathcal{L} &= T^{-1/2} L T^{-1/2} = T^{1/2} \Delta T^{-1/2} \\ \Delta &= T^{-1} L = T^{-1/2} \mathcal{L} T^{1/2}. \end{aligned} \tag{I.1}$$

The Laplace operator satisfies $\Delta = I - P$, where P is the transition probability matrix determined by $P(x,y) = \chi(x \sim y)/d_x$. Thus P governs the random walk on Γ where a walk in state x at time t transitions to an adjacent state y at time $t+1$ with probability $1/d_x$.

Throughout this document, we label the eigensystems of L and $\mathcal{L}$ as follows. The eigenvalues of L are $\sigma_0 \leq \sigma_1 \leq \cdots \leq \sigma_{|V|-1}$ with corresponding eigenvectors $\psi_0, \psi_1, \ldots, \psi_{|V|-1}$. The eigenvalues of $\mathcal{L}$ are $\lambda_0 \leq \lambda_1 \leq \cdots \leq \lambda_{|V|-1}$ with corresponding eigenvectors $\phi_0, \phi_1, \ldots, \phi_{|V|-1}$. We can choose the eigenvectors to be orthonormal when necessary. We now list some important and relatively straightforward properties of L and $\mathcal{L}$, mostly following the presentation of [29, pp. 6-7].

Lemma I.1 (Eigensystems of L and $\mathcal{L}$). *Suppose Γ has n vertices.*

(i) $\sum_i \sigma_i = vol(\Gamma)$, *and* $\sum_i \lambda_i \leq n$.

(ii) *L and $\mathcal{L}$ are positive semidefinite, and so the σ_i's and λ_i's are real and nonnegative.*

(iii) *Γ has $i+1$ connected components if and only if $\sigma_0, \ldots, \sigma_i = \lambda_0, \ldots, \lambda_i = 0$ and $\sigma_{i+1}, \lambda_{i+1} > 0$.*

(iv) *For all $0 \leq i \leq n-1$, we have $\sigma_i \leq 2\, d_{\max}$ and $\lambda_i \leq 2$. Equality is achieved for σ_{n-1} if and only if a connected component of Γ is $d_{\max}$-regular and bipartite, and for λ_{n-1} if and only if a connected component of Γ is bipartite.*

Proof. For (i), simply consider the traces of L and $\mathcal{L}$. Equality is achieved iff there is no isolated vertex.

For (ii), since L and $\mathcal{L}$ are real and symmetric, it suffices to show that $\langle f, Lf \rangle \geq 0$ and $\langle g, \mathcal{L}g \rangle \geq 0$ for all functions $f, g : V \to \mathbb{R}$. Without loss of generality, we assume Γ has no isolated vertices, so that $T^{-1/2}$ exists. We have

$$\langle f, Lf \rangle \;=\; \sum_x f(x) \sum_{y \sim x} (f(x) - f(y)) \;=\; \sum_{x \sim y} (f(x) - f(y))^2, \tag{I.2}$$

which as a sum of squares is nonnegative. Also for $\mathcal{L}$, we have

$$\langle g, \mathcal{L}g \rangle \;=\; \left\langle T^{1/2} f, T^{-1/2} L T^{-1/2} T^{1/2} f \right\rangle \;=\; \langle f, Lf \rangle \,, \tag{I.3}$$

where $g = T^{1/2} f$ defines f in terms of an arbitrary g. Therefore L and $\mathcal{L}$ are positive semidefinite and have real nonnegative eigenvalues.

For (iii), suppose Γ is connected. Let ψ be an eigenvector of L having eigenvalue 0. Thus $L\psi = 0$, and by (I.2)

$$\sum_{x \sim y} (\psi(x) - \psi(y))^2 = 0.$$

Therefore ψ must be constant on all connected components of Γ, and the eigenspace of L corresponding to the eigenvalue 0 is 1-dimensional. The eigenspace of $\mathcal{L}$ corresponding to eigenvalue 0 is also 1-dimensional, because any eigenvector ϕ with eigenvalue 0 satisfies $\mathcal{L}\phi = 0$; by (I.3),

$$\langle \phi, \mathcal{L}\phi \rangle \;=\; \sum_{x \sim y} (f(x) - f(y))^2 \;=\; 0,$$

where $\phi = T^{1/2} f$; therefore $\lambda_1 > 0$. When Γ is not connected, the result follows from the definitions of L and $\mathcal{L}$; in particular, L and $\mathcal{L}$ may be block diagonalized in terms of the Laplacians and normalized Laplacians, respectively, of the connected components of Γ.

To show (iv), we characterize the largest eigenvalues σ_{n-1} and λ_{n-1} in terms of the Rayleigh quotient, which for a given matrix M and vector $\mathbf{x}$ is defined as (cf. [73, pp. 176])

$$\frac{\langle \mathbf{x}, M\mathbf{x} \rangle}{\langle \mathbf{x}, \mathbf{x} \rangle}\,. \tag{I.5}$$

In particular, the Rayleigh quotient for matrix M and eigenvector $\mathbf{x}$ evaluates to the corresponding eigenvalue. Noting (I.2), the Rayleigh quotient for L is

$$\frac{\langle f, Lf \rangle}{\langle f, f \rangle} \;=\; \frac{\sum_{x \sim y} (f(x) - f(y))^2}{\sum_x f^2(x)}\,, \tag{I.6}$$

and so σ_{n-1} is determined by (cf. [73, Theorem 4.2.2])

$$\sigma_{n-1} \;=\; \max_{f \neq 0} \frac{\langle f, Lf \rangle}{\langle f, f \rangle} \;=\; \max_{f \neq 0} \frac{\sum_{x \sim y} (f(x) - f(y))^2}{\sum_x f^2(x)}\,. \tag{I.7}$$

Now $\sum_{x \sim y} (f(x) - f(y))^2 \leq \sum_{x \sim y} (2f^2(x) + 2f^2(y))$ with equality achieved if and only if $f(x) = -f(y)$ whenever $x \sim y$. Combining this with (I.7), we have

$$\sigma_{n-1} \;\leq\; \sup_f \frac{2 \sum_x f^2(x) d_x}{\sum_x f^2(x)} \;\leq\; 2\, d_{\max}.$$

If $\sigma_{n-1} = 2d_{\max}$, then $\psi_{n-1}(x) = -\psi_{n-1}(y)$ for all $x \sim y$, forcing Γ to have a bipartite connected component on which $\psi \neq 0$, and $d_x = d_{\max}$ for all $x \in V$ for which $\psi(x) \neq 0$, forcing Γ to be $d_{\max}$-regular in that component. On the other hand, if Γ has a bipartite $d_{\max}$-regular component, we can simply choose ψ_{n_1} to be $+1$ on one part of the vertices, -1 on the other part in that component, and 0 elsewhere in Γ.

The argument for λ_{n-1} is similar, except the Rayleigh quotient for $\mathcal{L}$ is, noting (I.3),

$$\frac{\langle g, \mathcal{L}g \rangle}{\langle g, g \rangle} \;=\; \frac{\langle f, Lf \rangle}{\left\langle T^{1/2} f, T^{1/2} f \right\rangle} \;=\; \frac{\sum_{x \sim y} (f(x) - f(y))^2}{\sum_x f^2(x) d_x}\,, \tag{I.8}$$

where $g = T^{1/2} f$. Therefore λ_{n-1} is given by

$$\lambda_{n-1} = \max_{f \neq 0} \frac{\sum_{x \sim y} (f(x) - f(y))^2}{\sum_x f^2(x) d_x}.$$

Again, $\lambda_{n-1} = 2$ can only be achieved if $\phi_{n-1}(x) = -\phi_{n-1}(y) \neq 0$ for all $x \sim y$ everywhere on some connected component of Γ. □

Recall that the *eigenspace* E_λ of a square matrix M corresponding to an eigenvalue λ is the set of vectors $E_\lambda = \{\mathbf{x} : M\mathbf{x} = \lambda \mathbf{x}\}$. In particular, E_λ is a vector space. When Γ is connected, L and $\mathcal{L}$ both have a null space, or 0-eigenspace, of dimension 1 corresponding to an eigenvector with all-positive entries, described as follows.

Lemma I.2 (Null space eigenvector). *Let Γ be connected. Then $\vec{1}$ ($T^{1/2}\vec{1}$) spans the eigenspace of L ($\mathcal{L}$) corresponding to eigenvalue 0.*

Proof. The eigenspaces of L and $\mathcal{L}$ corresponding to eigenvalue 0 both have dimension 1 by Lemma I.1(iii). Since every row of L sums to 0, $L\vec{1} = 0$, and $\mathcal{L}(T^{1/2}\vec{1}) = T^{-1/2} L \vec{1} = 0$. □

The corresponding normalized eigenvectors for $\vec{1}$ and $T^{1/2}\vec{1}$ are $\psi_0 = \vec{1}/\sqrt{|V(\Gamma)|}$ and $\phi_0 = T^{1/2}\vec{1}/vol(\Gamma)$. An immediate consequence of Lemma I.2 is that, when Γ is connected, eigenvectors corresponding to all other eigenvalues are negative in at least one coordinate.

For the rest of the eigensystems, we may specify the eigenvalues and eigenvectors of L and $\mathcal{L}$ by using the Rayleigh quotient, defined in (I.5), and applying the Courant-Fischer Theorem (cf. [73, Theorem 4.2.11]). The following theorem appears in [29, pp. 5-6].

Theorem I.3 (General eigenvalues and eigenvectors). *Let $k = 0, \ldots, n-1$. Then the eigenvalue σ_k of L satisfies*

$$\sigma_k = \min_{f \neq 0,\ f \perp \psi_0, \ldots, \psi_{k-1}} \frac{\sum_{x \sim y} (f(x) - f(y))^2}{\sum_x f^2(x)}, \tag{I.9}$$

where ψ_k is the eigenvector achieving σ_k, and the eigenvalue λ_k of L satisfies

$$\lambda_k = \min_{f \neq 0,\ T^{1/2} f \perp \phi_0, \ldots, \phi_{k-1}} \frac{\sum_{x \sim y} (f(x) - f(y))^2}{\sum_x f^2(x) d_x}, \tag{I.10}$$

where $\phi_k = T^{1/2} f$ for a vector f achieving λ_k is the eigenvector for λ_k.

We note that for $k = 0$ minimization is over all nonzero vectors. We justify the use of maximum instead of supremum because we can further restrict the maximum to be over all vectors with norm 1, so that the set of vectors considered is compact.

I.B Examples of Laplacians and their spectra

We now give examples of Laplacians of families of graphs and their corresponding eigensystems. These examples are well known, appearing, for example, in [29, p. 6]. The reader may wish to revisit Example 3 after inspecting the material on product graphs in Section I.F.

Example 1 (Complete graph K_n). Let $\Gamma = K_n$ be the complete graph on n vertices. The Laplacians of K_n are given by

$$L(x,y) = \begin{cases} n-1, & x = y \\ -1, & x \neq y \end{cases} \qquad \text{and} \quad \mathcal{L} = \frac{1}{n-1} L,$$

since K_n is $(n-1)$-regular. L has eigenvector $\vec{1}$ with eigenvalue 0. Label the vertices $V(\Gamma) = \{1, \ldots, n\}$ and define f_i, for $i = 1, \ldots, n-1$, to be the vector which is 1 at vertex i, -1 at vertex $i+1$ and 0 elsewhere. Then the f_i's are linearly independent eigenvectors of L each with eigenvalue n. Since $\mathcal{L} = L/(n-1)$, $\mathcal{L}$ has the same eigenvectors with corresponding eigenvalues multiplied by $1/(n-1)$.

Example 2 (Complete bipartite graph $K_{m,n}$). Let Γ be the complete bipartite graph on $m+n$ vertices, where the vertex bipartition is the disjoint union $V(\Gamma) = A \cup B$ with $|A| = m$ and $|B| = n$. Then the Laplacians of K_n are given by

$$L(x,y) = \begin{cases} n, & x = y \text{ and } x \in A \\ m, & x = y \text{ and } x \in B \\ -1, & x \in A \text{ and } y \in B \\ 0, & \text{otherwise} \end{cases} \qquad \text{and}$$

$$\mathcal{L}(x,y) = \begin{cases} 1, & \text{x=y} \\ -1/\sqrt{mn}, & x \in A \text{ and } y \in B \\ 0, & \text{otherwise.} \end{cases}$$

Label the vertices of Γ by $A = \{1, \ldots, m\}$ and $B = \{m+1, \ldots, m+n\}$. For $i = 1, \ldots, m-1$ define the vector f_i to be 1 on vertex i, -1 on vertex $i+1$ and 0 elsewhere. For $j = m+1, \ldots, m+n-1$ define the vector g_j to be 1 on vertex j, -1 on vertex $j+1$ and 0 elsewhere. Define the vector h to be n on A and $-m$ on B. Then $\vec{1}$ is an eigenvector of L with eigenvalue 0, the f_i's are $m-1$ linearly independent eigenvectors of L with eigenvalue m, the g_j's are $n-1$ linearly independent eigenvectors of L with eigenvalue n, and h is an eigenvector of L with eigenvalue $m+n$.

Now define the vector h_1 to be $\sqrt{n}$ on A and $\sqrt{m}$ on B, and define the vector h_2 to be $\sqrt{n}$ on A and $-\sqrt{m}$ on B. Then h_1 is an eigenvector of $\mathcal{L}$ corresponding to eigenvalue 0, h_2 corresponds to eigenvalue 2, and the f_i's and g_j's already defined are eigenvectors of $\mathcal{L}$ all corresponding to eigenvalue 1.

The next example shows how the combinatorial structure of the graph may be exploited in order to compute the eigensystems of its Laplacians.

Example 3 (Hypercube Q_k). We require $k \geq 1$. The 2^k vertices of the hypercube Q_k can be labeled by the set of vectors $x = (x_1, \ldots, x_k) \in \{0,1\}^k$. Two vertices are adjacent iff their corresponding vectors differ in exactly one coordinate. The Laplacian of Q_k is given by

$$L(x,y) = \begin{cases} k, & x = y \\ -1, & x \sim y \\ 0, & \text{otherwise} \end{cases} \qquad \text{and} \quad \mathcal{L} = \frac{1}{k} L,$$

since Q_k is k-regular. The eigenvectors of L and $\mathcal{L}$ are the same, but the eigenvalues for $\mathcal{L}$ are obtained by multiplying those of L by $1/k$. From now on we concentrate on the eigensystem of L only.

Suppose for a fixed $j \in \{0, \ldots, k\}$ we could construct a vector f with the following property. For any vertex x, $f(y) = -f(x)$ for j neighbors y of x, and $f(y) = f(x)$ for the remaining $k-j$ neighbors y of x. If such a vector can be constructed, we would have

$$Lf(x) = k \cdot f(x) + j \cdot f(x) - (k-j) \cdot f(x) = 2j \cdot f(x),$$

showing f to be an eigenvector of L with eigenvalue $2j$.

In fact, there are 2^k ways to construct a set of orthogonal f's of the above form, and they can even be indexed by the vertices themselves in a natural way. Let $v \in \{0,1\}^k$ be a vertex. Define

$$f_v(x) \quad = \quad (-1)^{\langle v,x \rangle}.$$

Set $j = \langle v, v \rangle$ and consider the values of f_v on x and its neighbors $y \sim x$. If y differs from x in a coordinate i for which $v_i = 1$, then $f_v(y) = -f_v(x)$. Otherwise, $f_v(y) = f_v(x)$. Therefore x has j neighbors y for which $f_v(y) = -f_v(x)$ and $k - j$ neighbors y for which $f_v(y) = f_v(x)$, and so f_v is an eigenvector of L with eigenvalue $2j$.

To show that $\{f_v : v \in \{0,1\}^k\}$ is the entire set of eigenvectors of L, it suffices to show that $\langle f_u, f_v \rangle = 0$ for all $u \neq v$. This inner product is just the sum

$$\sum_{x \in \{0,1\}^k} f_u(x) f_v(x). \tag{I.11}$$

We show this sum is 0 by matching every vector x with a distinct vector y such that $f_u(x)f_v(x) = -f_u(y)f_v(y)$. The necessary matching is provided by finding the first coordinate i on which u and v differ, and then setting $y = x$ on all except the ith coordinate, at which $y_i = 1 - x_i$. Thus either $f_u(y) = -f_u(x)$ and $f_v(y) = f_v(x)$, or $f_u(y) = f_u(x)$ and $f_v(y) = -f_v(x)$, and the summands for x and y in (I.11) cancel. There are $\binom{k}{j}$ ways of choosing distinct vectors v with j 1's, and so the eigenvectors of L are $\{f_v : v \in \{0,1\}^k\}$, with $\binom{k}{j}$ orthogonal eigenvectors corresponding to eigenvalue $2j$. Additionally, we note that if $\hat{0}$ and $\hat{1}$ are the all 0's and all 1's vectors, respectively, then $f_{\hat{0}} = \vec{1}$, corresponding to eigenvalue 0, and $f_{\hat{1}}$ takes opposite values on any pair of adjacent vertices, and so corresponds to eigenvalue $2k$, achieving the maximum in Lemma I.1(iv).

I.C Dirichlet Laplacians and their spectra

Consider again a simple graph Γ, and suppose we wish to restrict our attention to only those functions $f : |V| \to \mathbb{R}$ which satisfy $f \equiv 0$ on a certain specified set of boundary vertices. Such a restriction is called a *Dirichlet boundary condition* for Γ.

In particular, let $S \subseteq V$ be a subset of the vertices of Γ. Then δS, or the set of *boundary vertices* of S, is defined by

$$\delta S = \{y \notin S : y \sim x \text{ and } x \in S\}.$$

The set of *boundary edges*, ∂S, is defined by

$$\partial S = \{\{x, y\} : x \in S, y \in \delta S\}.$$

$\Gamma(S)$ is the subgraph of Γ induced by S, and $E(S)$ is the set of edges in $\Gamma(S)$. We usually assume $V = S \cup \delta S$, revising our conception of the parent graph Γ if necessary. However, in general the choice of S partitions V into three sets: the "playing area" S, the "boundary" δS and the "spectators" $V \setminus (S \cup \delta S)$. The reason for this appellation of $V \setminus (S \cup \delta S)$ is that we generally ignore the behavior of functions on the "spectator" vertices, and are only concerned about their behavior on S and δS; however, for some graphs, such as the path with boundary in Section I.E.2, the behavior of functions on $V \setminus (S \cup \delta S)$ is important. We are particularly interested in cases in which $\Gamma(S)$ is connected and $\delta S \neq \emptyset$. It is also reasonable to think of cases in which every connected component of the subgraph induced by S is incident to a boundary vertex. Otherwise, we could consider a connected component of S not incident to any boundary vertices separately.

A function $f : V \to \mathbb{R}$ is a *Dirichlet function* provided that $f(x) = 0$ for $x \in V \setminus S$. Thus $f \equiv 0$ on the boundary δS, which is the Dirichlet boundary condition, and $f \equiv 0$ on $V \setminus (S \cup \delta S)$, since the region of importance is S. Define $D(\Gamma, S)$ as the set of such Dirichlet functions, which has dimension $|S|$ as a vector subspace of $\mathbb{R}^{|V|}$. We wish to consider those Dirichlet functions which behave like eigenfunctions on S; i.e., those Dirichlet functions f and g for which

$$\begin{aligned} Lf(x) &= \sigma f(x) \qquad \forall x \in S, \text{ and} \\ \mathcal{L}g(x) &= \lambda g(x) \qquad \forall x \in S. \end{aligned} \tag{I.14}$$

In this case f is a *Dirichlet eigenfunction* of L corresponding to *Dirichlet eigenvalue* σ, and similarly g is a Dirichlet eigenfunction of L corresponding to Dirichlet eigenvalue λ. When the context is clear, we may drop the adjective "Dirichlet"; also, eigenvectors and eigenfunctions will be used interchangeably. We do not require (I.14) to hold on δS for Dirichlet eigenfunctions, because Dirichlet functions are fixed at 0 on δS. In fact, forthcoming in Example 4 are Dirichlet eigenfunctions for which $Lf \neq \sigma f$ on the boundary δS.

Define the *Dirichlet Laplacian* L_S to be L restricted to the rows and columns of of S. The *Dirichlet normalized Laplacian* $\mathcal{L}_S$ and the *Dirichlet Laplace operator* Δ_S are defined similarly. Just as in (I.1), L_S, $\mathcal{L}_S$ and Δ_S are related by

$$\begin{aligned} L_S &= T^{1/2}\mathcal{L}_S T^{1/2} \;=\; T\Delta_S \\ \mathcal{L}_S &= T^{-1/2} L_S T^{-1/2} \;=\; T^{1/2}\Delta_S T^{-1/2} \\ \Delta_S &= T^{-1}L_S \;=\; T^{-1/2}\mathcal{L}_S T^{1/2}. \end{aligned}$$

The Laplace operator Δ_S again satisfies $\Delta_S = I - P$, where P is the transition probability matrix of a simple random walk on Γ, but now with absorbing states δS. The following Lemma, similar to Lemma 8.2 of [29], describes how a Dirichlet eigenfunction of a Laplacian can be considered simultaneously as an eigenfunction of the corresponding Dirichlet Laplacian. We define $f|_S$ to be the restriction of the function $f : V \to \mathbb{R}$ to the domain $S \subset V$.

Lemma I.4 (Dirichlet eigenfunctions). *A Dirichlet function $f : V \to \mathbb{R}$ is a Dirichlet eigenfunction of L iff $f|_S$ is an eigenfunction of L_S. Similarly, a Dirichlet function $g : V \to \mathbb{R}$ is a Dirichlet eigenfunction of $\mathcal{L}$ iff $g|_S$ is an eigenfunction of $\mathcal{L}_S$. Furthermore, the eigenvalue σ of L_S corresponding to f is given by (I.6); i.e.,*

$$\sigma \;=\; \frac{\sum_{x\sim y}(f(x)-f(y))^2}{\sum_x f^2(x)},$$

and the eigenvalue λ of $\mathcal{L}_S$ corresponding to g is given by (I.8); i.e.,

$$\lambda \;=\; \frac{\sum_{x\sim y}(f(x)-f(y))^2}{\sum_x f^2(x)d_x},$$

where $g = T^{1/2} f$.

Proof. We give the proof for L; the proof for $\mathcal{L}$ proceeds analogously. Let f be a Dirichlet function on Γ. Then for all $x \in S$

$$\begin{aligned} L_S f|_S(x) &= d_x f|_S(x) - \sum_{y\in S,\, y\sim x} f|_S(y) \\ &= d_x f(x) - \sum_{y\in V,\, y\sim x} f(y) \;=\; Lf(x). \end{aligned}$$

Thus for all $x \in S$, $Lf(x) = \sigma f(x)$ iff $L_S f|_S(x) = \sigma f|_S(x)$. The Rayleigh quotient of L_S shows that σ satisfies

$$\begin{aligned} \sigma &= \frac{\langle f|_S, L_S f|_S\rangle}{\langle f|_S, f|_S\rangle} = \frac{\sum_{x\in S} f|_S(x)\left(f|_S(x)d_x - \sum_{y\in S,\, y\sim x} f|_S(y)\right)}{\sum_{x\in S} f|_S^2(x)} \\ &= \frac{\sum_{\{x,y\}\in E(S)\cup\partial S}(f(x)-f(y))^2}{\sum_{x\in S} f^2(x)} = \frac{\sum_{\{x,y\}\in E(\Gamma)}(f(x)-f(y))^2}{\sum_x f^2(x)}, \end{aligned}$$

since $f \equiv 0$ on δS. □

This crucial observation allows us to simultaneously view Dirichlet eigenvectors as vectors acted upon by the corresponding Laplacian and as eigenvectors of the corresponding Dirichlet Laplacian. From now on, we may use f to represent both the function on V and its restriction $f|_S$ to S, if the context is clear. Letting $n = |S|$, we label the Dirichlet eigenvalues of L by $\sigma_1 \le \cdots \le \sigma_n$ with corresponding Dirichlet eigenvectors $\psi_1, \ldots, \psi_n$. Similarly, we label the Dirichlet eigenvalues of $\mathcal{L}$ by $\lambda_1 \le \cdots \le \lambda_n$ with corresponding Dirichlet eigenvectors $\phi_1, \ldots, \phi_n$. When it is necessary to distinguish Dirichlet eigenvalues and eigenvectors from non-Dirichlet eigenvalues and eigenvectors, we will write $\sigma_i^{(S)}$ or $\lambda_j^{(S)}$ for the Dirichlet eigenvalues and $\psi_i^{(S)}$ or $\phi_i^{(S)}$ for the Dirichlet eigenvectors. We start numbering the eigenvalues at 1 because whenever Γ is connected, $\sigma_1, \lambda_1 > 0$, as argued by the next Lemma.

Lemma I.5 (Dirichlet eigensystems of L and $\mathcal{L}$). *Let $n = |S|$ for $S \subsetneq V(\Gamma)$, and assume $\delta S = V \setminus S$. The following hold for the Dirichlet eigensystems of L and $\mathcal{L}$.*

(i) $\sum_{i=1}^n \sigma_i = vol(S)$, *and* $\sum_{i=1}^n \lambda_i \le n$.

(ii) L_S *and* $\mathcal{L}_S$ *are positive semidefinite, and so the* σ_i*'s and* λ_i*'s are real and nonnegative. Furthermore,* $\sigma_1, \lambda_1 > 0$ *iff every connected component of the subgraph* $\Gamma(S)$ *induced by* S *is incident to a vertex in* δS.

(iii) The subgraph $\Gamma(S)$ *induced by* S *has* i *boundary-less connected components if and only if* $\sigma_1 = \cdots = \sigma_i = \lambda_1 = \cdots = \lambda_i = 0$ *and* $\sigma_{i+1}, \lambda_{i+1} > 0$.

(iv) For all $1 \le i \le n$, *we have* $\sigma_i \le 2\,d_{\max}$ *and* $\lambda_i \le 2$. *Equality is achieved for* σ_n *if and only if there is a* $d_{\max}$*-regular bipartite connected component of* $\Gamma(S)$ *a boundary-less connected component of* $\Gamma(S)$ *is , and for* λ_n *if and only if a boundary-less connected component of* $\Gamma(S)$ *is bipartite.*

Proof. For (i), simply consider the traces of L_S and $\mathcal{L}_S$. The inequality is equality iff no vertex in S is isolated.

For (ii), note that Lemma I.4 expresses the σ_i's and λ_j's in terms of Rayleigh quotients of L and $\mathcal{L}$, respectively, which are all nonnegative. Therefore all Dirichlet eigenvalues are nonnegative. For the positivity of the smallest eigenvalues, we give a proof for the case of σ_1 and leave the similar computation for λ_1 to the reader. Using the Rayleigh quotient for L_S and Lemma (I.4), we have

$$\begin{aligned} \sigma_1 &= \min_{f|_S \neq 0} \frac{\langle f|_S, L_S f|_S \rangle}{\langle f|_S, f|_S \rangle} \\ &= \min_{f \in D(\Gamma,S), f \neq 0} \frac{\sum_{x \sim y} (f(x) - f(y))^2}{\sum_x f^2(x)}. \end{aligned}$$

The only way for σ_1 to be positive is for every Dirichlet eigenfunction f to have $f(x) \neq f(y)$ for some $\{x, y\} \in E(S) \cup \partial S$. In other words, $\sigma_1 > 0$ if and only if there does not exist a nonzero Dirichlet eigenfunction with $f(x) = f(y)$ for all $\{x, y\} \in E(S) \cup \partial S$, if and only if every connected component induced by S has at least one of its vertices adjacent to a vertex in the boundary δS.

For (iii), block diagonalize L_S and $\mathcal{L}_S$ first in terms of the boundary-less connected components of $\Gamma(S)$, and then any remaining vertices. The result is a block-diagonal matrix where all but the last block are Laplacians of connected graphs (without boundary), and the last block consists of connected components of $\Gamma(S)$ all having vertices incident to boundary vertices in δS. Lemma I.1(iii) shows that each of the blocks corresponding to a boundary-less graph yields exactly one eigenvalue of 0, and (ii) shows that the last block yields no zero eigenvalues. Therefore setting i equal to the number of boundary-less connected components of $\Gamma(S)$ gives the result.

The proof of (iv) follows directly from the proof of I.1(iv) by noting that requiring $f(x) = -f(y)$ for all connected components of $\Gamma(S)$ means that all such components incident to the boundary δS require $f \equiv 0$ on the component. Only on a boundary-less connected component of $\Gamma(S)$ can $f(x) = -f(y) \neq 0$, and equality be achieved. $\square$

Sometimes eigenfunctions will actually be Dirichlet eigenfunctions, but not always, as illustrated in the following example.

Example 4 (Transfer of eigenvectors). Consider the cycle C_4 on vertices $\{0,1,2,3\}$, and let $S=\{0,1,2\}$. Then $\delta S=\{3\}$, and the Laplacians L and L_S of C_4 are

$$L=\begin{bmatrix} 2 & -1 & 0 & -1 \\ -1 & 2 & -1 & 0 \\ 0 & -1 & 2 & -1 \\ -1 & 0 & -1 & 2 \end{bmatrix}, \quad \text{and} \quad L_S=\begin{bmatrix} 2 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 2 \end{bmatrix}.$$

L has eigenvectors $\psi_0=(1,1,1,1)$, $\psi_1=(1,0,-1,0)$, $\psi_2=(0,1,0,-1)$ and $\psi_3=(1,-1,1,-1)$ with eigenvalues 0, 2, 2 and 4, respectively. However, only $\psi_1=\psi_2^{(S)}$ is a Dirichlet eigenvector for L with respect to S and boundary δS. The other Dirichlet eigenvectors are $\psi_1^{(S)}=(1,\sqrt{2},1,0)$ and $\psi_3^{(S)}=(1,-\sqrt{2},1,0)$ with Dirichlet eigenvalues $2-\sqrt{2}$ and $2+\sqrt{2}$, respectively, giving $(\sigma_1^{(S)},\sigma_2^{(S)},\sigma_3^{(S)})=(2-\sqrt{2},2,2+\sqrt{2})$. Note in particular that $L\psi_1^{(S)}(4)\neq 0$ and $L\psi_3^{(S)}(4)\neq 0$, and so $\psi_1^{(S)}$ and $\psi_3^{(S)}$ are not eigenvectors of L. Furthermore, $2\pm\sqrt{2}$ are Dirichlet eigenvalues but not eigenvalues of L.

Because the Dirichlet eigenvalues arise from the principal submatrix L_S of L, they are controlled by the eigenvalues of L to a degree which depends upon the number of rows and columns deleted to obtain L_S. This is known as the *inclusion principle*, which appears in [73, Theorem 4.3.15], and is presented here in the context of the discussion.

Theorem I.6 (Inclusion principle). *Let $s=|S|$ and $n=|V|$ so that $n-s$ is the number of columns and rows deleted to obtain L_S from L. Then for each integer k such that $0\leq k\leq s-1$, we have*

$$\sigma_k \leq \sigma_{k+1}^{(S)} \leq \sigma_{k+n-s}. \tag{I.16}$$

Theorem I.6 could also be stated in terms of $\mathcal{L}$ and $\mathcal{L}_S$. Note that in Example 4, the inclusion principle guarantees a Dirichlet eigenvalue of 2, since there $2=\sigma_1\leq\sigma_2^{(S)}\leq\sigma_2=2$; the three Dirichlet eigenvalues are otherwise guaranteed to be staggered sequentially between the eigenvalues of L. Determining which Dirichlet eigenvalues of L are also eigenvalues is in general difficult, because as soon as the number of rows and columns deleted from L to obtain L_S increases past 1, the control given by (I.16) markedly decreases. There might be a Dirichlet eigenfunction $\psi^{(S)}$ of L corresponding to Dirichlet eigenvalue σ, where $\psi^{(S)}$ is not an eigenfunction of L but σ is an eigenvalue of L.

Whenever a Laplacian has an eigenspace of high dimension, if the Dirichlet Laplacian is large enough as a principal submatrix, Theorem I.6 guarantees Dirichlet eigenvectors with the same eigenvalue. However, we can exercise more care in how we treat the "spectator" region $V \setminus (S \cup \delta S)$ in order to construct more Dirichlet eigenfunctions from a high-dimensional eigenspace of a Laplacian. Let Ψ_σ be the eigenspace of L corresponding to eigenvalue σ, and let Φ_λ be the eigenspace of $\mathcal{L}$ corresponding to eigenvalue λ. For finite sets U and W with $U \subseteq W$ and a set of functions F mapping W to $\mathbb{R}$, define the restriction $F|_U := \{f|_U : f \in F\}$. The idea of the next theorem is to construct a Dirichlet eigenvector f with Dirichlet eigenvalue σ by choosing an eigenvector $f' \in \Psi_\sigma$ such that $f' \equiv 0$ on δS, and $f \in D(\Gamma, S)$ is defined to agree with f' on $S \cup \delta S$ as follows:

$$f(x) = \begin{cases} f'(x), & x \in S \cup \delta S \\ 0, & x \in V \setminus (S \cup \delta S). \end{cases}$$

The crucial observation is that the maximum number of linearly independent Dirichlet eigenfunctions constructed in this fashion depends only on the behavior of Ψ_σ on $S \cup \delta S$, and not on the "spectator" region $V \setminus (S \cup \delta S)$. This is an improvement over Theorem I.6, in which the number of linearly independent Dirichlet eigenvectors guaranteed to have a particular eigenvalue is limited by the size of $V \setminus (S \cup \delta S)$.

Theorem I.7 (Dirichlet eigenvector extraction). *The dimension of the set of Dirichlet eigenfunctions with Dirichlet eigenvalue σ which agree on $S \cup \delta S$ with eigenfunctions in Ψ_σ is*

$$\dim(D(\Gamma, S)|_{S \cup \delta S} \cap \Psi_\sigma|_{S \cup \delta S}) = \dim(\Psi_\sigma|_{S \cup \delta S}) - \dim(\Psi_\sigma|_{\delta S}) \qquad \text{(I.17)}$$

and similarly for $\mathcal{L}$,

$$\dim(D(\Gamma, S)|_{S \cup \delta S} \cap \Phi_\lambda|_{S \cup \delta S}) = \dim(\Phi_\lambda|_{S \cup \delta S}) - \dim(\Phi_\lambda|_{\delta S}).$$

Proof. We prove the result for L and note that the proof for $\mathcal{L}$ proceeds analogously. The left-hand side of (I.17) is the dimension of the vector subspace of Dirichlet eigenfunctions with Dirichlet eigenvalue σ which can be extracted as described previously. The proof proceeds by showing the two inequalities corresponding to

$$\dim(D(\Gamma, S)|_{S \cup \delta S} \cap \Psi_\sigma|_{S \cup \delta S}) + \dim(\Psi_\sigma|_{\delta S}) = \dim(\Psi_\sigma|_{S \cup \delta S}).$$

For ($\geq$), let $r = \dim(\Psi_\sigma|_{S\cup\delta S})$ and let $f_1, \ldots, f_r$ be linearly independent vectors in Ψ_σ whose restrictions to $S \cup \delta S$ are also linearly independent. Place $f_1, \ldots, f_r$ as rows of a matrix with columns indexed from the left by δS, S, and then $V \setminus (S \cup \delta S)$, and obtain a row echelon form of the matrix by Gaussian elimination. In the row echelon form, let $r_{\delta S}$ be the number of linearly independent rows with nonzero entries in columns indexed by δS, and let r_S be the number of linearly independent rows with only zero entries in columns indexed by δS (in particular, $r = r_S + r_{\delta S}$). Then by the properties of a row echelon matrix, $\dim(\Psi_\sigma|_{\delta S}) \geq r_{\delta S}$, and the restrictions to $S \cup \delta S$ of the bottom r_S rows lie within $D(\Gamma, S) \cap \Psi_\sigma|_{S\cup\delta S}$ and are also linearly independent, so $\dim(D(\Gamma, S)|_{S\cup\delta S} \cap \Psi_\sigma|_{S\cup\delta S}) \geq r_S$.

For ($\leq$), let $r_S = \dim(D(\Gamma, S)|_{S\cup\delta S} \cap \Psi_\sigma|_{S\cup\delta S})$ and let $r_{\delta S} = \dim(\Psi_\sigma|_{\delta S})$. Choose $f_1, \ldots, f_{r_S}$ to be linearly independent functions from $D(\Gamma, S)|_{S\cup\delta S} \cap \Psi_\sigma|_{S\cup\delta S}$. Then there exist linearly independent functions $f'_1, \ldots, f'_{r_S} \in \Psi_\sigma$, the restrictions of which are $f'_i|_{S\cup\delta S} = f_i$. Choose $g_1, \ldots, g_{r_{\delta S}}$ to be linearly independent functions from $\Psi_\sigma|_{\delta S}$. Then there exist linearly independent functions $g'_1, \ldots, g'_{r_{\delta S}} \in \Psi_\sigma$ such that $g'_i|_{\delta S} = g_i$. Now $\{f'_1|_{S\cup\delta S}, \ldots, f'_{r_S}|_{S\cup\delta S}, g'_1|_{S\cup\delta S}, \ldots, g'_{r_{\delta S}}|_{S\cup\delta S}\}$ are linearly independent by inspecting the linear combination

$$\sum_{j=1}^{r_S} a_j f'_j|_{S\cup\delta S} + \sum_{k=1}^{r_{\delta S}} b_k g'_k|_{S\cup\delta S} \;=\; 0.$$

Since $f'_j|_{S\cup\delta S} \equiv 0$ on δS for all $1 \leq j \leq r_S$, and the g'_k's are linearly independent on δS, $b_k = 0$ is forced for all $1 \leq k \leq r_{\delta S}$. Thus $a_j = 0$ is forced for all $1 \leq j \leq r_S$ since the $f'_j|_{S\cup\delta S}$'s are linearly independent. Therefore $dim(\Psi_\sigma|_{S\cup\delta S}) \geq r_S + r_{\delta S}$, which completes the proof. □

The practical usage of Theorem I.7 is the row reduction in the proof of the first inequality, which yields a linearly independent set of Dirichlet eigenvectors from the eigenspace. The proof of the second inequality shows that this set is as large as possible. This technique will be used in Lemma I.14 to derive the Dirichlet eigensystem of the path with boundary. In general, Dirichlet eigenfunctions and eigenvalues can be determined by applying the Courant-Fischer Theorem (cf. [73, Theorem 4.2.11]) to the Rayleigh quotient of the Dirichlet Laplacian, as in [29, p. 128].

Theorem I.8 (General Dirichlet eigenvalues and eigenvectors). *Let $n = |S|$ and let $1 \leq k \leq n$. Then the Dirichlet eigenvalue σ_k of L satisfies*

$$\sigma_k \quad = \quad \min_{f \neq 0, f \in D(\Gamma, S),\ f \perp \psi_1, \ldots, \psi_{k-1}} \frac{\sum_{x \sim y} (f(x) - f(y))^2}{\sum_x f^2(x)}, \tag{I.18}$$

where ψ_k is the Dirichlet eigenvector achieving σ_k, and the Dirichlet eigenvalue λ_k of $\mathcal{L}$ satisfies

$$\lambda_k \quad = \quad \min_{f \neq 0,\ T^{1/2} f \perp \phi_1, \ldots, \phi_{k-1}} \frac{\sum_{x \sim y} (f(x) - f(y))^2}{\sum_x f^2(x) d_x}, \tag{I.19}$$

where $\phi_k = T^{1/2} f$ for a vector f achieving λ_k is the Dirichlet eigenvector for λ_k.

I.D An eigenvalue diameter bound

Bounds involving the smallest positive eigenvalue of a Laplacian appear frequently in the literature in terms of graph diameter [33], expansion properties [3], and the isoperimetric number and Cheeger constant [98], for example. In this section, Lemma I.10 presents relationships between the diameter of a graph and the smallest positive eigenvalues of its Laplacians, L, L_S, $\mathcal{L}$ and $\mathcal{L}_S$. Variants of these results, which are almost folklore, have appeared in [3, 18, 29, 32]. Lemma I.10 follows easily from the next technical lemma, in which the Rayleigh quotients are minimized over a more general set than those used to obtain the first positive eigenvalues.

Lemma I.9. *Let Γ be a connected, simple graph with diameter D. For $\emptyset \neq U \subseteq V$, let $D^*(\Gamma, U)$ be the set of nonzero Dirichlet vectors $f \in D(\Gamma, U)$ which satisfy $f(u)f(v) \leq 0$ for some $u, v \in V$. Let $d \in \mathbb{R}^{|V|}$ be a nonnegative vector such that $f^2(x)d(x) > 0$ for at least one $x \in U$. Then*

$$\min_{f \in D^*(\Gamma, U)} \frac{\sum_{x \sim y} (f(x) - f(y))^2}{\sum_x f^2(x) d(x)} \quad \geq \quad \frac{1}{\sum_{x \in U} d(x) D}. \tag{I.20}$$

Proof. Let $f \in D^*(\Gamma, U)$ and choose $u_0 \in V$ to maximize $|f|$. The assumptions on u and v guarantee a choice of $v_0 \in V$ such that $f(u_0)f(v_0) \leq 0$. Let P be a simple shortest path in Γ from u_0 to v_0. Then

$$\frac{\sum_{x \sim y} (f(x) - f(y))^2}{\sum_x f^2(x) d(x)} \quad \geq \quad \frac{\sum_{\{x,y\} \in P} (f(x) - f(y))^2}{\sum_{x \in U} f^2(u_0) d(x)}$$

$$\geq \frac{\frac{1}{D}\left(\sum_{\{x,y\}\in P}(f(x)-f(y))\right)^2}{\sum_{x\in U} f^2(u_0)d(x)} \tag{I.21}$$

$$= \frac{\frac{1}{D}(f(u_0)-f(v_0))^2}{\sum_{x\in U} f^2(u_0)d(x)} \tag{I.22}$$

$$\geq \frac{1}{D\sum_{x\in U} d(x)},$$

where (I.21) is by Cauchy-Schwarz, (I.22) is by telescoping, and the last inequality is because $|f(u_0)-f(v_0)| \geq |f(u_0)|$. □

Lemma I.10 (Eigenvalue diameter bounds). *Let Γ be a connected, simple graph with diameter D. Let $\emptyset \neq S \subsetneq V$ induce a connected subgraph $\Gamma(S)$. Then the eigenvalues σ_1 and λ_1 and Dirichlet eigenvalues $\sigma_1^{(S)}$ and $\lambda_1^{(S)}$ are related to D as follows:*

(i) $\sigma_1 \geq 1/(|V|D)$,

(ii) $\sigma_1^{(S)} \geq 1/(|S|D)$,

(iii) $\lambda_1 \geq 1/(vol(\Gamma)D)$, *and*

(iv) $\lambda_1^{(S)} \geq 1/(vol(S)D)$.

Proof. We apply Lemma I.9 in all four cases. For σ_1 and $\sigma_1^{(S)}$, let $d(x)=1$, and for λ_1 and $\lambda_1^{(S)}$, let $d(x)=d_x$. Let $U=V$ for σ_1 and λ_1, and let $U=S$ for $\sigma_1^{(S)}$ and $\lambda_1^{(S)}$. The results all follow by noticing that the Rayleigh quotients (I.9), (I.18), (I.10) and (I.19) used to obtain the eigenvalues are minimized over a set of vectors which in each case is contained in $D^*(\Gamma, U)$. □

The fact that all four results follow from the generalized Lemma I.9 is strong evidence that there is room for improving these bounds. Nevertheless, the results are useful as is, and Lemma I.10(ii) will be cited later in Section III.B to bound the number of steps in a chip-firing game.

I.E Primary examples

In this section we consider the Laplacians of cycle graphs and the Dirichlet Laplacians of path graphs along with their eigensystems. We first derive eigensystems for cycle graphs by considering their Laplacians as special cases of a class of matrices called *circulant*. We then describe how a cycle can be mapped onto a path with boundary in order to obtain the eigensystem of the Dirichlet Laplacian of the path in terms of the eigensystem of the Laplacian of the cycle.

I.E.1 Circulants and cycles

A square matrix is *circulant* if each row is obtained by cycling the row above it to the right one position. It is straightforward to determine the eigensystem of a general circulant matrix using properties of roots of unity, and then to specialize to obtain eigensystems of Laplacians which happen to be circulant. We will proceed in this fashion to obtain the eigensystem of the cycle graph C_m.

For $k = 0, \ldots, n-1$, let $C^{(k)} = \left(c_{ij}^{(k)}\right)$ be the $m \times m$ square matrix satisfying

$$c_{ij}^{(k)} = \begin{cases} 1, & j - i \equiv k \pmod{m} \\ 0, & \text{otherwise.} \end{cases}$$

Therefore $C^{(k)}$ is simply the matrix which acts on a vector f by setting $C^{(1)} f(i) = f(i + k \pmod{m})$, and every circulant matrix M can be uniquely expressed as a sum $M = \sum_{k=0}^{n-1} b_k C^{(k)}$. We have the following well-known theorem.

Theorem I.11 (Eigensystem of a circulant matrix). *Let $M = \sum_{k=0}^{n-1} b_k C^{(k)}$ be an $m \times m$ circulant matrix whose rows and columns are indexed by $0 \le i, j < m$. Then an eigensystem of M is*

$$\left\{ \left(\sum_{k=0}^{m-1} b_k \theta^k, \Theta_\theta \right) : \theta^m = 1 \right\},$$

where θ ranges over all mth roots of unity, and Θ_θ is defined by $\Theta_\theta(i) = \theta^i$.

Proof. It suffices to show that for each $k \in \{0, \ldots, n-1\}$ and each θ an nth root of unity, Θ_θ is an eigenvector of $C^{(k)}$ corresponding to eigenvalue θ^k. In this event, Θ_θ is simultaneously an eigenvector for each $C^{(k)}$, and the eigenvalue of Θ_θ for M is taken directly from the coefficients describing M as a linear combination of the $C^{(k)}$'s. Now fix k and θ and note that

$$C^{(k)} \Theta_\theta(i) = \Theta_\theta \left(i + k \pmod{m} \right)$$

$$= \theta^{i+k}$$

$$= \theta^k \Theta_\theta(i),$$

for all $0 \leq i < m$, which completes the proof. $\square$

This theorem immediately raises the question of which graphs have Laplacians which are circulant. We now define the class of graphs which corresponds to the circulant Laplacians.

Definition 1 (Circulant graphs). A simple graph Γ on m vertices $V(\Gamma) = \{0, \ldots, m-1\}$ is a *circulant graph* provided there is a set $S \subseteq \{1, \ldots, \lfloor m/2 \rfloor\}$ such that $\{i, j\} \in E(\Gamma)$ iff $i - j \pmod{m} \in S$ or $m - (i - j \pmod{m}) \in S$.

Therefore the *cycle graph* C_m with vertices $V(C_m) = \{0, \ldots, m-1\}$ is a circulant graph with $S = \{1\}$, and the complete graph K_m is a circulant graph with $S = \{1, \ldots, \lfloor m/2 \rfloor\}$. The next lemma characterizes the relationship between circulant graphs and circulant matrices.

Lemma I.12 (Circulant Laplacians are from circulant graphs). *The Laplacian of a simple graph Γ is circulant if and only if Γ is a circulant graph.*

Proof. As in the discussion, let the vertex set be $\{0, \ldots, m-1\}$. L is circulant if and only if $L = \sum_{k=0}^{m-1} b_k C^{(k)}$ and $b_k = b_{m-k} \in \{0, 1\}$ for $0 < k < m$. But this occurs if and only if $\{i, j\} \in E(\Gamma)$ exactly when $i - j \equiv k \pmod{m}$ or $i - j \equiv m - k \pmod{m}$ for those $0 < k < m$ for which $b_k = 1$. This is true if and only if Γ is a circulant matrix on m vertices where $S = \{k : 0 < k \leq \lfloor m/2 \rfloor \text{ and } b_k = 1\}$. $\square$

Since all circulant graphs are regular of degree $-\sum_{k=1}^{m-1} b_k$ in the circulant representation, the normalized Laplacian $\mathcal{L}$ satisfies $\mathcal{L} = L/b_0$, and determining the eigensystem of L or $\mathcal{L}$ are essentially equivalent. We now present the eigensystem of the cycle graph C_m which will be used in Chapter II.

Lemma I.13 (Eigensystem of C_m). *Let $m \geq 3$. The normalized Laplacian $\mathcal{L}$ of the cycle graph C_m on vertices $\{0, \ldots, m-1\}$ has orthonormal eigensystem*

$$\left\{ \left(1 - \cos\left(\frac{2\pi j}{m} \right), \phi_j \right) : 0 \leq j < m \right\},$$

where

$$\phi_j(x) = \frac{1}{\sqrt{m}} \exp\left(-i\frac{2\pi jx}{m}\right).$$

Proof. C_m is a circulant matrix, and $\mathcal{L}$ is circulant with representation $\mathcal{L} = \sum_{k=0}^{m-1} b_k C^{(k)}$, where $b_0 = 1$ and $b_1 = b_{m-1} = -1/2$. By Lemma I.11, each mth root of unity θ contributes an eigenvalue $1 - (\theta^1 + \theta^{m-1})/2$ with corresponding eigenvector Θ_θ defined by $\Theta_\theta(x) = \theta^x$. We write the roots of unity as $\theta_0, \ldots, \theta_{m-1}$ where $\theta_j = \exp(-2\pi ji/m)$ to see that $\Theta_\theta(x) = \exp(-2\pi jxi/m)$ is an eigenvector of $\mathcal{L}$ corresponding to eigenvalue

$$\begin{aligned} 1 - \frac{\theta^1 + \theta^{m-1}}{2} &= 1 - \frac{\exp\left(-i\frac{2\pi j}{m}\right) + \exp\left(i\frac{2\pi j}{m}\right)}{2} \\ &= 1 - \cos\left(\frac{2\pi j}{m}\right). \end{aligned}$$

We verify that we have an orthonormal eigensystem by checking the inner product of two eigenvectors as follows. Let $j_1, j_2 \in \{0, \ldots, m-1\}$, and compute

$$\begin{aligned} \langle \phi_{j_1}, \phi_{j_2} \rangle &= \sum_{x=0}^{m-1} \phi_{j_1}(x)\overline{\phi_{j_2}(x)} \\ &= \sum_{x=0}^{m-1} \frac{1}{m} \exp\left(i\frac{2\pi(j_2 - j_1)x}{m}\right) \\ &= \sum_{x=0}^{m-1} \frac{1}{m} \theta_{j_1 - j_2}^x \;=\; \chi(j_1 = j_2), \end{aligned}$$

since any m consecutive integral powers of any nontrivial mth root of unity cancel additively. □

I.E.2 Paths with boundary

The *path graph* with boundary P_m can be thought of as a contiguous piece of a very large cycle on the vertices $V = \{\ldots, 0, 1, \ldots, m, m+1, \ldots\}$ where $S = \{1, \ldots, m\}$ and the boundary is $\delta S = \{0, m+1\}$. In this formulation P_m is a regular graph, and the Dirichlet Laplacian of P_m is a $m \times m$ tri-diagonal matrix with 2's on the main diagonal and -1's on the sub- and super-diagonals. The Dirichlet normalized Laplacian is obtained by multiplying by $1/2$. Thus the Dirichlet Laplacians are both tri-diagonal and *Toeplitz*; that is, having all entries m_{ij} depend only on $i - j$ [73, p. 27]. The latter is important because information about the eigensystem of a Toeplitz matrix can be gleaned by studying a corresponding circulant matrix; however, we will take a different approach below for P_m.

Subjectively, we will see that the Dirichlet eigenvectors of the Laplacian of P_m can be thought of as standing waves, anchored on either side at vertex 0 and $m+1$. Indeed, if we think of the vertices $\{0,\ldots,m+1\}$ as having equal horizontal spacing along a string of length $m+1$ held fixed at both ends, the Dirichlet eigenvectors are obtained by reading off the values of the first m harmonics of the string at the the vertices. Thus we will show that the harmonics

$$\sin\left(\frac{k\pi x}{m+1}\right), \qquad (k=1,\ldots,m)$$

are the Dirichlet eigenvectors for P_m. For an introduction to standing waves, see [61], for example.

We now compute the Dirichlet eigensystem of P_m by extracting Dirichlet eigenvectors from the eigenspaces of $C_{2(m+1)}$, following theorem I.7.

Lemma I.14 (Dirichlet eigensystem for P_m). *Let $m \geq 1$. The normalized Laplacian $\mathcal{L}_S$ of the path P_m on vertices $\{1,\ldots,m\}$ with boundary $\{0,m+1\}$ has orthonormal eigensystem*

$$\left\{\left(1-\cos\left(\frac{\pi j}{m+1}\right),\phi_j\right) : 1 \leq j < m\right\},$$

where

$$\phi_j(x) = \sqrt{\frac{2}{m+1}}\sin\left(\frac{j\pi x}{m+1}\right).$$

Proof. Consider the cycle $C_{2(m+1)}$ on vertices $\{0,\ldots,2m+1\}$, for which the eigenspaces Φ_{λ_j} of the normalized Laplacian $\mathcal{L}$ are given by Lemma I.13. For $1 \leq j \leq m$, $\lambda_j = \lambda_{2(m+1)-j} = 1-\cos\left(\pi j/(m+1)\right)$, and Φ_{λ_j} is 2-dimensional, spanning the set

$$\{\phi_{\lambda_j},\phi_{\lambda_{2(m+1)-j}}\} \;=\; \left\{\exp\left(-i\frac{\pi j x}{m+1}\right),\exp\left(i\frac{\pi j x}{m+1}\right)\right\}.$$

Define the path P_m by letting $S=\{1,\ldots,m\}$, so that $\delta S=\{0,m+1\}$, and the "spectator" region is $V\setminus(S\cup\delta S) = \{m+2,\ldots,2m+1\}$. Following the row reduction step in Theorem I.7, notice that $\phi_{\lambda_j}(0) = \phi_{\lambda_{2(m+1)-j}}(0) \neq 0$ and that $\phi_{\lambda_j}(m+1) = \phi_{\lambda_{2(m+1)-j}}(m+1) \neq 0$. Thus $\dim(\Phi_{\lambda_j})|_{\delta S} = 1$. Note further that $\phi_{\lambda_j}(1) \neq \phi_{\lambda_{2(m+1)-j}}(1)$. Therefore $\dim(\Phi_{\lambda_j})|_{S\cup\delta S} = 2$, and $\phi_j^{(S)} := \phi_{\lambda_j} - \phi_{\lambda_{2(m+1)-j}}$ is a Dirichlet eigenvector for P_m corresponding to Dirichlet eigenvalue $\lambda_j^{(S)} = \lambda_j$. As j ranges over $\{1, \ldots, m\}$, the $\lambda_j^{(S)}$'s are distinct, and so the $\phi_j^{(S)}$'s are orthogonal. The coefficient $\sqrt{2/(m+1)}$ is precisely what is necessary for normalization. □

I.F Product graphs

Most product graphs are constructed by choosing two factor graphs and building edges on the Cartesian Product of the vertex sets of the two factor graphs according to some rule. Various such rules and their resulting product graph formulations appear in [71, 75]. Here, we consider the *graph Cartesian Product*, defined as follows. Let $\Gamma(V, E)$ and $\Gamma'(V', E')$ be simple graphs. The graph Cartesian Product $\Gamma \times \Gamma'$ has vertex set $V^\times := V(\Gamma \times \Gamma') = V \times V'$ and edge set

$$\begin{aligned} E^\times := E(\Gamma \times \Gamma') &= \{\{(x, x'), (y, x')\} : \{x, y\} \in E(\Gamma)\} \\ &\quad \bigcup \{\{(x, x'), (x, y')\} : \{x', y'\} \in E(\Gamma')\}. \end{aligned}$$

From now on we will simply refer to the graph Cartesian Product as the product of graphs. The Laplacian $L^\times$ of $\Gamma \times \Gamma'$ is

$$L^\times((x, x'), (y, y')) = \begin{cases} d_{(x,x')}, & \text{if } (x, x') = (y, y') \\ -1, & \text{if } x = y \text{ and } x' \sim y' \\ -1, & \text{if } x \sim y \text{ and } x' = y' \\ 0, & \text{otherwise,} \end{cases}$$

where $d_{(x,x')} = d_x + d_{x'}$. Examples of graphs with a high degree of product structure include tori (products of cycles), grids (products of paths), and hypercubes (repeated products of a single edge). Processes on these sorts of product graphs can often be broken down into processes on the constituent factor graphs (e.g., [46]).

If factor graphs Γ and Γ' are presented along with specified subsets $S \subseteq V(\Gamma)$ and $S' \subseteq V'(\Gamma')$, we may consider the Dirichlet version of the product graph. The "playing area" of $\Gamma \times \Gamma'$ is $S_\times := S \times S'$, the "boundary" is $\delta S^\times = S \times \delta S' \cup \delta S \times S'$, and the "spectator area" is

$$V^\times \setminus (S^\times \cup \delta S^\times) = \big(\delta S \times \delta S'\big) \cup \big(V \times V' \setminus (S' \cup \delta S')\big) \cup \big(V \setminus (S \cup \delta S) \times V'\big),$$

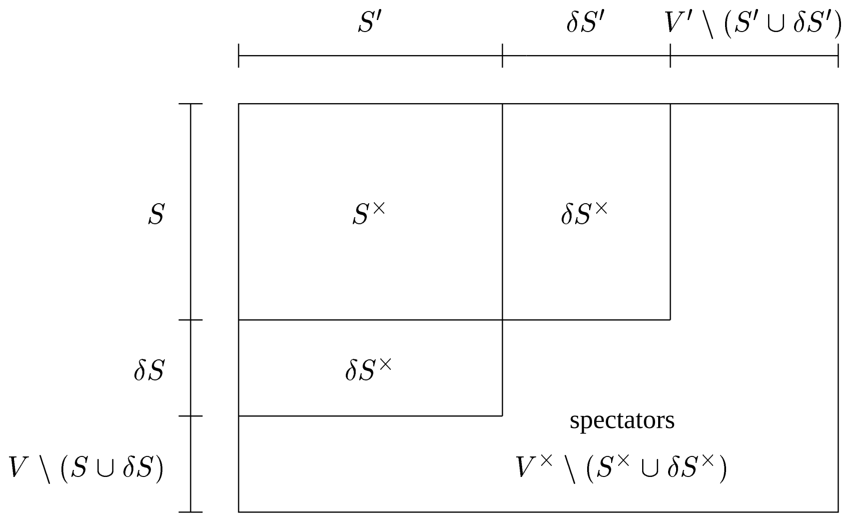

Figure I.1: Regions of a product graph whose factor graphs have boundary

as illustrated in Figure I.1. Of course, the playing area $S^\times$ of a product graph could be chosen after the graph is constructed, but we are primarily interested in the case where $S^\times$ is induced by S and S' in the factor graphs. Moreover, all definitions and results on Dirichlet Laplacians hold for product graphs with boundary conditions.

When both factor graphs are regular, the eigensystem of the Laplacians the product graph can be easily recovered from knowledge of the eigensystems of the Laplacians of the factors. This can be done for both Laplacians and Dirichlet Laplacians, and when the factor graphs are both regular but not of the same degree. In terms of boundary, there are three cases of product graphs: the product of two graphs with boundary ($S \subsetneq V$, $S' \subsetneq V'$), the product of a graph with boundary and a graph without boundary ($S \subsetneq V$, $S' = V'$), and the product of two graphs without boundary ($S = V$, $S' = V'$). Here a graph without boundary condition is denoted, without loss of generality, by specifying $S = V$. The three cases are combined in the following lemma, which is presented for the normalized Laplacian $\mathcal{L}$.

Lemma I.15. *Let Γ and Γ' be d- and d'-regular, respectively. Let $S \subseteq V$ and $S' \subseteq V'$. Suppose orthonormal eigensystems of the normalized Laplacians $\mathcal{L}_S$ of Γ and $\mathcal{L}'_{S'}$ of Γ' are given by $\{(\lambda_j, \phi_j) : j \in J\}$ and $\{(\lambda'_k, \phi'_k) : k \in K\}$, respectively. Then an orthonormal* *eigensystem of the normalized Laplacian* $\mathcal{L}^{\times}_{S\times S'}$ *of* $\Gamma\times\Gamma'$ *is*

$$\{(\Lambda_{j,k},\Phi_{j,k}) : j\in J, k\in K\} := \left\{\left(\frac{d}{d+d'}\lambda_j+\frac{d'}{d+d'}\lambda'_k,\phi_j\phi_k\right) : j\in J, k\in K\right\}.$$

Proof. Let $(x,y)\in S^{\times}=S\times S'$. By definition of the product graph,

$$\begin{aligned}
\mathcal{L}^{\times}_{S^\times}\Phi_{j,k}((x,x')) &= \Phi_{j,k}((x,x')) - \sum_{(y,y')\in S^\times,(y,y')\sim(x,x')}\frac{\Phi_{j,k}((y,y'))}{d+d'}\\
&= \phi_j(x)\phi'_k(x') - \sum_{y\in S,y\sim x}\frac{\phi_j(y)\phi'_k(x')}{d+d'} - \sum_{y'\in S',y'\sim x'}\frac{\phi_j(x)\phi'_k(y')}{d+d'}\\
&= \frac{d\phi'_k(x')}{d+d'}\left(\phi_j(x)-\sum_{y\in S,y\sim x}\frac{\phi_j(y)}{d}\right)\\
&\quad +\frac{d'\phi_j(x)}{d+d'}\left(\phi'_k(x')-\sum_{y'\in S',y'\sim x'}\frac{\phi'_k(y')}{d'}\right)\\
&= \left(\frac{d\lambda_j}{d+d'}+\frac{d'\lambda'_k}{d+d'}\right)\Phi_{j,k}((x,y)),
\end{aligned}$$

and so $\Phi_{j,k}$ is an eigenvector of $\mathcal{L}^{\times}_{S^\times}$ corresponding to eigenvalue $\Lambda_{j,k}=(d\lambda_j+d'\lambda'_k)/(d+d')$. Secondly, choose two eigenvectors Φ_{j_1,k_1} and Φ_{j_2,k_2} and note that

$$\begin{aligned}
\langle\Phi_{j_1,k_1},\Phi_{j_2,k_2}\rangle &= \sum_{(x,x')\in S^\times}\phi_{j_1}(x)\phi'_{k_1}(x')\overline{\phi_{j_2}(x)\phi'_{k_1}(x')}\\
&= \sum_{x\in S}\phi_{j_1}(x)\overline{\phi_{j_2}(x)}\sum_{x'\in S'}\phi'_{k_1}(x')\overline{\phi'_{k_1}(x')}\\
&= \langle\phi_{j_1},\phi_{j_2}\rangle\left\langle\phi'_{k_1},\phi'_{k_2}\right\rangle = \chi(j_1=j_2)\cdot\chi(k_1=k_2),
\end{aligned}$$

and so the Φ's form an orthonormal eigensystem. □

Whenever Γ is d-regular, the normalized Laplacian $\mathcal{L}_S$ and the Laplacian L_S are related by $\mathcal{L}_S=L_S/d$, and so the two matrices have the same eigenvectors, except that the corresponding eigenvalues of L_S are those of $\mathcal{L}_S$ multiplied by d. This property allows the derivation of the eigensystem of $L^{\times}_S$ from Lemma I.15.

Corollary I.16. *Under the same conditions as Lemma I.15, an orthonormal eigensystem of* $L^{\times}_{S^\times}$ *is*

$$\{(\Sigma_{j,k},\Psi_{j,k}) : j\in J, k\in K\} := \left\{\left(\sigma_j+\sigma'_k,\phi_j\phi_k\right) : j\in J, k\in K\right\},$$

where $\sigma_j=d\lambda_j$ *and* $\sigma'_k=d'\lambda'_k$.

Proof. The result follows easily from the facts that $L_S = d\mathcal{L}_S$, $L_{S'} = d'\mathcal{L}_{S'}$, and $L^{\times}_{S\times S'} = (d+d')\mathcal{L}^{\times}_{S\times S'}$. ☐

Because the Cartesian product of two graphs is associative, a graph formed by repeated products may written as the repeated product of factor graphs in arbitrary order. An orthonormal eigensystem of $\mathcal{L}^{\times}$ for the graph product $\Gamma^{(1)} \times \cdots \times \Gamma^{(t)}$, where $\Gamma^{(s)}$ is d_s-regular, is

$$\{(\Lambda_{j_1,\ldots,j_t}, \Phi_{j_1,\ldots,j_t}) : j_s \in J_s\} := \left\{ \left(\frac{d_1\lambda^{(1)}_{j_1} + \cdots + d_t\lambda^{(t)}_{j_t}}{d_1 + \cdots + d_t}, \phi_{j_1} \cdots \phi_{j_t} \right) : j_s \in J_s \right\}, \quad \text{(I.23)}$$

given that orthonormal eigensystems of $\mathcal{L}^{(s)}$ for $\Gamma^{(s)}$ are $\{(\lambda^{(s)}_{j_s}, \phi^{(s)}_{j_s}) : j_s \in J_s\}$, for $1 \le s \le t$. This fact holds even when $S^{(s)} \subseteq V^{(s)}$ determines the boundary condition for $\Gamma^{(s)}$; also, multiplying all eigenvalues through by the degree $\sum_{s=1}^{t} d_s$ of the corresponding regular product graph, as in Corollary I.16, yields the result for the Laplacian $L^{\times}$. Note that the hypercube Q_k is the product of k edges, or more formally, k K_2's; Example 3 could be completely re-derived in terms of Lemma I.15 and (I.23), using the eigensystem $\{(0, [1,1]^T), (2, [1,-1]^T)\}$ of the Laplacian of K_2.

We now present specific examples of product graphs with and without boundary which will reappear in Chapter II. All factors involved in these product graphs will be either cycles without boundary (Section I.E.1), or paths with boundary (Section I.E.2). If the product of t such factors is viewed as being laid out on the grid $\mathbb{Z}_{S^{(1)}} \times \cdots \times \mathbb{Z}_{S^{(t)}}$, a cycle factor provides a periodic boundary condition in its coordinate, and a path factor provides an absorbing boundary condition in its coordinate.

I.F.1 Tori

The t-dimensional torus $C_{m_1} \times \cdots \times C_{m_t}$, where $m_s \ge 3$ for $1 \le s \le t$, is the graph product of t factors which are all cycles. Using (I.23) and I.13 for the eigensystem of each factor, the eigensystem for the normalized Laplacian $\mathcal{L}^{\times}$ of $C_{m_1} \times \cdots \times C_{m_t}$ is given in the next lemma.

Lemma I.17 (Eigensystem for Tori). *An orthonormal eigensystem of the normalized Laplacian $\mathcal{L}^{\times}$ of the t-dimensional torus $C_{m_1} \times \cdots \times C_{m_t}$, where $m_s \ge 3$ for $1 \le s \le t$,* *is*

$$\left\{\left(\frac{1}{t}\sum_{s=1}^{t}\left(1-\cos\left(\frac{2\pi j_s}{m_s}\right)\right),\Phi_{j_1,\ldots,j_t}\right):0\le j_s<m_s,1\le s\le t\right\},$$

where for $(x_1,\ldots,x_t)\in\{0,\ldots,m_1-1\}\times\cdots\times\{0,\ldots,m_t-1\}=V^\times$,

$$\Phi_{j_1,\ldots,j_t}((x_1,\ldots,x_t))=\frac{1}{\sqrt{m_1\cdots m_t}}\exp\left(-2\pi i\sum_{s=1}^{t}\frac{j_s x_s}{m_s}\right).$$

The eigensystem of the Laplacian $L^\times$ of the t-dimensional torus is obtained from Lemma I.17 by multiplying the eigenvalues by $2t$, as the torus is $2t$-regular.

I.F.2 Grids with boundary

The t-dimensional grid $P_{m_1}\times\cdots\times P_{m_t}$, where $m_s\ge 1$ for $1\le s\le t$, is the graph product of t factors of paths with boundary. Thus travelling in either direction on a single coordinate of the grid will eventually reach the boundary. Unlike the cycle on 1 or 2 vertices, the paths P_1 and P_2 are simple graphs, and so we may consider the cases $m_s=1,2$. Having a factor of P_1 is an interesting case, because it means that every point in the resulting grid will be adjacent to the boundary in either direction on P_1's coordinate. The "playing area" $S^\times$ of the grid is simply $\{1,\ldots,m_1\}\times\cdots\times\{1,\ldots,m_t\}$. Using (I.23) and Lemma I.14 for the eigensystem of each factor, the eigensystem for the normalized Dirichlet Laplacian $\mathcal{L}^\times_{S^\times}$ of $P_{m_1}\times\cdots\times P_{m_t}$ is given in the next lemma.

Lemma I.18 (Dirichlet Eigensystem for Grids). *An orthonormal eigensystem of the normalized Dirichlet Laplacian* $\mathcal{L}^\times_{S^\times}$ *of the* t*-dimensional grid* $P_{m_1}\times\cdots\times P_{m_t}$*, where* $m_s\ge 1$ *for* $1\le s\le t$*, is*

$$\left\{\left(\frac{1}{t}\sum_{s=1}^{t}\left(1-\cos\left(\frac{\pi j_s}{m_s+1}\right)\right),\Phi_{j_1,\ldots,j_t}\right):1\le j_s\le m_s,1\le s\le t\right\},$$

where for $(x_1,\ldots,x_t)\in\{1,\ldots,m_1\}\times\cdots\times\{1,\ldots,m_t\}=S^\times$,

$$\Phi_{j_1,\ldots,j_t}((x_1,\ldots,x_t))=\frac{2^{t/2}}{\sqrt{(m_1+1)\cdots(m_t+1)}}\prod_{s=1}^{t}\sin\left(\frac{j_s\pi x}{m_s+1}\right).$$

The eigensystem of the Laplacian $L^\times_{S^\times}$ of the t-dimensional grid is obtained from Lemma I.18 by multiplying the eigenvalues by $2t$, as the grid is $2t$-regular.

I.F.3 Hybrids

The product graph construction and Lemma I.15, which describes how to generate the eigensystem of the product graph's Laplacian, do not require the factor graphs to be of the same class. Factor graphs may be chosen from any class of simple regular graphs with any choice of boundary conditions. Products of cycles and paths are of particular interest because the structure of the "playing area" is naturally a finite rectangular grid with absorbing or periodic boundary on any given coordinate. Examples of physical applications for which the underlying structure of the model is a product graph of this general hybrid class are the Ising [104] Potts [120], and sandpile models [6, 7, 45]. One interesting intersection of vertex-transitive (degree-regular) graph products, the Potts model, and the Cheeger constant appears in [107], which investigates phase transitions on general homogeneous lattices.

Chapter II

Discrete Green's Functions for Products of Regular Graphs

Discrete Green's functions are the inverses or pseudo-inverses of combinatorial Laplacians, which were introduced and discussed in Chapter I. Green's functions in the continuous case are used in the solution of differential equations; the seminal work on Green's functions is [70], summarized more recently in [69]. A treatment of Green's functions for partial differential equations can be found in [106]. Examples of contributions to the literature in which the Green's function is computed or approximated for a discrete region are [42, 84, 85]. The first major work on discrete Green's functions as the (pseudo-)inverses of combinatorial Laplacians is [35], wherein formulas are found for general families of graphs, and the Green's function is used to solve the discrete Laplace equation. Just as Green's functions in the continuous case depend on the domain and boundary conditions, discrete Green's functions are associated with the underlying graph and boundary conditions, if any. Thus a new set of discrete Green's functions must be determined for each new class of graphs. Certainly, a discrete Green's function can be determined by brute force (pseudo-)inversion of the corresponding Laplacian, but this is no advancement toward compact or closed-form functions.

In this chapter, we consider such compact formulas for discrete Green's functions. Results are illustrated with the cycle, torus, and the t-dimensional torus. Section II.A presents the necessary definitions and background. Section II.B illustrates these definitions by deriving the Green's function for the cycle. In Section II.C, we derive formulas for products of regular graphs with or without boundary, extending a result of [29]. In Section II.D, we illustrate the case of products of regular graphs without boundary by deriving the Green's function for the t-dimensional torus and addressing its computational complexity, with explicit Green's functions given for $t = 2$ and $t = 3$. The hitting time for a random walk on the torus is discussed in Section II.E.

II.A Preliminaries

The necessary definitions related to Laplacians L, $\mathcal{L}$ and Δ, and Dirichlet Laplacians L_S, $\mathcal{L}_S$ and Δ_S, are found in Chapter I, primarily in Sections I.A and I.C. We again consider a simple connected graph Γ, and for the Dirichlet versions specify a subset $S \subseteq V = V(\Gamma)$, whose boundary vertices are $\delta S = \{y \notin S : y \sim x \text{ and } x \in S\}$. For simplicity, we take the subgraph generated by S to be connected.

When $S \subsetneq V$, L_S, $\mathcal{L}_S$ and Δ_S are invertible, and the *Green's function* G, the *normalized Green's function* $\mathcal{G}$ and the *fundamental matrix* Z are defined by their relations with the corresponding Dirichlet Laplacians:

$$\begin{aligned} L_S G &= G L_S = I_S \\ \mathcal{L}_S \mathcal{G} &= \mathcal{G} \mathcal{L}_S = I_S \\ \Delta_S Z &= Z \Delta_S = I_S. \end{aligned} \tag{II.1}$$

Therefore by (I.1) on p. 4, the Green's functions are related to one another as follows:

$$\begin{aligned} G &= T^{-1/2} \mathcal{G} T^{-1/2} = Z T^{-1} \\ \mathcal{G} &= T^{1/2} G T^{1/2} = T^{1/2} Z T^{-1/2} \\ Z &= G T = T^{-1/2} \mathcal{G} T^{1/2}. \end{aligned} \tag{II.2}$$

We say that Z is the fundamental matrix because of the literature on random walks (e.g., [1]), but we may also think of Z as the discrete Green's function corresponding to the Dirichlet Laplace operator Δ_S. We can tie these definitions to random walks as follows. Let $P = [p_{xy}]$ be the transition probability matrix for the simple irreducible *transient* random walk on S with absorbing states δS, where the probability p_{xy} of moving to state y from state x is $1/d_x$ if x and y are adjacent and 0 otherwise. Then $\Delta_S = I - P$, and

$(I-P)^{-1} = I + P + P^2 + \cdots$ gives

$$Z(x,y) = \sum_{n\geq 0} P_n(x,y), \tag{II.3}$$

where $P_n(x,y)$ is the n-step transition probability matrix (cf. [112, p. 31]).

When the graph has no boundary vertices, which may be thought of as when $S = V$, the Laplacians are not invertible, and we require an alternate definition of the Green's functions. Recalling the properties and labeling of the eigensystems of L and $\mathcal{L}$ from Section I.A, we define G, $\mathcal{G}$ and Z as follows:

$$\begin{aligned} G &= \sum_{\sigma_i>0} \frac{1}{\sigma_i}\psi_i\psi_i^*, \\ \mathcal{G} &= \sum_{\lambda_j>0} \frac{1}{\lambda_j}\phi_j\phi_j^*, \\ Z &= T^{-1/2}\mathcal{G}T^{1/2}. \end{aligned} \tag{II.4}$$

Throughout the chapter, we omit the subscript of S from the non-singular Green's functions because the presence or absence of a boundary condition can be determined from the Laplacian it is associated with. In (II.4), the ψ_i's and ϕ_j's are taken to be orthonormal eigenvectors of L and $\mathcal{L}$, respectively, and as usual ψ_i and ϕ_j correspond to eigenvalues σ_i and λ_j, respectively. Recall from Sections I.A and I.C that the eigenvalues are labeled in increasing order. Since L and $\mathcal{L}$ are real Hermitian, the ψ's and ϕ's could be chosen to have all real entries, but sometimes a more natural eigenvector is preferred (e.g., Lemma I.13). The definitions of G and $\mathcal{G}$ in II.4 are equivalent to the two pairs of relations

$$\begin{aligned} GL = LG &= I - R_0 = I - \psi_0\psi_0^*, \\ \text{and} \quad GR_0 &= 0; \\ \mathcal{G}\mathcal{L} = \mathcal{L}\mathcal{G} &= I - \mathcal{R}_0 = I - \phi_0\phi_0^*, \\ \text{and} \quad \mathcal{G}\mathcal{R}_0 &= 0, \end{aligned} \tag{II.5}$$

where $R_0 = \psi_0\psi_0^*$ is the rank 1 projection of ψ_0, and $\mathcal{R}_0 = \phi_0\phi_0^*$ is the rank 1 projection of ϕ_0. By Lemma I.2 in Section I.A,

$$\begin{aligned} R_0 &= \frac{1}{|V|}J, \qquad \text{and} \\ \mathcal{R}_0(x,y) &= \frac{\sqrt{d_x d_y}}{vol(\Gamma)} \quad \forall x,y \in V. \end{aligned}$$

It is also important to note that when $\mathcal{G}$ is invertible, the definitions in (II.1) and (II.4) are equivalent; we simply consider the sums in (II.4) over the Dirichlet eigensystems. The definition of the fundamental matrix Z in II.4 is exactly what is required to have the relations

$$\begin{aligned} Z\Delta &= \left(T^{-1/2}\mathcal{G}T^{1/2}\right)\left(T^{-1/2}\mathcal{L}T^{1/2}\right) \\ &= T^{-1/2}\left(I-\mathcal{R}_0\right)T^{1/2} \\ &= I-\frac{1}{vol(\Gamma)}D_y, \\ \text{and} \qquad ZD_y &= 0, \end{aligned} \tag{II.6}$$

where $D_y(x,y)=d_y$ for all $x,y\in V$. The relations corresponding to those in (II.2) also hold for G, $\mathcal{G}$ and Z. The definition of Z in (II.6) is equivalent to the definition of Z more often used in random walks; i.e.,

$$Z(x,y) := \sum_{n=0}^{\infty}(P_n(x,y)-\pi_y), \tag{II.7}$$

where π is the stationary distribution of the random walk on Γ. To verify this alternate definition of Z, simply verify that $T^{1/2}ZT^{-1/2}$ satisfies (II.4) or (II.5) when used to replace $\mathcal{G}$. We think of Z as the Green's function corresponding to the Laplace operator. See [1, Ch. 3, p. 17] for relationships between Z and hitting times and [49] for an introduction to random walks.

II.B Green's function for the cycle C_m

In this section we illustrate the definition of the Green's function $\mathcal{G}$ in the case of the cycle, which has no boundary. The high degree of symmetry in the cycle allows the matrix equation involving the Green's function to be converted into a linear recurrence. The techniques developed here will be used in Section II.D to construct the Green's function for a t-dimensional torus.

Denote the vertex set of the cycle C_m be denoted by $\{0,1,\ldots,m-1\}$. The various Laplacians are related by $\Delta=\mathcal{L}=L/2$. Applying the definition in (II.5), the normalized Green's function $\mathcal{G}$ is determined by the relations

$$\begin{aligned} \mathcal{G}\mathcal{L} \;=\; \mathcal{L}\mathcal{G} &= I-\frac{1}{m}J, \\ \text{and} \qquad \mathcal{G}J &= 0, \end{aligned} \tag{II.8}$$

where $\phi_0(x) = \sqrt{1/m}$, and J is the $m \times m$ matrix with entries all 1's. In developing a formula for $\mathcal{G}$, it is useful to observe that the cycle is invariant under translation. Thus the values $\mathcal{L}(x, y)$ and $\mathcal{G}(x, y)$ depend only on the distance $|y - x|$ between x and y, and the following definition of $\mathcal{G}(a)$ is well-defined: for all $0 \leq a < m$,

$$\mathcal{G}(a) = \mathcal{G}(x, y), \qquad \text{if } a = |y - x|.$$

Since distance between x and y on the cycle can be measured by travelling in either direction, for all $0 < a < m$ we have

$$\mathcal{G}(a) \;=\; \mathcal{G}(m - a).$$

We are ready to derive the Green's function for the cycle.

Theorem II.1. *Let $m \geq 3$. For $0 \leq x, y \leq m-1$, the cycle C_m has normalized Green's function*

$$\mathcal{G}(x, y) = \frac{(m+1)(m-1)}{6m} - |y - x| + \frac{(y-x)^2}{m}. \tag{II.9}$$

Proof. From (II.8) we have the recurrence

$$2\mathcal{G}(x, y) - \mathcal{G}(x, y-1) - \mathcal{G}(x, y+1) \;=\; \begin{cases} 2 - 2/m, & x = y \\ -2/m, & x \neq y, \end{cases} \qquad \text{or}$$

$$2\mathcal{G}(a) - \mathcal{G}(a-1) - \mathcal{G}(a+1) \;=\; \begin{cases} 2 - 2/m, & a = 0, \\ -2/m, & a > 0, \end{cases}$$

provided that we define $\mathcal{G}(-1) = \mathcal{G}(1)$ for simplicity of representing the case $a = 0$. The following recurrence on differences results:

$$\mathcal{G}(a+1) - \mathcal{G}(a) \;=\; \mathcal{G}(a) - \mathcal{G}(a-1) \;+\; \frac{2}{m} \;-\; 2\chi(a = 0). \tag{II.10}$$

The second constraint in (II.8) determines that the sum of $\mathcal{G}$ across any row must be 0; i.e.,

$$\sum_{a=0}^{m-1} \mathcal{G}(a) \;=\; 0. \tag{II.11}$$

By considering the difference $(\mathcal{G}(a+1) - \mathcal{G}(a)) - (\mathcal{G}(a) - \mathcal{G}(a-1)) = 2/m$ in II.10 for $a > 0$, $\mathcal{G}(a)$ is quadratic in a with leading coefficient $1/m$, which we write as

$$\mathcal{G}(a) \;=\; \frac{a^2}{m} + Ba + C. \tag{II.12}$$

In order to obtain B, set $\mathcal{G}(a) = \mathcal{G}(m-a)$ to see that

$$\begin{aligned} \frac{a^2}{m} + Ba + C &= \frac{(m-a)^2}{m} + B(m-a) + C \\ Ba &= m - 2a + Bm - Ba, \end{aligned}$$

from which $B = -1$. Now applying the row sum constraint (II.11) allows us to compute the value of $C = \mathcal{G}(0)$.

$$\begin{aligned} 0 &= \sum_{a=0}^{m-1} \left(C - a + \frac{a^2}{m} \right) \\ mC &= \sum_{a=0}^{m-1} \left(a - \frac{a^2}{m} \right) \\ C &= \frac{(m+1)(m-1)}{6m} . \end{aligned} \tag{II.13}$$

Plugging B and C into (II.12) and letting $a = |y - x|$ achieves the desired result. $\square$

Using the alternate definition of $\mathcal{G}$ in (II.4) we have a whole class of identities formed by choosing any orthonormal eigensystem for C_m and equating (II.4) for $\mathcal{G}$ with (II.9). The following version arises from the orthonormal eigensystem for C_m derived in Lemma I.13.

Theorem II.2. *Let $m \geq 3$ and let $0 \leq x, y < m$. Then*

$$\frac{1}{m} \sum_{j=1}^{m-1} \frac{\exp\big((2\pi i j/m)(y-x)\big)}{1 - \cos(2\pi j/m)} = \frac{(m+1)(m-1)}{6m} - |y-x| + \frac{(y-x)^2}{m} .$$

II.C Green's functions for products of regular graphs

In this section, we extend Theorem 4 of [35] to include the normalized Green's function of the Cartesian product of a graph with boundary and a graph without boundary. Originally, [35] gives the normalized Green's function of the product of two graphs, each with boundary. Next, we present the normalized Green's function for a product of two graphs without boundary. The key observation for the second formula is as follows. When both graphs have an eigenvalue of 0, the residues of the contour integral associated with the normalized Green's function of the product graph are less easily calculated, and a separate formulation is needed. On the other hand, the normalized Green's function of the product graph is easy to calculate not only when both graphs have boundary [35], but also when one has boundary and the other does not; in either subcase, at least one graph does not have an eigenvalue of 0.

Throughout the remainder of this chapter, we will use the following notation. Let $\Gamma = (V, E)$ and $\Gamma' = (V', E')$ be simple connected undirected regular graphs of degree d and d' with specified vertex subsets $S \subseteq V$ and $S' \subseteq V'$, respectively. For simplicity, we require the subgraphs generated by S and S' to be connected. In the case of $S = V$, recall that $\mathcal{L}_S = \mathcal{L}$ and the subgraph induced by S is $\Gamma(S) = \Gamma$.

For any $\alpha \in \mathbb{C}$, let $\mathcal{G}_\alpha$ denote the symmetric matrix satisfying the relation $(\mathcal{L}_S + \alpha)\mathcal{G}_\alpha = I_S$, if $S \subsetneq V$; and the relations

$$\begin{aligned} (\mathcal{L}_S + \alpha)\mathcal{G}_\alpha &= I_S - P_0, \qquad \text{and} \\ \mathcal{G}_\alpha P_0 &= 0, \end{aligned} \tag{II.14}$$

if $S = V$ ($\mathcal{L}_S$ is singular). In either case, this is equivalent to

$$\mathcal{G}_\alpha(x, y) = \sum_{\lambda_j > 0} \frac{1}{\lambda_j + \alpha} \phi_j(x)\overline{\phi_j(y)}, \tag{II.15}$$

where the ϕ_j's are the orthonormal eigenfunctions of $\mathcal{L}_S$ associated with the eigenvalues λ_j. We call $\mathcal{G}_\alpha$ the *generalized Green's function*; it is a rational function of α which will be used in a contour integral to derive the normalized Green's function of the product graph. The analogous definitions of $\mathcal{L}'_{S'}$, $\mathcal{G}'_\alpha$, ϕ'_k, and λ'_k are made for Γ'.

Recalling the definitions in Section I.F, the Cartesian product $\Gamma \times \Gamma'$ has "playing area" $S^\times = S \times S'$, boundary $\delta S^\times$, normalized Laplacian $\mathcal{L}^\times_{S^\times}$, and normalized Green's function $\mathcal{G}^\times_{S^\times}$. The orthonormal eigensystem of $\mathcal{L}^\times_{S^\times}$ is labeled by eigenvalues $\Lambda_{j,k}$ with corresponding eigenvectors $\Phi_{j,k}$, because they are expressed in terms of the eigensystems of the factor graphs. Throughout the rest of the chapter, we may refer to a Laplacian in terms of S, S', or $S^\times$ to emphasize whether it is a Dirichlet Laplacian or not.

II.C.1 At least one graph has boundary

Suppose $S \subsetneq V$, so that S generates a connected subgraph with boundary in Γ. We allow $S' \subseteq V'$ to generate an arbitrary connected subgraph in Γ'. Recall that the

λ_j's are ordered by $0 < \lambda_1 \leq \cdots \leq \lambda_{|S|}$. We consider two cases, where the factor graphs are regular of the same degree or regular of different degrees.

Factor graphs are regular of same degree

Let C denote a contour in the complex plane consisting of all $\alpha \in \mathbb{C}$ satisfying $|\alpha - 1| = 1 + \lambda_1/2$. The contour C encloses all of the λ'_k's but none of $-\lambda_1, \ldots, -\lambda_{|S|}$. We have the following minor extension of Theorem 4 in [35].

Theorem II.3. *Let $\Gamma = (V, E)$ and $\Gamma' = (V', E')$ be d-regular, and let $S \subsetneq V$ and $S' \subseteq V'$. The normalized Green's function $\mathcal{G}^\times$ of the Cartesian product $\Gamma \times \Gamma'$ with $S^\times = S \times S'$ and boundary $\delta S^\times$ is*

$$\mathcal{G}^\times((x, x'), (y, y')) = \frac{1}{\pi i} \int_C \mathcal{G}_\alpha(x, y) \mathcal{G}'_{-\alpha}(x', y') d\alpha.$$

Proof. By Lemma I.15, the eigenvalues of the normalized Dirichlet Laplacian $\mathcal{L}^\times_{S^\times}$ of $\Gamma \times \Gamma'$ are $\{(\lambda_j + \lambda'_k)/2 : j, k\}$, with corresponding orthonormal eigenvectors $\Phi_{j,k} = \phi_j \phi'_k$. Starting from the formal definition of $\mathcal{G}^\times$ in (II.4), we have

$$\begin{aligned}
\mathcal{G}^\times((x, x'), (y, y')) &= 2 \sum_{j,k} \frac{\Phi_{j,k}(x, x') \overline{\Phi_{j,k}(y, y')}}{\lambda_j + \lambda'_k} \\
&= \frac{1}{\pi i} \int_C \sum_{j=1}^{|S|} \sum_k \frac{\phi_j(x) \overline{\phi_j(y)} \phi'_k(x') \overline{\phi'_k(y')}}{(\lambda_j + \alpha)(\lambda'_k - \alpha)} d\alpha \\
&= \frac{1}{\pi i} \int_C \mathcal{G}_\alpha(x, y) \mathcal{G}'_{-\alpha}(x', y') d\alpha,
\end{aligned}$$

where the integral is simplified by using (II.15). $\square$

Note that the above contour integral picks up exactly the residues at $\alpha = \lambda'_k$. For example, the residue at $\alpha = \lambda'_k$ is exactly

$$\sum_{\lambda'_K, \lambda'_K = \lambda'_k} \sum_{j=1}^{|S|} \frac{\phi_j(x) \overline{\phi_j(y)} \phi'_K(x') \overline{\phi'_K(y')}}{(\lambda_j + \lambda'_k)} = \sum_{\lambda'_K, \lambda'_K = \lambda'_k} \phi'_K(x') \overline{\phi'_K(y')} \cdot \mathcal{G}_{\lambda'_k}(x, y). \tag{II.16}$$

Because an eigenspace may be multi-dimensional, there could be many λ'_K's equal to a particular λ'_k. For convenience, for a fixed k we assign the term of the residue in (II.16) corresponding to $K = k$ to λ'_k. This observation gives us the computational formula for $\mathcal{G}^\times$ in the following corollary.

Corollary II.4. *Under the same conditions as in Theorem II.3, we have*

$$\mathcal{G}^\times((x,x'),(y,y')) = 2\sum_k \phi'_k(x')\overline{\phi'_k(y')}\mathcal{G}_{\lambda'_k}(x,y).$$

In practice, the corollary may be applied to a product graph in order to compute a closed formula for $\mathcal{G}^\times$, or to generate a non-trivial identity involving $\mathcal{G}_\alpha$ and the eigensystems of $\mathcal{L}_S$, $\mathcal{L}_{S'}$, and $\mathcal{L}^\times_{S^\times}$.

Factor graphs are regular of different degrees

Suppose we have the same conditions as Theorem II.3, except that the graphs Γ and Γ' are d- and d'-regular, respectively. By Lemma I.15, the eigenvalues of the normalized Dirichlet Laplacian of the Cartesian product $S \times S'$ are

$$\frac{d}{d+d'}\lambda_j + \frac{d'}{d+d'}\lambda'_k,$$

with corresponding orthonormal eigenvectors $\Phi_{j,k} = \phi_j\phi'_k$. The poles of $\mathcal{G}_{\alpha/d}$ are at $\alpha = -d\lambda_j$, and the poles of $\mathcal{G}'_{-\alpha/d'}$ are at $\alpha = d'\lambda'_k$. Let C denote a contour in the complex plane consisting of all $\alpha \in \mathbb{C}$ satisfying $|\alpha - d'| = d' + d\lambda_1/2$; thus C contains all of the $d'\lambda'_k$'s but none of $-d\lambda_1, \ldots, -d\lambda_{|S|}$. We obtain the following minor extension to Theorem 5 of [35].

Theorem II.5. *Let $\Gamma = (V,E)$ and $\Gamma' = (V',E')$ be d- and d'-regular, respectively, and let $S \subsetneq V$ and $S' \subseteq V'$. The normalized Green's function $\mathcal{G}^\times$ of the Cartesian product $\Gamma \times \Gamma'$ with $S^\times = S \times S'$ and boundary $\delta S^\times$ is*

$$\mathcal{G}^\times((x,x'),(y,y')) = \frac{d+d'}{2\pi i dd'}\int_C \mathcal{G}_{\alpha/d}(x,y)\mathcal{G}'_{-\alpha/d'}(x',y')d\alpha.$$

Proof. Beginning with the definition of $\mathcal{G}^\times$ in (II.4), we have

$$\begin{aligned}
\mathcal{G}^\times((x,x'),(y,y')) &= \sum_{j,k}\frac{d+d'}{d\lambda_j + d'\lambda'_k}\Phi_{j,k}(x,x')\overline{\Phi_{j,k}(y,y')} \\
&= \frac{d+d'}{2\pi i}\int_C \sum_{j=1}^{|S|}\sum_k \frac{\phi_j(x)\overline{\phi_j(y)}\phi'_k(x')\overline{\phi'_k(y')}}{(d\lambda_j+\alpha)(d'\lambda'_k-\alpha)} \\
&= \frac{d+d'}{2\pi i dd'}\int_C \sum_{j=1}^{|S|}\sum_k \frac{\phi_j(x)\overline{\phi_j(y)}\phi'_k(x')\overline{\phi'_k(y')}}{(\lambda_j+\alpha/d)(\lambda'_k-\alpha/d')}
\end{aligned}$$

$$= \frac{d+d'}{2\pi i d d'} \int_C \mathcal{G}_{\alpha/d}(x,y)\mathcal{G}'_{-\alpha/d'}(x',y')d\alpha. \qquad \square$$

Analogous to Corollary II.4, by inspecting the residues of the above contour integral at all values $\alpha = d'\lambda'_k$, we have the following.

Corollary II.6. *Under the same conditions as Theorem II.5, we have*

$$\mathcal{G}^{\times}((x,x'),(y,y')) = \frac{d+d'}{d} \sum_k \phi'_k(x')\overline{\phi'_k(y')}\mathcal{G}_{d'\lambda'_k/d}(x,y).$$

II.C.2 Neither graph has boundary

Here we consider the case of $S = V$ and $S' = V'$; in other words, there is no boundary condition on Γ, Γ', or $\Gamma \times \Gamma'$. We desire to compute the (non-invertible) normalized Green's function for the product graph. In particular, let $m = |V|$ and $n = |V'|$. Again, we consider the cases $d = d'$ and $d \neq d'$.

Factor graphs are regular of same degree

Recall from Section I.A that the orthonormal eigensystems of $\mathcal{L}$ and $\mathcal{L}'$ are $\{(\phi_j, \lambda_j) : 0 \leq j \leq m-1\}$ and $\{(\phi'_k, \lambda'_k) : 0 \leq k \leq n-1\}$, respectively. By Lemma I.15, the eigenvalues of $\mathcal{L}^{\times}$ of $\Gamma \times \Gamma'$ are $(\lambda_j + \lambda'_k)/2$, with corresponding orthonormal eigenvectors $\Phi_{j,k} = \phi_j \phi'_k$. Let C denote a contour in the complex plane consisting of all $\alpha \in \mathbb{C}$ satisfying $|\alpha - (2 + \lambda'_1/2)| = 2$. The contour C is designed to enclose $\lambda'_1, \ldots, \lambda'_{n-1}$ but not $-\lambda_0, \ldots, -\lambda_{m-1}$ or λ'_0.

Theorem II.7. *Let Γ and Γ' be d-regular and without boundary. The normalized Green's function $\mathcal{G}^{\times}$ of the Cartesian product $\Gamma \times \Gamma'$ is*

$$\mathcal{G}^{\times}((x,x'),(y,y')) = \frac{1}{\pi i} \int_C \mathcal{G}_{\alpha}(x,y)\mathcal{G}'_{-\alpha}(x',y')d\alpha + \frac{2}{n}\mathcal{G}(x,y) + \frac{2}{m}\mathcal{G}'(x',y').$$

Proof. By Lemma I.2, The eigenvector ϕ_0 corresponding to eigenvalue 0 is determined by $\phi_0(x) = \sqrt{(d_x/vol(\Gamma))}$. Starting from the formal definition of $\mathcal{G}^{\times}$ in (II.4), and noting that $d_v = d_{v'} = d$, $vol(\Lambda) = d \cdot m$, and $vol(\Lambda') = d \cdot n$, we have

$$\mathcal{G}^{\times}((x,x'),(y,y')) = 2 \sum_{j=1}^{m-1} \sum_{k=1}^{n-1} \frac{\Phi_{j,k}(x,x')\overline{\Phi_{j,k}(y,y')}}{\lambda_j + \lambda'_k}$$

$$
\begin{aligned}
& +2\sum_{j=1}^{m-1}\frac{\Phi_{j,0}(x,x')\overline{\Phi_{j,0}(y,y')}}{\lambda_j}+2\sum_{k=1}^{n-1}\frac{\Phi_{0,k}(x,x')\overline{\Phi_{0,k}(y,y')}}{\lambda'_k} \\
= \; & \frac{1}{\pi i}\int_C\sum_{j=1}^{m-1}\sum_{k=1}^{n-1}\frac{\phi_j(x)\overline{\phi_j(y)}\phi_k(x')\overline{\phi_k(y')}}{(\lambda_j+\alpha)(\lambda'_k-\alpha)}d\alpha \\
& +2\frac{\sqrt{d_{x'}d_{y'}}}{vol(\Gamma')}\sum_{j=1}^{m-1}\frac{\phi_j(x)\overline{\phi_j(y)}}{\lambda_j}+2\frac{\sqrt{d_x d_y}}{vol(\Gamma)}\sum_{k=1}^{n-1}\frac{\phi_k(x')\overline{\phi_k(y')}}{\lambda'_k} \\
= \; & \frac{1}{\pi i}\int_C \mathcal{G}_\alpha(x,y)\mathcal{G}'_{-\alpha}(x',y')d\alpha+\frac{2}{n}\mathcal{G}(x,y)+\frac{2}{m}\mathcal{G}'(x',y'),
\end{aligned}
$$

where the integral is simplified by using (II.15). □

Analogous to Corollary II.4, inspecting the residues of the above contour integral at $\lambda'_1,\ldots,\lambda'_{n-1}$ yields the following corollary.

Corollary II.8. *Under the same conditions as in Theorem II.7, we have*

$$
\mathcal{G}^\times((x,x'),(y,y'))=2\sum_{k=1}^{n-1}\phi'_k(x')\overline{\phi'_k(y')}\mathcal{G}_{\lambda'_k}(x,y)+\frac{2}{n}\mathcal{G}(x,y)+\frac{2}{m}\mathcal{G}'(x',y').
$$

Factor graphs are regular of different degrees

Suppose we have the same conditions as Theorem II.8, except that the graphs Λ and Λ' are d- and d'-regular, respectively. By Lemma I.15, the eigenvalues of the normalized Laplacian $\mathcal{L}^\times_{S^\times}$ of the Cartesian product $\Gamma\times\Gamma'$ are

$$
\frac{d}{d+d'}\lambda_j+\frac{d'}{d+d'}\lambda'_k
$$

with corresponding orthonormal eigenvectors $\Phi_{j,k}=\phi_j\phi'_k$. Let C denote a contour in the complex plane consisting of all $\alpha\in\mathbb{C}$ satisfying $|\alpha-(d'+d'\lambda'_1/2)|=d'$. By Lemma I.1(iv), $d'\lambda'_{n-1}\le 2d'$, and C contains $d'\lambda'_1,\cdots,d'\lambda'_{n-1}$, but not $-d\lambda_0,\ldots,-d\lambda_{m-1}$ or $d'\lambda'_0$. We obtain the following theorem.

Theorem II.9. *Let Γ and Γ' be d- and d'-regular, respectively, and both without boundary. The normalized Green's function $\mathcal{G}^\times$ of the Cartesian product $\Gamma\times\Gamma'$ is*

$$
\begin{aligned}
\mathcal{G}^\times((x,x'),(y,y')) \; = \; & \frac{d+d'}{2\pi i d d'}\int_C \mathcal{G}_{\alpha/d}(x,y)\mathcal{G}'_{-\alpha/d'}(x',y')d\alpha \\
& +\frac{d+d'}{dn}\mathcal{G}(x,y)+\frac{d+d'}{d'm}\mathcal{G}'(x',y').
\end{aligned}
$$

Proof. Beginning with the definition of $\mathcal{G}^\times$ in (II.4), we have

$$\begin{aligned}
\mathcal{G}^\times((x,x'),(y,y')) &= \sum_{j=1}^{m-1}\sum_{k=1}^{n-1} \frac{d+d'}{d\lambda_j + d'\lambda'_k}\Phi_{j,k}(x,x')\overline{\Phi_{j,k}(y,y')} \\
&\quad + \sum_{j=1}^{m-1} \frac{d+d'}{d\lambda_j}\Phi_{j,0}(x,x')\overline{\Phi_{j,0}(y,y')} \\
&\quad + \sum_{k=1}^{n-1} \frac{d+d'}{d'\lambda'_k}\Phi_{0,k}(x,x')\overline{\Phi_{0,k}(y,y')} \\
&= \frac{d+d'}{2\pi i d d'}\int_C \frac{dd'\phi_j(x)\overline{\phi_j(y)}\phi_k(x')\overline{\phi_k(y')}}{(d\lambda_j+\alpha)(d'\lambda_k-\alpha)}d\alpha \\
&\quad + \frac{d+d'}{d}\frac{\sqrt{d_{x'}d_{y'}}}{vol(\Gamma')}\mathcal{G}(x,y) + \frac{d+d'}{d}\frac{\sqrt{d_x d_y}}{vol(\Gamma)}\mathcal{G}'(x',y') \\
&= \frac{d+d'}{2\pi i d d'}\int_C \mathcal{G}_{\alpha/d}(x,y)\mathcal{G}'_{-\alpha/d'}(x',y')d\alpha \\
&\quad + \frac{d+d'}{dn}\mathcal{G}(x,y) + \frac{d+d'}{d'm}\mathcal{G}'(x',y'). \qquad \square
\end{aligned}$$

Analogous to Corollary II.4, by inspecting the residues of the above contour integral at $d\lambda'_1,\dots,d\lambda'_{n-1}$, we have the following.

Corollary II.10. *Under the same conditions as in Theorem II.9, we have*

$$\begin{aligned}
\mathcal{G}^\times((x,x'),(y,y')) &= \frac{d+d'}{d}\sum_{k=1}^{n-1}\phi'_k(x')\overline{\phi'_k(y')}\mathcal{G}_{d'\lambda'_k/d}(x,y) \\
&\quad + \frac{d+d'}{dn}\mathcal{G}(x,y) + \frac{d+d'}{d'm}\mathcal{G}'(x',y').
\end{aligned}$$

II.D Green's functions examples

Application of the integral formula in the previous section to specific examples is limited only to cases where the necessary raw materials can be computed. The results in Section II.C.1 for the product where at least one graph has boundary require the eigensystem of one graph and the generalized Green's function $\mathcal{G}_\alpha$ of the other graph. As written, Corollaries II.4 and II.6 assume that the generalized Green's function is known for the graph with boundary, and the eigensystem is known for the graph without boundary; however, corresponding versions can be easily re-derived when the reverse is true. For example, the version of Corollary II.4 used is important when considering the Cartesian product of a cycle and a path with boundary. The Green's function and generalized Green's function of a path with boundary appear in [35], along with the integral formula for products of paths with boundary.

The results in Section II.C.2 for the product of two graphs without boundary require knowledge of the eigensystem of one graph, the generalized Green's function $\mathcal{G}_\alpha$ of the other graph, and of the Green's functions $\mathcal{G}$ and $\mathcal{G}'$ of both graphs. Thus if we desire to compute $\mathcal{G}^\times$ for a product graph, we can look for any possible decomposition of the graph into two factor graphs for which this information is known. This observation is particularly useful in building the normalized Green's function inductively where each additional factor graph is from a specific family.

II.D.1 The torus $C_m \times C_n$

Following Corollary II.8, determination of the Green's function of the torus requires the Greens function $\mathcal{G}$ and generalized Green's function $\mathcal{G}_\alpha$ of the cycle. In obtaining a compact formula for the torus, it is critical to simplify $\mathcal{G}_\alpha$ as much as possible before incorporating it into Corollary II.8.

Theorem II.11. *Let $m,n \geq 3$. For $0 \leq x,y \leq m-1$ and $0 \leq x',y' \leq n-1$, the torus $C_m \times C_n$ has normalized Green's function*

$$\begin{aligned}
\mathcal{G}^\times((x,x'),(y,y')) = {} & \frac{2}{n}\sum_{k=1}^{n-1} \exp\left((2\pi i k/n)(y'-x')\right)\Bigg[-\frac{1}{m(1-\cos(2\pi k/n))} \\
& + \frac{T_{m/2-|y-x|}(2-\cos(2\pi k/n))}{(1-\cos(2\pi k/n))(3-\cos(2\pi k/n))U_{m/2-1}(2-\cos(2\pi k/n))}\Bigg] \\
& + \frac{2}{n}\left(\frac{(m+1)(m-1)}{6m} - |y-x| + \frac{(y-x)^2}{m}\right) \\
& + \frac{2}{m}\left(\frac{(n+1)(n-1)}{6n} - |y'-x'| + \frac{(y'-x')^2}{n}\right)
\end{aligned}$$

where T and U are the Chebyshev polynomials of the first and second kind, respectively.

Note that the formula depends only on the distances between y and x and between y' and x', which is expected due to the translational symmetries of the torus. The first step of the proof is to obtain a closed form for $\mathcal{G}_\alpha$ for the cycle C_m ($\mathcal{G}$ was determined in Theorem II.1). The proof of Theorem II.11 is deferred until after Cor. II.13.

Theorem II.12. *For a cycle C_m with vertices $0, 1, \ldots, m-1$, complex α, and $0 \leq x, y \leq m-1$, the normalized Green's function $\mathcal{G}_\alpha$ satisfies*

$$\mathcal{G}_\alpha(x, y) \;=\; -\frac{2}{m\,(r + r^{-1} - 2)} + \frac{2(r^{m/2-|x-y|} + r^{-m/2+|x-y|})}{(r - r^{-1})(r^{m/2} - r^{-m/2})},$$

where $2(1+\alpha) = r + r^{-1}$.

Proof. Because C_m is vertex-transitive, $\mathcal{G}_\alpha(x, y)$ depends only on the distance $\min(|y - x|, m - |y - x|)$ between x and y. Therefore define $\mathcal{G}_\alpha(a) := \mathcal{G}_\alpha(x, y)$, where $a = |y - x|$; this induces the additional relation $\mathcal{G}_\alpha(a) = \mathcal{G}_\alpha(m - a)$ for $1 \leq a \leq m - 1$. From equation (II.14), we have

$$\begin{aligned}
\chi(x = y) - \frac{1}{m} &= (\mathcal{L}_S + \alpha)\,\mathcal{G}_\alpha(x, y) \\
&= \frac{1}{2}\,(2(1+\alpha)\mathcal{G}_\alpha(x, y) - \mathcal{G}_\alpha(x+1, y) - \mathcal{G}_\alpha(x-1, y)) \\
&= \frac{1}{2}\left((r + r^{-1})\mathcal{G}_\alpha(x, y) - \mathcal{G}_\alpha(x+1, y) - \mathcal{G}_\alpha(x-1, y)\right),
\end{aligned}$$

where $\mathcal{L}_S$ is the normalized Laplacian of C_m. We can rewrite this as

$$\mathcal{G}_\alpha(x-1, y) - r\mathcal{G}_\alpha(x, y) \;=\; \frac{2}{m} - 2\chi(x = y) + \frac{1}{r}(\mathcal{G}_\alpha(x, y) - r\mathcal{G}_\alpha(x+1, y)),$$

which for $a > 0$ becomes

$$\begin{aligned}
\mathcal{G}_\alpha(a+1) - r\,\mathcal{G}_\alpha(a) &= \frac{2}{m} + \frac{1}{r}\,(\mathcal{G}_\alpha(a) - r\,\mathcal{G}_\alpha(a-1)) \\
&= \qquad \vdots \\
&= \frac{2}{m} + \cdots + \frac{1}{r^{a-1}}\frac{2}{m} + \frac{1}{r^a}\,(\mathcal{G}_\alpha(1) - r\,\mathcal{G}_\alpha(0))\,. \qquad \text{(II.17)}
\end{aligned}$$

When $a = 0$, we have

$$\mathcal{G}_\alpha(1) - r\,\mathcal{G}_\alpha(0) = \frac{2}{m} - 2 + \frac{1}{r}\,(\mathcal{G}_\alpha(0) - r\,\mathcal{G}_\alpha(m-1)),$$

and since $\mathcal{G}_\alpha(1) = \mathcal{G}_\alpha(m-1)$, we obtain

$$\begin{aligned}
\mathcal{G}_\alpha(1) &= \frac{1}{m} - 1 + \frac{r + r^{-1}}{2}\,\mathcal{G}_\alpha(0) \\
\mathcal{G}_\alpha(1) - r\mathcal{G}_\alpha(0) &= \frac{1}{m} - 1 + \frac{-r + r^{-1}}{2}\,\mathcal{G}_\alpha(0) \qquad \text{(II.18)}
\end{aligned}$$

From this point, the reader who wishes to verify details is encouraged to employ any standard computer algebra system. (II.17) and (II.18) define a recurrence and initial condition on differences of $\mathcal{G}_\alpha$, which is resolved by substituting $\mathcal{G}_\alpha(1) - r\mathcal{G}_\alpha(0)$ from (II.18) into (II.17) and simplifying the geometric series. For $a \geq 0$ this yields

$$\mathcal{G}_\alpha(a+1) - r\,\mathcal{G}_\alpha(a) = \frac{2}{r^{a-1}m}\frac{1-r^a}{1-r} + \frac{1}{r^a}\left(\frac{1}{m} - 1 + \frac{-r+r^{-1}}{2}\mathcal{G}_\alpha(0)\right). \tag{II.19}$$

Now denote the right-hand side of (II.19) by $D_\alpha(a)$; thus for $a > 0$ we have

$$\begin{aligned} \mathcal{G}_\alpha(a) &= r\,\mathcal{G}_\alpha(a-1) + D_\alpha(a-1) \\ &= \vdots \\ &= r^a\mathcal{G}_\alpha(0) + r^{a-1}D_\alpha(0) + r^{a-2}D_\alpha(1) + \cdots + r^0 D_\alpha(a-1). \end{aligned} \tag{II.20}$$

A careful but straightforward summing of geometric series in (II.20) yields, for $a > 0$,

$$\begin{aligned} \mathcal{G}_\alpha(a) &= \frac{1}{2}\mathcal{G}_\alpha(0)\frac{1+r^{2a}}{r^a} \\ &\quad + \frac{2}{m}\frac{1}{r^{a-2}}\frac{1-r^a}{1-r}\left(\frac{1+r^a}{1-r^2} + \frac{r^{a-1}}{1-r} + \frac{1+r^a}{1+r}\frac{1-m}{2r}\right). \end{aligned} \tag{II.21}$$

Now using (II.21), we set $\mathcal{G}_\alpha(1) = \mathcal{G}_\alpha(m-1)$ and solve for $\mathcal{G}_\alpha(0)$, obtaining

$$\mathcal{G}_\alpha(0) = -\frac{2}{m}\frac{r}{(r-1)^2} + \frac{2r(1+r^m)}{(r^2-1)(r^m-1)}, \tag{II.22}$$

which together with (II.21) and simplification yields

$$\begin{aligned} \mathcal{G}_\alpha(a) &= \mathcal{G}_\alpha(0) - \frac{2\left(r^{a/2} - r^{-a/2}\right)\left(r^{m/2-a/2} - r^{-(m/2-a/2)}\right)}{\left(r - r^{-1}\right)\left(r^{m/2} - r^{-m/2}\right)} \\ &= \frac{-2}{m\left(r + r^{-1} - 2\right)} + \frac{2\left(r^{m/2} + r^{-m/2}\right)}{\left(r - r^{-1}\right)\left(r^{m/2} - r^{-m/2}\right)} \\ &\quad - \frac{2\left(r^{a/2} - r^{-a/2}\right)\left(r^{m/2-a/2} - r^{-(m/2-a/2)}\right)}{\left(r - r^{-1}\right)\left(r^{m/2} - r^{-m/2}\right)} \\ &= \frac{-2}{m\left(r + r^{-1} - 2\right)} + \frac{2(r^{m/2-|x-y|} + r^{-m/2+|x-y|})}{(r - r^{-1})(r^{m/2} - r^{-m/2})}. \end{aligned}$$

Substituting $|y-x|$ for a gives the desired formula for $\mathcal{G}_\alpha$. $\square$

By the definition of α and r, we may use the substitution $r = e^{i\theta}$ to rewrite $(r^z + r^{-z})/2 = \cos z\theta$ and $(r^z - r^{-z})/2i = \sin z\theta$. Together with the definition of the Chebyshev polynomial of the first and second kinds, T_n and U_n, respectively; i.e.,

$$\begin{aligned} T_n(x) &:= \cos n\theta \quad \text{and} \\ U_n(x) &:= \frac{\sin(n+1)\theta}{\sin\theta}, \end{aligned}$$

where $x = \cos\theta$, we obtain the following corollary to Theorem II.12.

Corollary II.13. *For a complex α and $0 \le x, y \le m-1$, the normalized Green's function $\mathcal{G}_\alpha$ for a cycle C_m with vertices $0, 1, \ldots, m-1$ satisfies*

$$\mathcal{G}_\alpha(x,y) = -\frac{1}{m\alpha} + \frac{T_{m/2-|y-x|}(1+\alpha)}{\alpha(2+\alpha)U_{m/2-1}(1+\alpha)}$$

where T and U are the Chebyshev polynomials of the first and second kinds, respectively.

Proof of Theorem II.11: The theorem follows by applying the integral formula for products of graphs without boundary in Corollary II.8 to the torus, where $\Gamma = C_m$, $\Gamma' = C_n$, the ϕ''s are the orthonormal basis described in Lemma I.13, $\mathcal{G}$ and $\mathcal{G}'$ are given by Theorem II.1, and $\mathcal{G}_\alpha$ is given by Corollary II.13. $\square$

Combining Theorem II.11 with (II.4) using the orthonormal eigensystem of Lemma I.13 for both C_m and C_n yields the following nontrivial identity.

Corollary II.14. *Let $0 \le x, y \le m-1$ and $0 \le x', y' \le n-1$. Then*

$$\begin{aligned}
&\frac{1}{mn} \sum_{(j,k)\neq(0,0)} \frac{\exp\big((2\pi i j/m)(y-x)\big)\exp\big((2\pi i k/n)(y'-x')\big)}{\big(1-\cos(2\pi j/m)/2-\cos(2\pi k/n)/2\big)} \\
&= \frac{2}{n}\sum_{k=1}^{n-1} \exp\big((2\pi i k/n)(y'-x')\big)\Bigg[-\frac{1}{m(1-\cos(2\pi k/n))} \\
&+ \frac{T_{m/2-|y-x|}(2-\cos(2\pi k/n))}{(1-\cos(2\pi k/n))(3-\cos(2\pi k/n))U_{m/2-1}(2-\cos(2\pi k/n))}\Bigg] \\
&+ \frac{(m+1)(m-1)}{3mn} - \frac{|y-x|}{n} + \frac{(y-x)^2}{mn} \\
&+ \frac{(n+1)(n-1)}{3mn} - \frac{|y'-x'|}{m} + \frac{(y'-x')^2}{mn},
\end{aligned}$$

where T and U are the Chebyshev polynomials of the first and second kinds, respectively.

The Laplacian of C_m has a 1-dimensional eigenspace corresponding to eigenvalue 0, and a second 1-dimensional eigenspace corresponding to eigenvalue 2 iff C_m is bipartite (when m is even). Otherwise, all eigenspaces are 2-dimensional, since $\lambda_j = \lambda_{m-j}$ for all $1 \le j \le m-1$. This means that Corollary II.14 is only one of a class of identities constructed by choosing orthonormal eigensystems for C_m and C_n for the left-hand side, and a possibly distinct orthonormal eigensystem for C_n on the right-hand side.

II.D.2 The t-dimensional torus $C_{m_1} \times C_{m_2} \times \cdots \times C_{m_t}$

Computation of the normalized Green's function for the repeated product of cycles by use of Corollary II.8 requires a careful decomposition into factor graphs. Under the factor decomposition we are considering, the bottleneck lies in the computation of the generalized Green's function $\mathcal{G}_\alpha$, which we now have for the cycle C_m, but not for the torus for $t \geq 2$. This leads to a decomposition of the repeated product into $\Gamma = C_{m_1}$ and $\Gamma' = C_{m_2} \times \cdots C_{m_t}$.

Before giving the normalized Green's function of $C_{m_1} \times \cdots \times C_{m_t}$, we present the information on the components still needed. Choose and label the eigensystem of each C_{m_s} by

$$\{(\lambda_{j_s}^{(s)}, \phi_{j_s}^{(s)}) : 0 \leq j_s \leq m_s - 1\},$$

where $m_s \geq 3$, $0 = \lambda_0^{(s)} < \lambda_0^{(s)} \leq \cdots \leq \lambda_{m_s-1}^{(s)}$, and the $\{\phi_{j_s}^{(s)} : 0 \leq j_s \leq m_s - 1\}$ are orthonormal. The eigenvalues of $C_{m_2} \times \cdots \times C_{m_t}$ are averages of the eigenvalues of the factors C_{m_s}, and the corresponding eigenvectors are products of the eigenvectors of the factors. This is summarized in the next lemma, whose proof is a straightforward induction on Lemma I.15.

Lemma II.15. *The eigenvalues of $C_{m_2} \times \cdots \times C_{m_t}$ are*

$$\Lambda_{j_2,\ldots,j_t} = \frac{\lambda_{j_2}^{(2)} + \cdots + \lambda_{j_t}^{(t)}}{t-1},$$

where $0 \leq j_s \leq m_s - 1$ for all $2 \leq s \leq t$, with corresponding eigenvectors

$$\Phi_{j_2,\ldots,j_t}(x_2, \ldots, x_t) = \prod_{s=2}^{t} \phi_{j_s}^{(s)}(x_s).$$

For the following theorem, let $\mathcal{G}$ be the normalized Green's function for C_{m_1} from Theorem II.1, and $\mathcal{G}'$ the normalized Green's function for $C_{m_2} \times \cdots C_{m_t}$.

Theorem II.16. *Let $t \geq 2$. Let $0 \leq x_{j_s}, y_{j_s} \leq m_s - 1$ where $m_s \geq 3$ for $1 \leq s \leq t$. The t-dimensional torus $C_{m_1} \times \cdots \times C_{m_t}$ has normalized Green's function*

$$\begin{aligned} \mathcal{G}^{\times}((x_1, \ldots, x_t), (y_1, \ldots, y_t)) &= t \sum_{K \neq (0,\ldots,0)} \Phi_K(x_2, \ldots, x_t) \overline{\Phi_K(y_2, \ldots, y_t)} \mathcal{G}_{\Lambda_K}(x_1, y_1) \\ &+ \frac{t}{(t-1)m_1} \mathcal{G}'((x_2, \ldots, x_t), (y_2, \ldots, y_t)) + \frac{t}{m_2 \cdots m_t} \mathcal{G}(x_1, y_1), \end{aligned} \tag{II.23}$$

where K ranges over all indices $(j_2,\ldots,j_t)\neq(0,\ldots,0)$, Φ and Λ are defined in Lemma II.15, and $\mathcal{G}_\alpha$ is defined as in Corollary II.13.

Proof. The proof proceeds by using $\Gamma = C_{m_1}$ and $\Gamma' = C_{m_2}\times\cdots\times C_{m_t}$ in Corollary II.10. The degree of Γ is $d = 2$, and the degree of Γ' is $d' = 2(t-1)$. The result follows. $\square$

Although $\mathcal{G}'$ in Theorem II.16 may not already be known, it can be computed inductively from repeated applications of the theorem. Determination of $\mathcal{G}_\alpha$ for any small product $C_1\times\cdots\times C_{t'}$ would allow the reduction in the number of applications required by a factor of t'.

Corollary II.17. *For $0\le x_1,y_1,x_2,y_2,x_3,y_3\le m-1$ where $m\ge 3$, the 3-dimensional torus $C_m\times C_m\times C_m$ has normalized Green's function*

$$\begin{aligned}\mathcal{G}^\times((x_1,x_2,x_3),(y_1,y_2,y_3)) \;=\; & \frac{3}{m^2}\sum_{(j,k)\neq(0,0)}\Big[\exp\big((2\pi ij/m)(y_2-x_2)\big)\\ & \exp\big((2\pi ik/m)(y_3-x_3)\big)\mathcal{G}_{(1-\cos(2\pi j/m)/2-\cos(2\pi k/m)/2)}(x_1,y_1)\Big]\\ & +\frac{3}{m^2}\sum_{j=1}^{m}\exp\big((2\pi ik/m)(y_3-x_3)\big)\mathcal{G}_{(1-\cos(2\pi j/m))}(x_2,y_2)\\ & +\frac{3}{m^2}\left(\frac{(m+1)(m-1)}{6m}-|y_3-x_3|+\frac{(y_3-x_3)^2}{m}\right)\\ & +\frac{3}{m^2}\left(\frac{(m+1)(m-1)}{6m}-|y_2-x_2|+\frac{(y_2-x_2)^2}{m}\right)\\ & +\frac{3}{m^2}\left(\frac{(m+1)(m-1)}{6m}-|y_1-x_1|+\frac{(y_1-x_1)^2}{m}\right).\end{aligned}$$

where $\mathcal{G}_\alpha$ is defined as in Corollary II.13.

Proof. The proof proceeds by applying the inductive formula for t-dimensional tori in Theorem II.16 twice, where we first take the product of $\Gamma = C_m$ with $\Gamma' = C_m\times C_m$, and then the product of $\Gamma = C_m$ with $\Gamma' = C_m$. Substitution for all values gives the result. $\square$

These compact formulas for Green's functions of tori offer very fast alternatives to computing pseudo-inverses of their Laplacians directly. This is mainly because the Chebyshev polynomials T_n and U_n arising from the integral formula can be computed in $O(\log n)$ time. Various algorithms for computing T_n and U_n are given in [80], and a more theoretical treatment of types of polynomials computable in $O(\log n)$ appears in

[57]. The following corollary to Theorem II.16 is significant because the Laplacian ($\mathcal{L}$, L, or Δ) of the torus on n vertices has rank $n-1$, and so computing its pseudo-inverse provides along the way the inverse of an $(n-1)\times(n-1)$ matrix.

Corollary II.18. *Matrix pseudo-inversion of the Laplacian of the t-dimensional torus with n vertices via its Green's function is $O(t\cdot n^{2-1/t}\log n)$, provided that the matrix itself is not completely reconstructed.*

Proof. We assume the t-dimensional torus is $C_{m_1}\times\cdots\times C_{m_t}$, where $m_s\geq 3$ for $1\leq s\leq t$ and $\prod_{s=1}^{t} m_s = n$. It suffices to compute one row of the pseudo-inverse of the normalized Laplacian in order to know the entire inverse, due to the translational symmetry of the torus; i.e., since

$$\mathcal{G}^{\times}((x_1,\ldots,x_t),(y_1,\ldots,y_t)) \;=\; \mathcal{G}^{\times}((0,\ldots,0),(|y_1-x_1|,\ldots,|y_t-x_t|)).$$

(In fact, because $|y_s-x_s|$ can be replaced by $m-|y_s-x_s| \pmod m$ without changing the value of $\mathcal{G}^{\times}$, only $\prod_{s=1}^{t}\lceil m_s/2\rceil$ of these entries must actually be computed.) Order the coordinates of the torus so that $m_1\geq\cdots\geq m_t$. Then the summation term on the right-hand side of (II.23) has at most $n^{1-1/t}$ summands, which can each be computed in $O(t\log n)$ time. The second and third terms can also be computed in $O(t\,n^{1-1/t}\log n)$ time, and we must compute n terms total to know all entries of the pseudo-inverse of $\mathcal{L}$. □

For example, the time complexity of computing the Green's function for the torus $C_m\times C_m\times C_m$ is $O(n^{5/3}\log n)$, where $n=m^3$ is the number of vertices. Such a quick pseudo-inversion formula is surprising, since matrix inversion in general is the same complexity as matrix multiplication (see [21]). Matrix multiplication is now known to be $O(n^{\omega})$, where $2\leq\omega\leq 2.376$ (see [36]). Surprisingly, for large n we can compute all of the values for the pseudo-inverse of the Laplacian for the torus faster than we can write down the whole matrix. Of course, requiring the presentation of the whole matrix rather than just the first row increases the complexity to $O(t\,n^{1-1/t}\log n+n^2)$.

II.E Hitting times from Green's functions

Since the normalized Green's function $\mathcal{G}$ for a graph without boundary is equivalent under similarity transformation to the fundamental matrix Z in (II.7), many quantities in random walks may be computed using $\mathcal{G}$. The *hitting time* $Q(x, y)$ of a random walk starting at vertex x with target vertex y is the expected number of steps to reach vertex y. In [35], Chung and Yao show the relationship between $\mathcal{G}$ and Q as follows.

Theorem II.19 (Chung, Yao). *The hitting time* $Q(x, y)$ *satisfies*

$$Q(x,y) = \frac{vol(\Gamma)}{d_y}\mathcal{G}(y,y) - \frac{vol(\Gamma)}{\sqrt{d_x d_y}}\mathcal{G}(x,y).$$

We immediately have a computational formula for the hitting time whenever $\mathcal{G}$ is known. For instance, whenever Γ is regular with n vertices,

$$Q(x,y) = n\left(\mathcal{G}(y,y) - \mathcal{G}(x,y)\right). \tag{II.24}$$

The resulting formula in the case of the torus is obtained by using $\mathcal{G}$ from Theorem II.11 or II.16. Figure II.1 illustrates numerical values of hitting times for the 2-dimensional torus $C_{49} \times C_{49}$. The vertices of the torus may be laid out as a square grid if we imagine the boundary to be periodic, making opposite ends adjacent. The vertical axis plots the

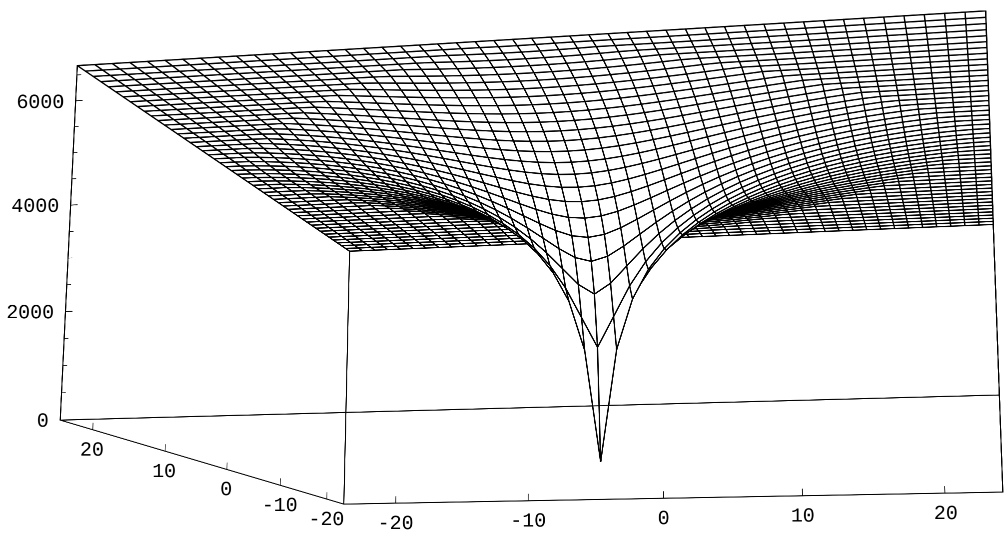

Figure II.1: Graph of the hitting time of the torus $C_{49} \times C_{49}$, laid out as a square with periodic boundary hitting time of a random walk initiated at $(0,0)$ with target (x,y). The hitting time at $(0,0)$ is 0 since the walk starts at $(0,0)$, and levels off at just above 6000 steps to reach vertices furthest from the start of the walk.

If (II.24) is computed using techniques such as Corollary II.13, the hitting time expression will involve orthogonal polynomials. Aldous and Fill claim in [1] that orthogonal polynomials may appear whenever Γ has sufficient symmetry, but the dependence remains largely unstudied.

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Chapter III

The Dirichlet Chip-Firing Game

Chip-firing is a game played on a graph Γ. Each vertex of Γ contains an integral number of chips. A vertex may be *fired* provided that it has at least as many chips as its degree, and upon firing it sends one chip along each edge to the other vertex incident to the edge. The game proceeds by firing a sequence of vertices in succession, whereby firing leads from one *configuration* of the game to another, terminating when no vertex may be fired. Interesting questions include the number of firings before termination (game *length*), the structure of the intermediate configurations which might arise, and the determination of a suitable representative set of terminating configurations known as *critical configurations*. Precursors of chip-firing include *balancing games* of various kinds, concerning sets [103], vectors [108, 109, 110], and matrices [8, 9]. Another forerunner of chip-firing is the *probabilistic abacus* introduced by Engel [53], which relates certain discrete configurations to Markov chains. Chip-firing has been studied previously in terms of classification of legal game sequences [17, 18], critical configurations [14], and by use of the chromatic polynomial [15], the Tutte polynomial [14, 88], and matroids [89, 90]. Issues of computational complexity are discussed in [54, 66, 111, 116]. The lattice structure of game configurations is considered in [67, 83]. Parallel versions of chip-firing, in which all ready vertices fire simultaneously, are studied in [50, 79, 105]. Variants of chip-firing include a generalized firing game [113], source-reversal in directed graphs [68], node-firing [55], and chip-firing on graphs where edges may be added or deleted during the game [56]. Chip-firing is closely related to *self-organized criticality* [6, 7], *avalanche models* [62], and the *abelian sandpile model* [64, 65, 102, 117], introduced by Dhar [44, 45].

The two most important aspects of chip-firing games are the classes of algebraic and combinatorial objects related to game configurations and game play, and the close ties between chip-firing and random walks. Critical configurations of the basic game are in bijection with both the set of spanning trees of the graph and the elements of the *critical group* [13], or *sandpile group* [37], of the graph. The set of legal game sequences of many types of chip-firing games forms a language called a *greedoid* [18, 19, 81], for which certain exchange and confluence properties hold. The number of steps needed to reach a terminating configuration is related to the *mixing time* of a random walk (the authority on relationships between chip-firing and random walks is [87]).

In this chapter we consider a new variant of the chip-firing game, in which chips are removed from the game when they are fired across a boundary. This modified chip-firing game is motivated in part by communication network models in which the chips represent packets or jobs and the boundary nodes represent processors with unlimited computational power. We will refer to this variant as the chip-firing game with *Dirichlet boundary condition*, and hereafter simply refer to it as the "Dirichlet game" unless otherwise specified. The *Dirichlet eigenvalues* (defined in Section I.C) of the Laplacian of the graph with rows and columns of boundary vertices deleted are important in analyzing the game. After preliminary definitions in Section III.A, in Section III.B we obtain a bound on the length of the Dirichlet game in terms of the number of chips and the Dirichlet eigenvalues of the graph. In Sections III.C-III.E we consider three families of structures associated with an induced subgraph of Γ on a subset S of vertices:

(1) The set of spanning forests on S with roots on the boundary of S;

(2) A set of "critical configurations" that are special distributions of chips (detailed definition to be given later in Section III.D);

(3) A coset group, that is often called the "sandpile" group.

As it turns out, all three families have the same cardinalities. We will discuss the bijections among these three families. Some questions and remarks are included in Section III.G.

III.A Preliminaries

The Dirichlet chip-firing game takes place in the setting of a simple loopless connected graph $\Gamma = (V, E) = (V(\Gamma), E(\Gamma))$ with vertex set $V(\Gamma)$. The notion of boundary is the same as is developed in Section I.C. Let S denote a fixed proper subset of $V(\Gamma)$, called the *playing area.* S induces a *boundary* $\delta S := \{y \notin S : y \sim x \text{ and } x \in S\}$ and the *spectators* $V \setminus (S \cup \delta S)$. For convenience, throughout the chapter we will make the following assumptions on Γ with respect to S. The induced subgraph $\Gamma(S)$ must be connected; otherwise, we could decompose the game with respect to connected components of $\Gamma(S)$. The boundary δS of S is nonempty; otherwise, the game reduces to the basic chip-firing game already studied. Furthermore, we assume $V(\Gamma) = S \cup \delta S$, since chip movement ignores the spectators, and that the subgraph $\Gamma(\delta S)$ induced by the boundary δS has no edges, since chips cannot move between boundary vertices.

We begin by placing a nonnegative number of chips on each vertex in S. Any vertex $v \in S$ is *ready* to be fired if it has at least as many chips as its degree. Firing a vertex sends one chip to each of its neighbors. If the firing of one vertex causes a second vertex to go from not ready to ready, then we say the first *primes* the second, or the second is *primed*. Chips fired from a vertex in S to a vertex in δS are instantly processed and removed from the game. Thus a configuration c of the Dirichlet game is a vector $c : V(\Gamma) \to \mathbb{Z}^+ \cup \{0\}$ which satisfies the *Dirichlet boundary condition* $c(v) = 0$ for all $v \in \delta S$. A configuration is *stable* if no vertex $v \in S$ is ready. Let c_0 denote the initial configuration of a Dirichlet game. We may fire vertices in succession provided that they are ready at the time of their firing, yielding a finite *firing sequence* (elsewhere known as a *record*) $\mathcal{F} = (\mathcal{F}(1), \mathcal{F}(2), \mathcal{F}(3), \ldots)$ (finiteness is proven in Lemma III.5). The final configuration achieved after the firing sequence, when no vertices are ready, is denoted by c_E. In general, if a firing sequence $\mathcal{F}$ leads from a configuration c_1 to another configuration c_2, we say that c_1 yields c_2 under $\mathcal{F}$. The *score* of a Dirichlet game with firing sequence $\mathcal{F}$ is the vector $f : S \to \mathbb{Z}^+ \cup \{0\}$ defined by $f(v) = \left|\mathcal{F}^{-1}(\{v\})\right|$, where $f(v)$ may be interpreted as the number of times the vertex $v \in S$ is fired during the Dirichlet game. The *length* of the Dirichlet game may thus be defined as the total number of firings, $\sum_v f(v)$. A configuration c is *recurrent* if there exists a configuration

b and a firing sequence $\mathcal{F}$ such that $c+b$ yields c under $\mathcal{F}$. We think of this as being able to add chips to the configuration c and play the game until returning to c. A configuration is *Dirichlet-critical* if it is both stable and recurrent.

III.A.1 Chip-firing and Laplacians

The combinatorial Laplacian L of a graph Γ (defined in Section I.A) may also be defined by its operation on a vector $f \in \mathbb{Z}^{|V(\Gamma)|}$:

$$Lf(u) = \sum_{v \sim u} f(u) - f(v).$$

Let x_v be the standard basis vector $(0, \ldots, 0, 1, 0, \ldots, 0) \in \mathbb{Z}^{V(\Gamma)}$ with a 1 in the position corresponding to v. Firing a vertex $v \in S$ which has no neighbors in δS at the configuration c_j to obtain the configuration c_{j+1} may be expressed as

$$c_j(u) - c_{j+1}(u) = Lx_v(u),$$

but in general for the Dirichlet game, this must be expressed as

$$c_j(u) - c_{j+1}(u) = \begin{cases} Lx_v(u) & \text{if } u \in S \\ 0 & \text{if } u \in \delta S, \end{cases} \tag{III.1}$$

More generally, if f is the score of a Dirichlet game, then $Lf = c_0 - c_E$ on S.

In this chapter we are interested in the eigenvalues of the restriction L_S of L to the rows and columns corresponding to S. L_S is the *Dirichlet Laplacian* (defined in Section I.C) of Γ with respect to the playing area S. A chip configuration in the Dirichlet game can be viewed simultaneously as a nonnegative function on S or as a nonnegative *Dirichlet function* on V (equal to 0 on δS). Recall that the set of Dirichlet functions on Γ with specified playing area S is $D(\Gamma, S)$. If we identify a vector $f \in \mathbb{Z}^{|S|}$ with a Dirichlet function $g \in D(\Gamma, S)$ satisfying $g(v) = f(v)$ for $v \in S$, then we have

$$L_S f(v) = Lg(v)$$

for $v \in S$. As an alternative to (III.1), we may encode firing a vertex $v \in S$ in the configuration c_j to obtain the configuration c_{j+1} by

$$c_j(u) - c_{j+1}(u) = \begin{cases} L_S x_v(u) & \text{if } u \in S \\ 0 & \text{if } u \in \delta S, \end{cases} \tag{III.2}$$

where this time $x_v \in \mathbb{Z}^{|S|}$. Due to (III.1) and (III.2), we will interchangeably consider configurations and score vectors of the Dirichlet game to reside in either $\mathbb{Z}^{|V|}$ or $\mathbb{Z}^{|S|}$. Recall from Section I.C that the Dirichlet eigenvalues of Γ with respect to vertex set S and boundary set δS are the eigenvalues of L_S, and are written in order as

$$0 < \sigma_1 \leq \sigma_2 \leq \cdots \leq \sigma_{|S|}.$$

In particular, if $f|_S$ is the restriction of f to S, σ_1 satisfies the following:

$$\begin{aligned} \sigma_1 &= \inf_{f|_S \neq 0} \frac{\langle f|_S, L_S f|_S \rangle}{\langle f|_S, f|_S \rangle} \\ &= \inf_{f \in D(\Gamma, S), f \neq 0} \frac{\sum_{x \sim y} (f(x) - f(y))^2}{\sum_x f^2(x)}, \end{aligned} \tag{III.3}$$

where the second infimum ranges over all f satisfying the Dirichlet boundary condition and the "$\sum_{x \sim y}$" can be thought of as ranging over all unordered pairs of vertices x and y so that x is adjacent to y and at least one of x and y is in S. Because we are dealing with a restricted Laplacian, there is no eigenvalue of 0, and so the infimum is over all nonzero vectors f instead of over all vectors f orthogonal to an eigenvector for the eigenvalue 0. Furthermore, we can take the infimum to be over all vectors f with norm 1, which is a compact space, and so there is an f which achieves the infimum.

III.A.2 Chip-firing variants

Analysis of the Dirichlet game is similar to that of three other games already studied: the basic chip-firing game, the dollar game, and the abelian sandpile model. Proofs of facts about these three games can be converted to proofs of similar facts about the Dirichlet game by constructing the appropriate graph.

The *basic chip-firing game*, or *basic game*, is simply the Dirichlet game with empty boundary. This is the game called the "chip-firing game" in [18]. Chip configurations and score vectors in the basic game are defined over the entire set of vertices of the graph. Vertex readiness and firing are the same as in the Dirichlet game, except that chips are never removed from play since there is no boundary. Firing a vertex is encoded by the Laplacian of the graph as in (III.1), where $\delta S = \emptyset$.

The *dollar game*, defined in [13], is the same as the basic game except that one vertex q is reserved as the "government," which may only fire when no other vertex is ready. Chips in the game may be considered as money, and q is fired only when the "economy" gets stuck. The value of the configuration at q is defined to be nonpositive, such that the total number of chips in the game is 0. The dollar game is nearly equivalent to the Dirichlet game with boundary size $|\delta S| = 1$, where q plays the role of δS, except that δS never fires. In particular, a configuration in the dollar game is *critical* iff the same configuration in the Dirichlet game with $\delta S = \{q\}$ is Dirichlet-critical.

The Dirichlet game with $|\delta S| = 1$ is equivalent to the *abelian sandpile model*, or *sandpile model*, in [37]. In the sandpile model on a graph Γ with $V(\Gamma) = \{x_1, \ldots, x_n\}$, the vertex x_n is called the *root* and never topples (fires); x_n plays the role of a single boundary vertex in the corresponding Dirichlet game. Configurations of the sandpile model are sometimes allowed to take on negative values, and the value of the configuration at the root vertex is arbitrary since it cannot fire. We now present several definitions and theorems associated with the sandpile model from [37] and discuss their implications for the Dirichlet game.

In order to distinguish definitions, we add the modifier "sandpile" in front of terms related to the sandpile model. Also, given any vector $c \in \mathbb{Z}^{|V|}$, the vector $\overline{c}$ is equal to c except on δS, where $\overline{c} \equiv 0$; this is to allow seamless transfer of configurations between the sandpile model with root x_n and Dirichlet game with $\delta S = \{x_n\}$. A nonnegative configuration c is *sandpile-stable* provided that $c(v) < d_v$ for all $v \neq x_n$. Thus c is sandpile-stable iff $\overline{c}$ is stable. A nonnegative stable configuration c in the sandpile model is *sandpile-recurrent* provided there exists a nonnegative configuration b such that $c + b$ yields c under some firing sequence. Thus c is sandpile-recurrent iff $\overline{c}$ is Dirichlet-critical.

We now define two special configurations which facilitate the study of sandpile-recurrent configurations. The configuration δ is defined to have d_x chips on each vertex x. In particular, δ is not sandpile-stable, and $\overline{\delta}$ is not stable. For two configurations c_1 and c_2, define $c_1 \oplus c_2$ to be the terminating configuration resulting from playing either the sandpile model or the Dirichlet game on $c_1 + c_2$; the game played will be clear from the context. The configuration ϵ is defined to be

$$\epsilon \;=\; \delta + (\delta - \delta \oplus \delta).$$

In particular, ϵ is a nonnegative configuration. The following appears as [37, Lemma

2.4].

Lemma III.1 (Cori, Rossin). *A configuration c in the sandpile model on Γ with $V(\Gamma) = \{x_1, \ldots, x_n\}$ and root x_n is sandpile-recurrent iff $c + \epsilon$ yields c under some firing sequence.*

This lemma can be adapted to the Dirichlet game to give a specific configuration which can be added to a Dirichlet-critical configuration in order to certify that it is in fact Dirichlet-critical.

Corollary III.2. *A configuration $\overline{c}$ on Γ with boundary δS is Dirichlet-critical iff $\overline{c} + \overline{\epsilon}$ yields $\overline{c}$ under some firing sequence.*

Proof. Define Γ' from Γ by contracting all vertices of δS in into a single vertex x_n, where the vertices in S are labeled $\{x_1, \ldots, x_{n-1}\}$. Without loss of generality, we consider the configurations $\overline{c}$ and $\overline{\epsilon}$ to be defined on Γ'. By Lemma III.1 and the discussion above, the configuration $\overline{c}$ is Dirichlet-critical iff $\overline{c}$ is sandpile-recurrent, iff $\overline{c} + \epsilon$ in the sandpile game yields $\overline{c}$ under some firing sequence, iff $\overline{c} + \overline{\epsilon}$ in the Dirichlet game yields $\overline{c}$ under the same firing sequence. $\square$

An alternate characterization of sandpile-recurrent configurations or Dirichlet-critical configurations is in terms of adding chips to those vertices adjacent to the root vertex or the boundary vertices, respectively. The following lemma appears as Corollary 2.6 of [37] (the equivalent result for the dollar game appears as Lemma 3.6 of [13]). Define the nonnegative (sandpile) configuration β to be $e_{j,n}$ on x_j, where $e_{j,n}$ is the number of edges between x_j and the root x_n, and $-d_{x_n}$ on x_n.

Lemma III.3 (Cori, Rossin). *The configuration c is sandpile-recurrent iff $c + \beta$ yields c under some firing sequence which is a permutation of $\{x_1, \ldots, x_{n-1}\}$.*

The proof of the following corollary proceeds analogously to that of Corollary III.2. Define the configuration $\overline{\beta}$ for $v \in S$ by setting $\overline{\beta}(v)$ to be the number of vertices in δS adjacent to v. Let $\overline{\beta} \equiv 0$ elsewhere. Then $\overline{\beta}$ plays the same role for a Dirichlet-critical configuration as β plays for a sandpile-recurrent configuration.

Corollary III.4 (Burning Algorithm). *The configuration $\overline{c}$ in the Dirichlet game with boundary δS is Dirichlet-critical iff $\overline{c}+\overline{\beta}$ yields $\overline{c}$ under some firing sequence which is a permutation of S.*

This result and its equivalent formulations for the sandpile model and dollar game are called as "burning algorithms" because of the similarity to the progress of forest fire; a blaze ignited in one location spreads throughout adjacent forested area but cannot re-burn charred trees. Thus every vertex is fired (burned) exactly once. The above results for the sandpile model hold when Γ has multiple edges. Implicit in the construction of Γ' in Corollary III.2 is the possibility of creating multiple edges, although our assumptions on the Dirichlet game do not explicitly allow multiple edges. We remark that the Dirichlet game can be extended in a straightforward fashion to allow for multiple edges, and furthermore that the constructions used above can be thought of as a way of bookkeeping for the Dirichlet game that is actually occurring on the simple graph Γ. Corollary III.4 will be revisited in Section III.D, where Dirichlet-critical configurations are more explicitly characterized.

III.B Convergence bounds for the Dirichlet game

Given the setting of a chip-firing game with Dirichlet boundary condition, we may wish to determine the length of a game based on its initial configuration. Starting from an initial configuration c_0, we fire vertices successively for as long as possible. A game terminates when it reaches a stable configuration, in which no vertex $v \in S$ is ready. That the game must terminate when Γ is connected and $\delta S \neq \emptyset$ is a minor variant on Lemma 3.1 of [18]:

Lemma III.5. *Every Dirichlet game must terminate in a finite number of firings.*

Proof. With the same assumptions on Γ as in Section III.A, recall that only vertices in S may be fired, and that vertices in δS immediately remove any chips that are sent to them. Let $N = \sum_v c_0(v)$ be the total number of chips at the start of the game. Now suppose to the contrary that a game does not terminate. Then there is a vertex $v_1 \in S$ that is fired infinitely often. Let $P = v_1, \ldots, v_k$ be a simple path from v_1 to some vertex

$v_k \in \delta S$, with all vertices except for v_k in S. For each $i \in \{1, \ldots, k-1\}$, if vertex v_i is fired infinitely often, then vertex v_{i+1} receives infinitely many chips, and must also be fired infinitely often if it is in S. This is because each vertex may have no more than N chips at a single time. Therefore infinitely many chips are removed from the game, which is a contradiction. This completes the proof of the lemma. $\square$

A fascinating result on the characterizations of score vectors of games is that the score vector depends only on the initial configuration and not on the firing sequence used to go from the initial configuration to the final configuration. As long as two such distinct firing sequences are legal, they will have the same score. We give the corresponding result [18, Theorem 2.1] for the basic game, stated for our assumptions on Γ.

Theorem III.6 (Björner, Lovász, Shor). *Given an initial configuration, every basic chip-firing game either continues indefinitely or terminates with the same score and the same final configuration.*

The proof considers properties of the language $\mathbf{L}$ of firing sequences of all possible basic games (the same properties appear in the study of greedoids [81] and antimatroids [51]). For conciseness, the three properties considered in [18] are that $\mathbf{L}$ is

- *left-hereditary*, because any prefix of a firing sequence is also a firing sequence;
- *locally free*, because either of two vertices may be fired if both are ready; and
- *permutable*, because the readiness of a vertex depends only on the set of vertices previously fired and not the order of firing.

These properties are sufficient to show that a vertex is fired the same number of times in any terminating basic game. An argument parallel to that of Lemma III.5 gives that every vertex is fired infinitely often in non-terminating basic games. The terminating case of Theorem III.6 can be adapted for the Dirichlet game as follows.

Corollary III.7. *Given an initial configuration, every Dirichlet game terminates with the same score and same final configuration.*

Proof. Extend the graph Γ of the Dirichlet game to the graph Γ' as follows. Let N be the total number of chips in the initial configuration c_0. Add vertices $v_1, \ldots, v_N$ to Γ, and add $N \cdot |\delta S|$ edges connecting each of these vertices to every vertex in δS. Consider the basic game on the new graph with initial configuration c_0' such that $c_0' = c_0$ on the original vertices and $c_0' \equiv 0$ on $v_1, \ldots, v_N$. Because the degree of any boundary vertex in Γ' is now larger than the number of chips in play, none of the vertices of δS are fired in any basic game starting from c_0'. Therefore a firing sequence $\mathcal{F}$ is valid either for both the basic game on Γ' and the Dirichlet game on Γ or neither. The score of the Dirichlet game is exactly the score of the basic game, and the final configuration of the Dirichlet game is determined by removing all chips from δS in the final configuration of the basic game. $\square$

Because every Dirichlet game has the same score vector f, the initial and final configurations c_0 and c_E of a Dirichlet game are related precisely by

$$L_S f \quad = \quad c_0 - c_E. \tag{III.4}$$

This expression of the score vector in terms of the Dirichlet Laplacian leads us to obtain a bound on game length $\sum_x f(x)$ using Dirichlet eigenvalues. By Corollary III.7, we may consider this bound simultaneously valid for all Dirichlet games with the same initial configuration.

Theorem III.8. *Let f be the score vector of a Dirichlet game on Γ. Then the length of the game is at most*

$$\sum_{x \in S} f(x) \leq \frac{1}{\sigma_1} \sqrt{2} N n^{1/2} ,$$

where N is the total number of chips in the initial configuration, and $n = |S|$ is the size of the playing area.

Proof. With the same assumptions on Γ as in Section III.A, recall that c_0 and c_E are the initial and final configurations of the game; thus $N = \sum_{x \in S} c_0(x)$. Also, we have eigenvalues $0 < \sigma_1 \leq \sigma_2 \leq \cdots \leq \sigma_n$ of the Dirichlet Laplacian L_S of Γ, corresponding to orthonormal eigenvectors $\phi_1, \ldots, \phi_n$. Accordingly, write $f = \sum a_i \phi_i$. We may bound each a_i using (III.4).

$$\begin{aligned} a_i &= \langle f, \phi_i \rangle = \frac{1}{\sigma_i} \langle f, \sigma_i \phi_i \rangle \\ &= \frac{1}{\sigma_i} \langle f, L_S \phi_i \rangle = \frac{1}{\sigma_i} \langle L_S f, \phi_i \rangle = \frac{1}{\sigma_i} \langle c_0 - c_E, \phi_i \rangle . \end{aligned} \tag{III.5}$$

The number of firings in the game is simply the sum of the entries of f; i.e.,

$$\sum_{x\in S} f(x) \quad = \quad \langle 1_S, f\rangle \,. \tag{III.6}$$

Putting (III.5) and (III.6) together, we obtain

$$\begin{aligned}
\sum_{x\in S} f(x) &= \left\langle 1_S, \sum_i a_i\phi_i \right\rangle = \left\langle 1_S, \sum_i \frac{1}{\sigma_i}\left\langle c_0 - c_E, \phi_i\right\rangle \phi_i \right\rangle \\
&= \sum_i \frac{1}{\sigma_i}\left\langle c_0 - c_E, \phi_i\right\rangle \left\langle 1_S, \phi_i\right\rangle \\
&\le \frac{1}{\sigma_1}\left(\sum_i \left\langle c_0 - c_E, \phi_i\right\rangle^2\right)^{1/2}\left(\sum_i \left\langle 1_S, \phi_i\right\rangle^2\right)^{1/2} \qquad \text{(III.7)} \\
&= \frac{1}{\sigma_1}||c_0 - c_E||_2||1_S||_2 \\
&\le \frac{1}{\sigma_1}||c_0 - c_E||_2\sqrt{|S|} \\
&\le \frac{1}{\sigma_1}\sqrt{2}Nn^{1/2}\ ,
\end{aligned}$$

where (III.7) is by Cauchy-Schwarz, and $||c_0 - c_E||_2 \le ||c_0||_2$ is bounded above by $\sqrt{2}N$. This completes the proof of the theorem. □

This result can be stated in terms of the diameter of Γ rather than in terms of σ_1, by invoking the eigenvalue-diameter bound developed in Lemma I.10, which in this context states that $\sigma_1 \ge 1/(nD)$. We have the following corollary to Theorem III.8.

Corollary III.9. *Let D be the diameter of Γ. Under the same conditions as Theorem III.8, the length of the Dirichlet game is at most*

$$\sum_{x\in S} f(x) \quad \le \quad D\sqrt{2}\cdot Nn^{3/2}.$$

Theorem III.8 can also be used to address the game length of a terminating basic game. A result of Tardos [111] gives that every terminating basic game has a vertex which is never fired. Otherwise if all vertices are fired, consider the vertex v whose last appearance in the firing sequence is as early as possible. All neighbors of v appear in the firing sequence after v, and so v is ready at the end of the firing sequence, which is a contradiction. This observation leads to the following improvement by a factor of $\sqrt{2}n^{1/2}$ over Theorem 4.2 of [18], which states that any terminating basic game on Γ has length at most $2n^2DN$, where the quantities have the same definition as in Corollary III.9.

Corollary III.10. *Every terminating basic chip-firing game with N chips on a graph Γ with diameter D has length at most $D\sqrt{2}\cdot Nn^{3/2}$ steps, where $n = |V(\Gamma)|$.*

Proof. Given the initial configuration c_0 of N chips and the fact that the basic game terminates, Theorem III.6 gives that every possible game played to termination starting from c_0 has the same score vector. By the result of Tardos discussed above, there is a vertex v which every possible basic game leaves unfired. Then the basic game on Γ starting with c_0 is equivalent to the Dirichlet game on Γ with $\delta S = \{v\}$ starting with the initial configuration c_0' obtained from c_0 by setting $c_0'(v) = 0$. The two games have the same firing sequence and length, which is bounded above by Theorem III.9. □

III.C A matrix-tree theorem for induced subgraphs with Dirichlet boundary condition

For a graph Γ and vertex set $S \subsetneq V(\Gamma)$ chosen according to our assumptions in Section III.A, we define a *rooted spanning forest* of S to be a subgraph F satisfying

(1) F is an acyclic subgraph of Γ,

(2) F has vertex set $S \cup \delta S$,

(3) Each connected component of F contains exactly one vertex in δS.

The following theorem relates the product of Dirichlet eigenvalues of S with the enumeration of rooted spanning forests of S. The proof method is quite similar to the original proof of the matrix-tree theorem as well as the proof in [34]. For completeness, we will briefly sketch the proof here.

Theorem III.11. *For an induced subgraph $\Gamma(S)$ of S in a graph Γ with $\delta S \neq \emptyset$, the number $\tau(S)$ of rooted spanning forests of S is*

$$\tau(S) = \prod_{i=1}^{|S|} \sigma_i$$

where σ_i are the Dirichlet eigenvalues of the Laplacian L_S of Γ.

Proof. Let $s = |S|$. We consider the incidence matrix B with rows indexed by vertices in S and columns indexed by edges in Γ as follows:

$$B(x,e) = \begin{cases} 1 & \text{if } e = \{x,y\}, x < y \\ -1 & \text{if } e = \{x,y\}, x > y \\ 0 & \text{otherwise} \end{cases}$$

We have

$$L_S = B\ B^* \tag{III.8}$$

where B^* denotes the transpose of B.

We have

$$\begin{aligned} \prod_{i=1}^{s} \sigma_i &= \det L_S \\ &= \det B\ B^* \\ &= \sum_X \det B_X \det B_X^* \end{aligned}$$

where X ranges over all possible choices of s edges and B_X denotes the square submatrix of B whose s columns correspond to the edges in X. This expansion over X, known as the Cauchy-Binet expansion, is described in [82].

Claim 1: If the subgraph with vertex set $S \cup \delta S$ and edge set X contains a cycle, then $\det B_X = 0$.

The proof is similar to that in the classical matrix-tree theorem and will be omitted.

Claim 2: If the subgraph formed by edge set X contains a connected component having two vertices in δS, then $\det B_X = 0$.

Let Y denote a connected component of the subgraph formed by X. If Y contains more than one vertex in δS, then Y has no more than $|E(Y)| - 1$ vertices in S. The submatrix formed by the columns corresponding to edges in Y has rank at most $|E(Y)| - 1$. Consequently, $\det B_X = 0$.

Claim 3: If the subgraph formed by X is a rooted forest of S with roots δS, then $|\det B_X| = 1$.

The claim follows by definition of B_X.

Combining Claims 1-3, we have

$$\prod_{i=1}^{|S|} \sigma_i = \det L_S = \sum_X \det B_X \det B_X^* = |\{\text{rooted spanning forests of } S\}|,$$

which completes the proof of the theorem. □

We remark that the usual matrix-tree theorem can be viewed as a special case of Theorem III.11. Namely, for a graph Γ, we apply Theorem III.11 to Γ with $\delta S = \{v\}$ for some vertex v in Γ. The rooted spanning forests of $S = V(\Gamma) \setminus \{v\}$ are all spanning trees on Γ.

III.D Dirichlet-critical configurations and rooted spanning forests

The Dirichlet-critical configurations of the Dirichlet game can be characterized in several non-trivially different ways, and as a set have the same cardinality as the number of spanning forests of Γ rooted in δS. In fact, a bijection between the two sets may be obtained algorithmically by playing a chip-firing game using the Dirichlet-critical configuration as a starting point. This bijection will be described after we state and discuss the following useful facts on Dirichlet-critical configurations.

Lemma III.12. *Let c be a stable configuration of the Dirichlet game. Then the following are equivalent:*

(a) *c is Dirichlet-critical.*

(b) *There exists a configuration b and a firing sequence $\mathcal{F}$ such that b yields c under $\mathcal{F}$ and each vertex in S appears at least once in $\mathcal{F}$.*

(c) *There exists a configuration b and a firing sequence $\mathcal{F}$ such that b yields c under $\mathcal{F}$ and each vertex in S appears exactly once in $\mathcal{F}$.*

(d) *Starting with c, if one chip is added at every vertex v for each edge crossing into δS to obtain a second configuration b, then there is a firing sequence $\mathcal{F}$ which is a permutation of S such that b yields c under $\mathcal{F}$.*

Proof. The equivalence of (a), (c), and (d) follows directly from Corollary III.4. The chips added to c in (d) corresponds to adding the configuration $\overline{\beta}$ defined for Corollary III.4. The resulting configuration $b = c + \overline{\beta}$ both certifies that c is Dirichlet-critical and yields c under a firing sequence which is a permutation of S.

We have (c)$\Rightarrow$(b) trivially, and prove (b)$\Rightarrow$(c) as follows. Consider a configuration b and a firing sequence $\mathcal{F} = (\mathcal{F}(1), \ldots, \mathcal{F}(L))$ in which each vertex in S appears at least once such that $b + c$ yields c under $\mathcal{F}$. We assume the length of $\mathcal{F}$ is more than $|S|$ to avoid the trivial case. We will rearrange $\mathcal{F}$ to obtain a new allowable firing sequence for the Dirichlet game starting in configuration $b + c$ whose last $|S|$ vertices are a permutation of S. Define the *complete tail* $\mathcal{T}$ of $\mathcal{F}$ to be the shortest possible firing sequence $\mathcal{T} = (\mathcal{F}(k), \ldots, \mathcal{F}(L))$ in which every vertex appears at least once. If $\mathcal{T}$ is of length $|S|$, we are done, and the configuration b' determined by the Dirichlet game played on $b+c$ with firing sequence $(\mathcal{F}(1), \ldots, \mathcal{F}(k-1))$ yields c under $\mathcal{T}$. Now suppose $\mathcal{T}$ has length less than $|S|$. Let $u = \mathcal{F}(k)$. Then there is some vertex $v \neq u$ in S which occurs twice in $\mathcal{T}$. Choose as v the vertex whose second occurrence in $\mathcal{T}$ is as early as possible. Let the first two appearances of v in $\mathcal{T}$ be denoted by $\mathcal{F}(r)$ and $\mathcal{F}(s)$, where $k < r < s \leq L$. Let c_1 be the configuration which $b + c$ yields under the firing sequence $(\mathcal{F}(1), \ldots, \mathcal{F}(k-1))$. Then v must be ready in configuration c_1, because each neighbor of v appears at most in the firing subsequence $(\mathcal{F}(k), \ldots, \mathcal{F}(s-1))$. Thus we can move the first occurrence of v in $\mathcal{T}$ at $\mathcal{F}(r)$ left in the sequence to replace $\mathcal{F}(k)$; all vertices it is moved over shift to the right one place in the sequence. Specifically, this defines a new firing sequence $\mathcal{F}'$ such that

$$\mathcal{F}'(t) = \begin{cases} \mathcal{F}(t+1), & \text{if } k \leq t < r \\ \mathcal{F}(r), & \text{if } t = k \\ \mathcal{F}(t), & \text{otherwise.} \end{cases}$$

$\mathcal{F}'$ is also an allowable firing sequence for $b + c$ which yields c, and the complete tail $\mathcal{T}'$ of $\mathcal{F}'$ is one vertex shorter than $\mathcal{T}$. We replace $\mathcal{F}$ with $\mathcal{F}'$ and repeat the process until the complete tail is of length $|S|$. Denoting this final firing sequence by $\mathcal{F}$, let b' be the configuration yielded by firing $(\mathcal{F}(1), \ldots, \mathcal{F}(L - |S|))$ starting with the initial configuration $b + c$. Then b' is the required configuration which yields the Dirichlet-critical configuration c under the firing sequence $(\mathcal{F}(L - |S| + 1), \ldots, \mathcal{F}(L))$, which is a permutation of S. $\square$

We note that the equivalence of (b) with the other three properties was proved independently as Theorem 3.6 of [116]. An alternate way of obtaining the results for the general case from the case for $|\delta S| = 1$, thus preserving the structure of the boundary, is as follows. Beginning with the Dirichlet game on Γ, create Γ_q by attaching a distinguished vertex q by a single edge to each vertex in δS. Now take $S_q = S \cup \delta S$ and δS_q to be only this vertex q. For a Dirichlet-critical configuration c from the original game, define the configuration c_q on the new game by

$$c_q(v) = \begin{cases} c(v) & \text{if } v \in S, \\ \deg_{\Gamma_q}(v) - 1 & \text{if } v \in \delta S, \\ 0 & \text{if } v = q. \end{cases} \tag{III.9}$$

Whenever c is Dirichlet-critical, c_q is a critical configuration of the dollar game with specified "government" vertex q. All of the necessary information about the Dirichlet-critical configuration c may be obtained by using existing theorems on c_q for the dollar game in [15]. This leads us to the main theorem of the section.

Theorem III.13. *The number of Dirichlet-critical configurations of the Dirichlet game on Γ is the same as the number of spanning forests of Γ rooted in δS.*

Proof. In the case of $|\delta S| = 1$, Biggs and Winkler have proved the theorem for the equivalent dollar game in Theorems 1-3 of [15]. For completeness, we sketch the proof in the language of the Dirichlet game as follows. Consider the Dirichlet game on Γ with boundary $\delta S = \{q\}$. Note that spanning forests of Γ rooted in δS can be viewed as spanning trees of Γ. Fix once and for all a total ordering on the edges of Γ. Let c be a Dirichlet-critical configuration of Γ. We require a bijective mapping

$$\theta : \{\text{Dirichlet-critical configurations}\} \to \{\text{spanning trees of } \Gamma\}.$$

Define $\theta(c) = T$ as follows.

Algorithm A

(i) Initialize $T = \{\}$, the tree to be constructed.

(ii) Add chips to the game as if q were fired (equivalent to adding $\overline{\beta}$ defined in Section III.A.2 to c). The number of chips at q remains 0. Add $\{q, u\}$ to T for each u adjacent to q which becomes ready.

(iii) Fire a vertex v that is ready. Ties are broken by firing the vertex v where the shortest path from q to v has an ordered edge list which is least possible in the lexicographic ordering on tuples of edges. If v primes any vertex u, add edge $\{u, v\}$ to T.

(iv) Repeat (iii) until all vertices have been fired.

That this process is well-defined and completes with T a spanning tree of Γ is a result of part (d) of Lemma III.12. We observe that by Corollary III.4, each vertex is both primed and fired exactly once in Algorithm A, and so T is in fact a spanning tree rooted in $\delta S = \{q\}$. The details of proving that θ is a bijection may be viewed in [15]. This completes the sketch of the proof for $|\delta S| = 1$.

Now, let Γ be a general Dirichlet game with boundary δS where $|\delta S| \geq 1$. We require a bijective mapping

$$\theta_q : \{\text{Dirichlet-critical configurations on } \Gamma\} \to \{\text{spanning forests of } \Gamma \text{ rooted in } \delta S\}.$$

Define θ_q as follows. Convert Γ to a Dirichlet game with boundary of size 1 by constructing Γ_q from Γ as previously described, recalling that $S_q = S \cup \delta S$ and $\delta S_q = \{q\}$. Let c be a Dirichlet-critical configuration of Γ. Define a configuration c_q of Γ_q according to (III.9). Use c_q to construct a spanning tree T of Γ_q using Algorithm A. Remove the edges $\{q, v\}$ for all $v \in \delta S$ from T to obtain a spanning forest F rooted in δS. Let $\theta_q(c_q) = F$. We must show that θ_q defined in this way is a bijection.

First we show that θ_q is well-defined. To show that c_q is Dirichlet-critical for the game on Γ_q, note that c_q is stable. Also, c_q must be recurrent. Adding one chip to each vertex adjacent to q in Γ_q primes each vertex in δS. Firing each vertex of δS in succession causes one chip to be added at each vertex $v \in S$ for each edge crossing into δS. Then by Lemma III.12(d) for the Dirichlet game on Γ, there is a permutation in which the vertices of S may be legally fired. Every vertex $v \neq q$ has now been fired, yielding the original configuration c_q. By Lemma III.12(d) for the Dirichlet game on Γ_q, c_q is Dirichlet-critical. Also, we must show that F is a spanning forest of Γ rooted in δS. But all that is required for this is that the tree T produced in Algorithm A contain all edges $\{q, v\}$ for $v \in \delta S$. This is true since Step 2 of the algorithm primes every vertex in δS (recall that $c_q(v) = \deg_{\Gamma_q}(v) - 1$ for all $v \in \delta S$). Therefore F is a spanning forest of Γ rooted in δS and θ_q is well-defined.

Now we must show that θ_q is one-to-one. The preparatory mapping from c to c_q is one-to-one because the values of c on S are preserved. The Biggs-Winkler bijection θ gives a one-to-one mapping from the Dirichlet-critical configurations on Γ_q (critical configurations of the equivalent dollar game) to the spanning trees T of Γ_q. In going from T to F, the exact same edges, $\{\{q, v\} | v \in \delta S\}$, are removed from T in each case, so this step is also a one-to-one mapping. Thus θ_q as the composition of three one-to-one mappings is one-to-one.

Finally, we must show that θ_q is onto. Let F be a spanning forest of Γ rooted in δS. Construct T in Γ_q by adding all edges $\{\{q, v\} | v \in \delta S\}$. From the Biggs-Winkler bijection θ, we obtain the Dirichlet-critical configuration c_q for Γ_q which corresponds to this T. Because all edges $\{\{q, v\} | v \in \delta S\}$ are in T, Step 2 of Algorithm A must prime all vertices in δS, and thus $c_q(v) = \deg_{\Gamma_q}(v) - 1$ for all $v \in \delta S$. Define c on S by restricting c_q to S. Since c_q is Dirichlet-critical, after adding chips to all vertices adjacent to q there is a permutation in which all the other vertices may be legally fired. This implies that in the Dirichlet-game on Γ, after adding one chip to $v \in S$ for each edge incident to a vertex in δS, there is a permutation of S which is a legal firing sequence and yields the same original configuration, c. Thus c is Dirichlet-critical for Γ. Therefore $\theta_q(c) = F$, completing the proof of Theorem III.13. $\square$

III.E The sandpile group and rooted forests

The *sandpile group* originated from *abelian sandpile model*, sometimes called the *avalanche model*, which considers the behavior of grains of sand piled onto the nodes of a structure [44, 45]. Once the number of grains of sand at a particular node exceeds a threshold condition, the sand topples down (fires) from this more saturated node, possibly causing sand in adjacent nodes to exceed stability thresholds as well (thus the notion of avalanches). On a graph, the threshold at a vertex is exceeded when the vertex gets a number of grains of sand (chips) equal to its degree. The sandpile group of a graph models the allowable transitions which may occur when vertices topple in succession. A starting sandpile configuration is a member of one of the cosets of the sandpile group. As we wish to view the toppling of sand as leaving the underlying structure or dynamics of the sandpile unchanged, toppling is modeled by traveling to various other members of the same coset via the allowable transitions.

The sandpile group of a graph is defined as follows. Let $V(\Gamma) = \{1, \ldots, n\}$, and root the graph Γ at vertex n. Consider $\mathbb{Z}^n$ as a group under addition, and associate each vertex i with the standard basis vector $x_i \in \mathbb{Z}^n$. Define

$$\Delta_i = \deg_\Gamma(i) x_i - \sum_{j=1}^{n} A(i,j) x_j,$$

where $\deg_\Gamma(i)$ is the degree of i in Γ and A is the adjacency matrix of Γ. Δ_i may be interpreted as the i^{th} row vector of the Laplacian of Γ; subtracting Δ_i from a configuration corresponds to toppling (firing) vertex i. Then the sandpile group $\mathrm{SP}(\Gamma)$ of Γ is the group

$$\mathrm{SP}(\Gamma) = \mathbb{Z}^n / \langle \Delta_1, \ldots, \Delta_n, x_n \rangle .$$

The order of $\mathrm{SP}(\Gamma)$ is the number of spanning trees of Γ; this is a restatement of the *Matrix-Tree Theorem*. In fact, a group structure may be imposed on the Dirichlet-critical configurations of the Dirichlet game with boundary $|\delta S| = 1$ which yields a group isomorphic to $\mathrm{SP}(\Gamma)$. For the equivalent dollar game, critical configurations under the operation '$\oplus$' (defined in Section III.A.2) are shown to be isomorphic to $\mathrm{SP}(\Gamma)$ in [14]. For the equivalent sandpile model, sandpile-recurrent configurations under '$\oplus$' are shown to be isomorphic to $\mathrm{SP}(\Gamma)$ in [37].

We now define a more general sandpile group which is related to the Dirichlet-critical configurations of the Dirichlet game. Let $V(\Gamma) = \{1, \ldots, n, n+1, \ldots, n+m\}$ with $S = \{1, \ldots, n\}$ and $\delta S = \{n+1, \ldots, n+m\}$, by relabeling if necessary. Define

$$\mathrm{SP}_S(\Gamma) = \mathbb{Z}^{m+n} / \langle \Delta_1, \ldots, \Delta_{n+m}, x_{n+1}, \ldots, x_{n+m} \rangle .$$

The motivation for constructing $\mathrm{SP}_S(\Gamma)$ is to encode the firing rule for vertex $i \in S$ with the Δ_i and the processing of chips in δS by $x_{n+1}, \ldots, x_{n+m}$. As a result, two configurations of the Dirichlet game are in the same coset of the coset group $\mathrm{SP}_S(\Gamma)$ if one can be reached from the other by firing a sequence of vertices. The size of $\mathrm{SP}_S(\Gamma)$ is given by the next theorem.

Theorem III.14. *Let $SP_S(\Gamma)$ be the generalized sandpile group on Γ with specified vertex set S and boundary set δS. Then*

$$|SP_S(\Gamma)| = det\ L_S = \tau(S),$$

where L_S is the restricted Laplacian of Γ, and $\tau(S)$ is the number of spanning forests of Γ rooted in δS.

Theorem III.14 is a restatement of Theorem III.11, the generalized Matrix-Tree theorem for rooted spanning forests. Thus we know that the set of Dirichlet-critical configurations has the same size as the order of $\mathrm{SP}_S(\Gamma)$, which leads us to desire a meaningful bijection between the two sets. We now state the main theorem of the section, which Cori and Rossin proved as Theorem 1 of [37] for the equivalent sandpile model with a unique root vertex δS.

Theorem III.15. *$SP_S(\Gamma)$ is isomorphic to the set of Dirichlet-critical configurations of the chip-firing game with Dirichlet boundary $\delta S = \{n+1, \ldots, n+m\}$.*

Proof. The proof may be had as an extension of the proof of Theorem 1 of [37]. We now outline that extension. A configuration u of the Dirichlet game may be viewed as an element of $\mathrm{SP}_S(\Gamma)$ simply by extending u to be 0 on δS. For future reference, call this extension $\phi(u)$. Thus adding two configurations of the game corresponds to adding vectors in the group. Recall that we equip the set of Dirichlet-critical configurations with a candidate group operation $\oplus$ by defining $x \oplus y$ to be the unique Dirichlet-critical configuration obtained as the final configuration of the Dirichlet game played with initial configuration $x+y$. In order to prove the theorem by showing that $\oplus$ is a group operation for which ϕ is an isomorphism, it is sufficient to show that for any configuration u in the Dirichlet game there exists a unique Dirichlet-critical configuration v such that

$$u - v \in \Delta_S := \langle \Delta_1, \ldots, \Delta_{n+m}, x_{n+1}, \ldots, x_{n+m} \rangle . \tag{III.10}$$

That is, every Dirichlet-critical configuration matches with exactly one coset of the general sandpile group for Γ. In order to show existence of v in (III.10), there must be a way of starting with any configuration u and obtaining a Dirichlet-critical configuration in the same coset. This is achieved by adding u together with a cleverly chosen configuration $u' \in \Delta_S$ such that $u + u'$ yields a critical configuration v under a firing sequence. We may take $u' = k\overline{\epsilon}$ for sufficiently large $k \in \mathbb{N}$, where $\overline{\epsilon}$ is defined in Section III.A.2. Since $u' \in \Delta_S$, u and $u + u'$ are in the same coset, and the firing rules are encoded by elements of Δ_S; u and v are in the same coset. Thus the existence of v is ascertained. Uniqueness of v in (III.10) is shown by proving that if u and v are both Dirichlet-critical configurations with $u - v \in \Delta_S$, then $u = v$. □

Corollary III.16. *The mapping ϕ from Dirichlet-critical configurations of Γ to $SP_S(\Gamma)$, where $\phi(c)$ is defined by extending c to be 0 on δS, is a bijection from Dirichlet-critical configurations to cosets of the general sandpile group $SP_S(\Gamma)$.*

III.F Finding Dirichlet-critical configurations

By Theorem III.15, every configuration in the Dirichlet game corresponds to a unique Dirichlet-critical configuration which is in the same sandpile group coset. We now develop an algorithm which produces the Dirichlet-critical configuration corresponding to an arbitrary configuration. Subjectively, starting with an arbitrary configuration c, if enough chips are added to completely saturate the graph, playing the game will terminate in a Dirichlet-critical configuration. Corollary III.9 gives a bound on the length of this game, but the bound depends on the number of chips the game starts with. If c has an arbitrarily large number of chips, the game length bound may be unfavorable. This difficulty is circumvented by preconditioning c with the Green's function in order to obtain a configuration c' in the same coset as c but with a small number of chips. Then c' is saturated with enough chips to guarantee game termination in a Dirichlet-critical configuration. For the sandpile game, Cori and Rossin show [37, §2] that any initial configuration c satisfying $c(v) \geq d_v$ for all non-root vertices v terminates in a sandpile-recurrent configuration. The same technique of extension as in the previous section gives the analogous result for the Dirichlet game.

Lemma III.17. *Let c be a configuration of the Dirichlet game with $c(v) \geq d_v$ for all $v \in S$. Then the game terminates in a Dirichlet-critical configuration.*

The following lemma, extended from the case of $|\delta S| = 1$ [116, Lemma 8.3], describes how to precondition a configuration with a large number of chips. The proof is due to van den Heuvel and is included for completeness.

Lemma III.18. *Let $|\delta S| \geq 1$. Given a configuration c in the Dirichlet game and the (nonsingular) discrete Green's function G of Γ, the configuration c' defined by*

$$c' = c - L_S \lfloor Gc \rfloor$$

satisfies $|c'(v)| < d_v$ for all $v \in S$.

Proof. Let $t = Gc - \lfloor Gc \rfloor$ so that $0 \leq t(v) < 1$ for all $v \in S$. Then

$$L_S t = c - L_S \lfloor Gc \rfloor = c'.$$

Integrality of c' is guaranteed since c and $\lfloor Gc \rfloor$ are both integral. Now for $v \in S$,

$$\begin{aligned} c'(v) &= L_S t \\ &= t(v) d_v - \sum_{u \in S, u \sim v} t(u). \end{aligned}$$

The $t(v)d_v$ term contributes strictly less than d_v, and the summation contributes strictly more than $-d_v$. Combined with integrality of c', the result follows. □

The previous two steps are combined to yield an algorithm for determining the Dirichlet-critical configuration corresponding to an arbitrary configuration.

Theorem III.19. *Given a configuration c in the Dirichlet game with nonempty boundary, computing the corresponding Dirichlet-critical configuration requires at most*

$$7\sqrt{2}\, vol(S) D n^{3/2}$$

vertex firings and $O(n^{\omega})$ arithmetic operations, where D is the diameter of Γ, $n = |S|$, and $2 \leq \omega \leq 2.376$ is the power of the complexity of matrix multiplication.

Proof. Applying Lemma III.18 to c yields a new configuration c' which satisfies $|c'(v)| < d_v$ for all $v \in S$, and which is in the same sandpile coset in $\mathrm{SP}_S(\Gamma)$ as c. This is done at the cost of $O(n^\omega)$ arithmetic operations for matrix inversion and less complex operations. The configuration $\overline{\epsilon}$, defined in Section III.A.2, requires playing the game on $\delta \oplus \delta$, which by Corollary III.9 terminates in at most $2\sqrt{2}\,vol(S)Dn^{3/2}$ firings, since $\delta(v) = d_v$ for all $v \in S$. By the definition of $\overline{\epsilon}$, $d_v < \overline{\epsilon}(v) \leq 2d_v$ for all $v \in S$, and $\overline{\epsilon} \in \Delta_S$. Thus the configuration $c' + 2\overline{\epsilon}$ has at least d_v chips at each vertex $v \in S$ and corresponds to the same Dirichlet-critical configuration as c. By Lemma III.17, playing the Dirichlet game on $c' + 2\overline{\epsilon}$ terminates in a Dirichlet-critical configuration. Since $c' + 2\overline{\epsilon}$ has at most $5d_v$ chips at each vertex $v \in S$, applying the game length bound in Corollary III.9 with $N = 5\,vol(S)$ yields the result. □

If the discrete Green's function G is already known, the number of arithmetic operations required to compute c' is reduced to $O(n^2)$. If G is computed from a compact formula such as that in Theorem II.16, facing the full computational complexity of matrix inversion can be avoided. A result similar to Theorem III.19 appears as [116, Theorem 1.7], but uses edge-connectivity instead of diameter, and requires a much more complex analysis of a construct called the "oil game" to bound game length.

III.G Problems and remarks

There are several related versions of the Dirichlet game that we will mention here.

(i) The construction Γ_q in Section III.D is used instead of contracting all boundary vertices into one vertex in order to emphasize the geometry of the boundary δS. This emphasis might be important in, for example, grid graphs with boundary along the exterior. These graphs appear in load-balancing problems and in applications of statistical physics.

(ii) The technique in Lemma III.18 can also be used in the case of no boundary to find a "balanced" configuration c' corresponding to an initial configuration c with N

chips by setting

$$c' = c - L\lfloor Gc \rfloor.$$

The resulting configuration has the same number of chips and is balanced in the sense that $|c'(v) - N/n| < d_v$ for all vertices v, where $n = |V(\Gamma)|$.

(iii) The basic chip-firing game model is different in that it has no boundary vertices to process chips; therefore games may proceed indefinitely provided that there are enough chips in the right configuration (see [18, Theorem 3.3]). A directed version of the basic game may be found in [17].

(iv) The dollar game variant seems to capture properties of critical configurations especially well. Related results appear in [11, 13, 14, 15, 37, 88, 116].

(v) The sandpile model, dollar game, Dirichlet game, and other chip-firing variants have the special property that the resulting configuration of a game with a certain score vector (defined in Section III.A) is independent of the order in which the vertices appear in the firing sequence. This has led to parallel chip-firing games [16] in which all the vertices that are ready at one stage are fired simultaneously. A succession of configurations in a parallel chip-firing game will also be configurations in the corresponding non-parallel game, but in general not vice-versa. An infinite parallel chip-firing game will eventually stabilize with the same subsequence of configurations repeated over and over again, which leads naturally to questions concerning the periodicity of such recurrences. Parallel games are also considered in [50, 79, 105].

(vi) Chip-firing on the infinite path (infinite in both directions) has been studied extensively in [4]. The initial configuration considered is a finite number of chips placed on a single vertex. Every vertex may be fired. Results include the characterization of the possible final configurations and bounds on the number of firings required.

(vii) Sandpile models on finite dimensional lattices have been studied in detail, especially from the point of view of self-organized criticality. Computational complexity of sandpiles on lattices, and more specifically, the inherent complexity of computing stable and recurrent states, is treated in [102]. In fact, it is shown that any problem solvable with a polynomial time algorithm may be reduced to determining the final state of a sandpile model on a finite lattice. The reader is referred to the bibliography of this paper for references to work done on sandpile model variations of interest in physics.

There are numerous open questions concerning chip-firing which remain unsolved. Here we describe some of these problems and mention associated remarks:

- Of interest is to have an intuitive bijection between spanning forests rooted in δS and Dirichlet-critical configurations that does not depend on a total ordering of edges (cf. Theorem III.13). Van den Heuvel [115] claims to have such a bijection for the dollar game.
- There is an interesting connection between critical configurations and the Tutte polynomial by an 1-dimensional grading of critical configurations in terms of the number of chips [88]. In fact, it may be possible to obtain other or finer (e.g., 2-dimensional) gradings using the Tutte polynomial.
- Chip-firing games can be used to model several aspects of Internet computing, in particular, in connection with routing and fault tolerance. One such model assumes that chips are labeled by messages which they carry, and studies the propagation of messages in terms of informed and uninformed nodes of the network. Numerous directions remain to be explored.

Acknowledgement

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Chapter IV

Dummy Fill as a Reduction to Dirichlet Chip-Firing

In the manufacture of silicon wafer microchips containing extremely small metal features, non-uniformity of the density of these features can be a major source of loss in manufacturing yield [63]. Microchips are manufactured as successive layers of wafers and metal microchip layout features; each layer must be planarized before adding the next layer. The current planarization standard is known as *chemical-mechanical polishing* (CMP). Dummy metal features which we call *dummy fill* are superimposed on the layout features of a chip layer so that the total layout density is more uniform, and the logical function of the chip is unchanged. Due to variations in CMP effects, density of layout features and dummy fill has a direct effect on variations in the height of the surface

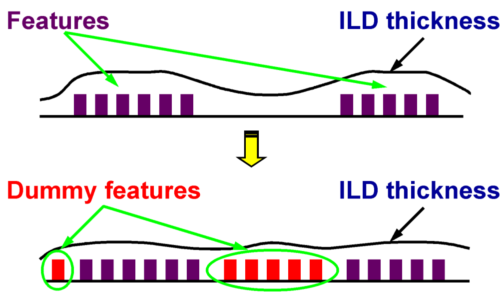

Figure IV.1: Insertion of dummy features to decrease post-CMP variation of ILD thickness.

of the microchip layer (interlayer dielectric height, or ILD height) after polishing (see Figure IV.1). As these height variations are undesirable, it is of interest to reduce density variations in order to obtain a smoother, flatter microchip layer surface. A more detailed explanation of the use of dummy fill for layout density control is found in [77].

In this chapter, we use a modified version of the Dirichlet game of Chapter III to achieve more uniform layout density. The microchip layer surface is divided into equal parts by a rectangular grid, with each cell of the grid corresponding to a vertex in the game. Placement of dummy fill corresponds to a choice of chip configuration in the game, where a chip corresponds to the smallest indivisible unit of dummy fill. We describe the particulars of the modifications used to address the layout density control problem in Sections IV.A and IV.B, discuss properties of the layout control game in Section IV.C, and present results on various real-world microchip layer density control problems in Section IV.D.

IV.A Layout density control in the r-dissection context

In practice, the post-planarization height of the chip layer depends only locally on the density of the surrounding metal. This leads to the choice of controlling layout density by examining and controlling density in square *windows* on the layout surface. We could examine and control density in every possible square window over the rectangular layout surface, but a more computationally tractable choice is to consider a finite number of evenly spaced, overlapping windows. To this end we consider the layout region as being partitioned into square *tiles* (cells) whose width is determined by the horizontal and vertical spacing between adjacent, overlapping windows. A square window is the union of r^2 tiles, where r is a positive integer, and can be identified with the tile which lies flush in its upper left-hand corner. This formulation is known as the *r-dissection context* (see Figure IV.2). The following parameters come into play:

- M, N, the length and height of the rectangular layout region,
- w, the fixed window width of the square windows
- U, the upper bound on the density of each window,

- L, the lower bound on the density of each window, and
- r, the number of tiles fitting across the side of a window (so that a window is the union of r^2 tiles), assumed to divide both M and N evenly.

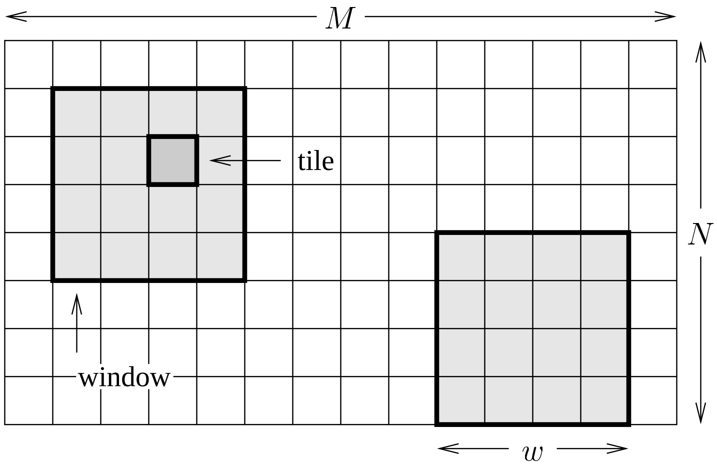

Figure IV.2: An $M \times N$ rectangular layout region in the r-dissection context with $r = 4$, window size $w \times w$ and tile size $w/r \times w/r$

We assume that the tile width w/r divides both M and N evenly; otherwise M and N are rounded up to the nearest tile by padding with blank layout space when necessary. Density bounds U and L lie in $[0, 1]$. For the sake of the reduction to the Dirichlet chip-firing game, we neglect side constraints presented in [77], such as preservation of design-rule correctness and geometric constraints. We justify this assumption in practice by referring to data which gives the maximum number of dummy fill units of a predetermined shape which can be added in a given tile in the grid; this data will introduce a new chip-firing constraint – the maximum number of chips that a tile (vertex) may have.

Possible objectives for placing dummy fill to control layout density include the following. Fill is placed in tiles so that no window violates the upper or lower bound on density, and

(i) **(Min Variation)** the variation in density of fill among all possible windows is minimized,

(ii) **(Max Fill)** the minimum density of all windows is maximized,

(iii) **(Min Fill)** the total amount of fill is minimized.

The imposition of a design objective such as the three above introduces a major new consideration to the chip-firing paradigm; in particular, choices of vertices (tiles) to fire must be made with the imposed design goal in mind, so that the final configuration of the game satisfies the objective. Because the nature of the basic chip-firing game (defined in Section III.A.2) is to balance a load with static total value (total number of chips), the most natural application of chip-firing is to approximate minimum variation with a fixed total amount of fill; therefore the pure minimum variation objective is more difficult to address. The maximum fill objective can be pursued using the basic chip-firing game by adding as many chips as possible while still allowing termination of the game in a configuration which satisfies all density constraints. The difficulty here lies in determining the quantity and location of chips to be added. The Dirichlet game is naturally adaptable to pursue the third density control objective, Min Fill, which we now present in the r-dissection context.

IV.B Reduction of Min-Fill objective to the Dirichlet game in the r-dissection context

The Min-Fill objective, described in [27, 28, 114], seeks to insert fill so that density of each window lies between L and U where the total amount of inserted fill is minimized. In the r-dissection context, the entire layout region is partitioned into an $(Nr/w) \times (Mr/w)$ grid of tiles. We formalize the reduction of density control with Min Fill objective to the Dirichlet game in the r-dissection context as follows. Let the function $f : \{T \mid T \text{ a tile}\} \to \mathbb{R}_{\geq 0}$ denote the quantity of fixed features preexisting in the tiles. Let $s : \{T \mid T \text{ a tile}\} \to \mathbb{Z}_{\geq 0}$ denote the new capacity constraint, i.e., the maximum number of chips each tile may have. The Min-Fill objective is to determine a function $c : \{T \mid T \text{ a tile}\} \to \mathbb{Z}_{\geq 0}$ so that for every square window W,

- $c(T) \leq s(T)$ for all tiles T,
- $L \leq \left(\sum_{T \in W} f(T) + c(T)\right) / \delta_{\max} \leq U$, and
- $\sum_T c(T)$ is minimized.

Here, $\delta_{\max}$ is the constant of normalization which gives the density of a window from the total quantity of fixed features and fill in the tiles of the window. This constant depends on manufacturing parameters but is typically proportional to the area w^2 of a window. We pursue the Min Fill objective by running the Dirichlet game of Chapter III *backwards*, adding chips from across the boundary to satisfy the lower bound on density for each window, in such a way that the upper bound on density is respected and the total number of chips is approximately minimized.

Throughout the chapter, the *normal Dirichlet game* refers to the Dirichlet chip-firing game defined in Chapter III. The reduction from the Min-Fill objective to Dirichlet chip-firing presented here will be called the *relaxed reverse fill Dirichlet game*, or more simply, the *fill game*. The game board Γ is defined with S considered to be the $(Mr/w) \times (Nr/w)$ grid graph of tiles, along with boundary tiles δS consisting of all "tiles" in the infinite grid of distance 1 from the game board. Edges of Γ are exactly those induced from the infinite grid graph (where each vertex has 4 neighbors in the cardinal directions) except that there are no edges between vertices of δS. It is a *reverse* game because tiles are fired backwards, or *banked*. When a tile is fired in the normal game, it sends one chip to each neighbor. When a tile is banked in the reverse game, it grabs one chip from each neighbor. It is a *relaxed* game because every tile is allowed to go into deficit by at most 4 chips (if each of its neighbors banks while it has no chips itself). Relaxation is required to avoid premature termination of the fill game before window density bounds are satisfied. It is a Dirichlet game because banking a tile adjacent to a boundary tiles causes a new chip to be created for each boundary tile adjacent to the tile banked.

The list of relevant quantities for the reduction of the Min-Fill objective to the fill game is summarized as follows.

- **Feature density.** $f : \{T \mid T \text{ a tile}\} \to \mathbb{R}_{\geq 0}$ denotes the amount of density due to fixed features in a given tile. $f(T)$ contributes additively to the density of each windows containing T.
- **Tile slack.** Let $s : \{T \mid T \text{ a tile}\} \to \mathbb{Z}_{\geq 0}$ denote the maximum number of fill units (chips) that may be added to a tile T. Tile slack limits the ability of a tile to be banked, when it grabs chips from its neighbors.

- **Fill (chip) configuration.** $c : \{T \mid T \text{ a tile}\} \to \mathbb{Z}$ denotes the distribution of movable fill units (chips) over all tiles T. Initially, $c \equiv 0$. $c(T)$ contributes additively to the density of each window containing T, and determines the number of fill units in play.

- **Window density.** Density of a window W is
$$\left(\sum_{T \in W} f(T) + c(T)\right) / \delta_{\max}.$$

- **Least dense containing window.** $MinWin : \{\text{tiles } T\} \to [0,1]$ denotes the density of the least dense window W containing a given tile T.

- **Most dense containing window.** $MinWin : \{\text{tiles } T\} \to [0,1]$ denotes the density of the most dense window W containing a given tile T.

The fill game has initial configuration $c_0 \equiv 0$ and final configuration c_E. The game progresses by banking a single tile and updating the configuration. This leads to a sequence of configurations $c_0, c_1, \ldots, c_E$. The characteristics of the initial and final configurations do not necessarily depend upon the readiness status of tiles, as in Chapter III, but rather upon satisfaction of the Min-Fill objective. The banking rules, or the readiness of tiles to be banked, are determined as follows. Any tile with deficit may be banked. If there are no tiles with deficit, then a tile T with $MinWin(T) < L$ and $MaxWin(T) < U$ may be banked. The *banking sequence* $\mathcal{B} = (b_1, \ldots, b_\mu)$ records the order in which tiles are banked. The length of the fill game is $|\mathcal{B}| = \mu$.

It is useful to compare the fill game to a normal Dirichlet game. With this in mind, the *relaxed forwards fill Dirichlet game*, or more simply, the *forwards fill game*, is just the fill game run in reverse. Thus the forwards game starts in configuration c_E, ends in configuration c_0, and has firing sequence $\mathcal{F} = \mathcal{B}^R := (b_\mu, \ldots, b_1)$, which determines the order in which tiles are fired. The forwards game is almost a normal Dirichlet game, except that tiles are allowed to go into deficit (by at most 4 chips). In particular, chips fired from a tile to an adjacent boundary tile are removed from the game. The length of the forwards fill game is also $|\mathcal{F}| = \mu$.

The *augmented forwards fill game* is constructed by adding enough chips (4 per tile suffices) to the initial configuration of the forwards fill game so that firing tiles according to the firing sequence $\mathcal{F}$ causes no tiles to go into deficit. If tiles may still be fired after that, game play continues according to the normal Dirichlet game. It will be useful to note that the length of the augmented forwards fill game is at least the length of the fill game. This allows us to develop a bound on the length of the fill game by using the bound on the length of the normal Dirichlet game in Corollary III.9.

The banking rules of the fill game are summarized as follows.

(i) **Negative fill chip correction.** Tiles in deficit, with $c(T) < 0$, are banked before considering other tiles.

(ii) **MinWin prioritization.** In a configuration c, a tile T may be banked provided that $MinWin(T) < L$, $c(T) \leq s(T) - 4$, $MaxWin(T) < U$, and there is no tile T' in deficit.

(iii) **Game termination.** The game terminates when no tile may be banked.

The condition that $c(T) \leq s(T) - 4$ ensures that after T is banked, the fill units in T do not exceed the tile's capacity for fill units. The negative fill chip correction stage may in fact cause $c(T) > s(T)$, or an overfilling of a tile with fill, but this overfilling is never by more than 3 units; furthermore, at the end of the fill game we may either remove all fill units exceeding slack, or attempt to migrate them to nearby tiles with excess slack. Either choice has only a minor effect on window densities.

IV.C Properties of the fill game

In the beginning of the game, when there are no fill chips, whatever tile is banked creates a deficit of chips at its neighbors. These neighbors must be banked, which cause a deficit at their neighbors, etc., until all the tiles next to the boundary are banked, and satisfy the deficit by "creating" chips corresponding to adjacent boundary vertices. Then the next tile with satisfying the banking criteria is banked, negative chips are expunged again, and so forth.

After game termination, we perform two post-processing steps: *migration* and *greedy deletion*. Migration is necessary when a tile T is banked in order to clear its deficit, but ends up containing more chips than it has room for at the end of the game

$(c(T) > s(T))$. An attempt is made to move the surplus chips to neighboring tiles having the same $MinWin$ value and excess slack for chips. Chips that fail to migrate are removed.

Greedy deletion occurs as follows. Greedily remove a single chip from any tile T that has a positive number of fill chips (i.e., $c_E(T) > 0$), and whose removal does not violate the lower bound L on window density. This post-processing takes no longer than the game itself; each tile is checked at most once, and removal of chips requires updates of $MinWin$.

The result after migration and greedy deletion is the fill solution for the Min-Fill objective returned by the fill game. Termination of the fill game is perhaps the most fundamental requirement, but the extra density constraints make it difficult to prove.

Lemma IV.1 (Conjectured). *The relaxed reverse fill Dirichlet game with Min-Fill objective terminates.*

Sketch of possible proof: It is conjectured that a given fill game will correspond to a uniquely determined augmented forwards fill game (which depends on implementation choices). It is not clear that the fill game will terminate, due to complexities introduced to mandatory bankings of tiles in deficit. The following is given as intuition towards a proof of the lemma.

The length of the fill game is at most the length of the corresponding augmented forwards fill game (the existence of which is conjectured). The augmented forwards fill game is a normal Dirichlet game, and so by Lemma III.5, it terminates in a finite number of steps, and so the fill game terminates in a finite number of steps. $\square$

We now show how terminating configurations of the fill game are close to locally optimal fill solutions. A fill solution describes where to add fill to existing features. A locally optimal fill solution $h : \{T \mid T \text{ a tile}\} \to \mathbb{Z}$ for the Min-Fill objective has the following properties.

Definition of a locally optimal fill solution. A fill solution h is locally optimal provided that the following hold.

(i) **Feasibility.**

(a) **Nonnegativity.** $h(T) \geq 0$ for all tiles T.

(b) **Density attainment.** $\left(\sum_{T \in W} f(T) + h(T)\right) / \delta_{\max} \geq L$, for all windows W.

(ii) **Local optimality.** For any tile T^*, the candidate solution

$$h_{T^*}(T) = \begin{cases} h(T) - 1, & \text{if } T = T^* \\ h(T), & \text{otherwise} \end{cases}$$

violates feasibility condition (i)-(a) or (i)-(b).

The expression for density in (i)-(b) is representative of the calculation for density, and is chosen with the density bounds L and U in mind. In more general terms, the set of all nonnegative feasible fill solutions h forms a partial order, where $h_1 \preceq h_2$ provided that $h_1(T) \leq h_2(T)$ for all tiles T. Starting with a feasible fill solution h, we may obtain a (possibly non-unique) locally optimal fill solution by greedily decreasing the value of h by 1 on any tile T such that nonnegativity and feasibility are not violated.

Based on the banking rules, the fill game can be viewed as iteratively banking a single tile T with $MinWin(T) < L$ followed by clearing any deficits that might result. With this in mind, we define a *bank and clear cycle* of the banking sequence $\mathcal{B}$, or more simply, a *cycle* of $\mathcal{B}$, to be a contiguous subsequence of $\mathcal{B}$ consisting of a tile banked while not in deficit followed by as many tiles banked while in deficit as possible. Thus a banking sequence $\mathcal{B}$ has a unique decomposition as the concatenation of some finite number of cycles. A cycle consists of a *head*, which is a tile T banked when no tiles are in deficit and $MinWinT < L$, and a *body*, which consists of all tiles banked to clear deficits before the head of the next cycle.

Lemma IV.2. *Each tile appears at most once in a bank and clear cycle.*

Proof. Let $\mathcal{D}$ be a cycle of $\mathcal{B}$ in a fill game. Write $\mathcal{D} = (T_1, \ldots, T_k)$. The configuration c of the fill game just before T_1 is banked has no deficit tiles, by definition of a cycle. Suppose to the contrary that some tile T is banked twice in the cycle $\mathcal{D}$. Let T_r be such a tile where $1 \leq r \leq k$ is minimal. Because r is minimal, at most 4 neighbors of T_r bank before T_r banks the second time. But then T_r could not be in deficit when it banks the second time, since it started not in deficit, previously banked 4 chips, and lost at most 4 chips to its neighbors. Therefore no tile appears twice in $\mathcal{D}$. $\square$

A starting configuration of a fill game may admit many possible banking sequences, and thus many possible cycles. The next lemma shows that the order in which deficits are cleared does not matter. The game essentially depends only on the order in which tiles are banked when there is no deficit. After playing several cycles of the fill game, we might have a choice of how to play the next cycle; that choice depends only on what the current configuration is. This is the setting of the next lemma, and the techniques in the proof are related to the language properties discussed in Section III.B.

Lemma IV.3. *Let c be a configuration in the fill game such that $c \geq 0$ (there are no tiles in deficit). Let $\mathcal{D}_1$ and $\mathcal{D}_2$ be two cycles for that configuration with the same first tile T_1. Then $|\mathcal{D}_1| = |\mathcal{D}_2|$ and $\mathcal{D}_2$ is just a reordering of the tiles of $\mathcal{D}_1$.*

Proof. Without loss of generality, suppose $|\mathcal{D}_1| \leq |\mathcal{D}_2|$. By Lemma IV.2, we know $|\mathcal{D}_1|, |\mathcal{D}_2| \leq n$. Therefore we may write

$$\begin{aligned} \mathcal{D}_1 &= (T_1, T_2, \ldots, T_j), \qquad \text{and} \\ \mathcal{D}_2 &= (T_1, U_2, \ldots, U_k). \end{aligned}$$

In $\mathcal{D}_1$, T_2 is in deficit after T_1 is banked, so T_2 must appear somewhere in $\mathcal{D}_2$. If not, $\mathcal{D}_2$ is not a cycle because it leaves T_2 in deficit. Let $U_{i_2} = T_2$ and construct $\mathcal{D}_2'$ from $\mathcal{D}_2$ by moving U_{i_2} to the beginning after T_1. We have

$$\mathcal{D}_2' = (T_1, U_{i_2}, U_1, \ldots, U_{i_2-1}, U_{i_2+1}, \ldots, U_k).$$

This move can only increase the deficit of all tiles to the left of U_{i_2} in $\mathcal{D}_2$ and leaves all tiles to the right of U_{i_2} in $\mathcal{D}_2$ with the same deficit. Thus $\mathcal{D}_2'$ is a cycle provided that $\mathcal{D}_2$ is a cycle; changing the order in which tiles are banked does not change the resulting configuration. Repeat the construction with $U_{i_r} = T_r$ for all $3 \leq r \leq j$ to obtain

$$\mathcal{D}_2' = (T_1, U_{i_2}, U_{i_3}, \ldots, U_{i_j}, V_1, \ldots V_{k-j}).$$

Thus $\mathcal{D}_1$ is a prefix of $\mathcal{D}_2'$. Since $\mathcal{D}_2'$ is a cycle, and no tile is in deficit after applying its prefix $\mathcal{D}_1$, then $j = k$ and $\mathcal{D}_2$ is just a reordering of the tiles of $\mathcal{D}_1$. ☐

Lemma IV.4 (Conjectured). *There exists a locally optimal fill solution h, such that the terminating configuration c_E of the relaxed reverse fill Dirichlet game satisfies $h \preceq c_E$ and $c_E(T) \leq h(T) + 3$ for all tiles T.*

Proof idea: A successful proof may argue that the firing rules cause the game to progress in a sufficiently monotone fashion so that only a small number of chips can be removed from c_E before it becomes infeasible. In particular, it will be argued that at most 3 chips need to be moved from each tile before a locally optimal solution is obtained. $\square$

Corollary III.9 gives a bound on the length of a Dirichlet game based on the number of chips in the game and the properties of the board, which may be applied directly to the augmented forwards fill game. In the r-dissection setting, let the number of chips in the augmented forwards fill game be $\eta = \sum_T b_0(T)$, where b_0 is the initial configuration of the augmented forwards fill game. Letting τ be the total number of tiles, the diameter of the grid (including boundary) is $(Nr/w) + (Mr/w) + 2$, which is roughly $2\sqrt{\tau} = 2\sqrt{NM}r/w$, by inspecting the distance between opposite diagonals. Thus the bound on the length the game is roughly $2\sqrt{2}\eta\tau^2$. In order to bound the fill game using the bound on the length of the augmented forwards fill game, we need the following lemma.

Lemma IV.5. *By adding at most 4 chips per tile to the initial configuration $c_0 \equiv 0$ of the relaxed reverse fill Dirichlet game, the game can be replayed with the same banking sequence, disregarding firing rules, so that all intermediate configurations are nonnegative.*

Proof. Since each tile appears at most once in a bank and clear cycle, never does a tile go into deficit below -4; the largest deficit occurs when all the neighbors of a tile bank before the tile itself does, and the original number of chips at the tile is 0. Playing a reverse game starting in initial configuration $c \equiv 4$ and using exactly the same banking sequence keeps all tiles out of deficit. The augmented forwards game is simply this fill game played backwards. $\square$

Combining the preceding (conjectured) lemmas and the Dirichlet game bound in Corollary III.9 gives the main result on the length of the fill game.

Theorem IV.6 (Conjectured). *Let c_E be the terminating configuration of the relaxed reverse fill Dirichlet game. Let $h \preceq c_E$ be the corresponding locally optimal solution, with $\eta_h = \sum_T h(T)$. Let τ be the number of tiles, and suppose $M \geq N$. Then the number of* *firings in the game is at most*

$$\sqrt{2}\left(2\frac{Nr}{w}+2\right)(\eta_h+7\tau)\tau^{3/2}.$$

Proof. Lemma IV.4 conjectures the existence of a locally optimal fill solution h with $c_E(T) \leq h(T) + 3$ for all tiles T. Let $\mathcal{B}$ be the banking sequence of the fill game. Lemma IV.5 guarantees that the augmented forwards fill game with initial configuration $b_0(T) = h(T) + 7$, and firing sequence $\mathcal{F}$, whose prefix is $\mathcal{B}^R$, will never cause a tile to go into deficit. Corollary III.9 bounds the length $|\mathcal{F}|$ of the augmented forwards fill game by the desired quantity, since the diameter of the grid is at most $(2(Nr/w)+2)$. Because $|\mathcal{B}| \leq |\mathcal{F}|$, the theorem follows. □

A more careful proof of the lemmas might tighten the 7τ term, but this would not guarantee significant speed improvement for any fill problem requiring a number of fill units on the order of $\Theta(\tau)$, which seems likely in most cases.

The following strategies may decrease the length of the fill game by reducing the number of times tiles are banked.

- **Clumped banking.** Bank a ready tile T $\lceil (L - MinWin(T))/4 \rceil$ times instead of once, in order to make up more of the shortfall at once; deficits created can be handled all at once, as well.
- **Configuration Preconditioning.** Precondition the initial configuration by adding as much fill as possible so that the game still terminates close to a locally optimal solution. The reduction in time complexity will be proportional to the percentage of total fill added that is involved in the estimate.
- **Lazy density updates.** Allow some constant number of cycles to execute before updating $MinWin$ and $MaxWin$ values. Strong confluence properties of balancing games will allow a tradeoff between gains in time complexity and error in approximating the solution to the Min Fill objective.

IV.D Experimental results and discussion

The results appearing in Table IV.D arise from the fill game being played with real-world layout data. The minimum and maximum densities over all windows of the fixed features in the layout data are 0.0159543 and 0.108103, respectively. All trials use $U = 0.108103$, and so there is at least one window to which no fill should be added. Trials 1, 2, and 3 set $L = .5U$, $.75U$, and $.9U$, respectively. The lazy update value l determines the number of cycles in the fill game which occur before window densities are updated. L^* and U^* are the actual extremal window densities returned by the linear programming and fill game solutions. The Min Fill objective in a given trial is thus to add as few chips as possible so that each window has density at least L and no window density exceeds U.

Ideally, an integer program the Min Fill objective for given layout data, L, and U is needed to return the optimal solution which can be used as a benchmark to judge the performance of the fill game. Such an integer program is intractable, but we may use the corresponding linear program, which is tractable, though quite computationally intensive. The linear program returns fractional configuration values, but rounding yields a solution that is almost optimal. The first row of each trial in Table IV.D gives the performance of this benchmark linear program. The meanings of the columns are as follows. The "# chips" is just $\sum_T c(T)$, the total chips in the solution configuration. The "extra chips" column gives the percentage of chips above the number given by the linear program solution. L^* and U^* are the minimum and maximum, respectively, over all window densities given by combining the original fixed features in the layout data and the fill solution. The last column gives the percentage by which the given fill solution causes a violation in the upper bound U on density. The value l, set to 1, 10, 50, and 100 for each trial, determines how many banking cycles occur before the density of all windows is updated.

The experimental results validate the use of the Dirichlet chip-firing model in the context of allocating dummy fill to make layout density uniform. Perhaps the most important observation is that the strong confluence properties of chip-firing allow a large value of l (number of banking cycles before density update) while still returning a reasonable solution. In these three trials, the game is most successful in observing the upper bound on density when $l = 1$, as expected. Violations in this upper bound are due to chips being added to tiles after they go into deficit. These violations arise from the discrete nature of the fill game, and would be reduced if chips were to correspond to

Table IV.1: Results for the fill game with Min Fill objective in achieving density between desired lower upper bounds

Trial 1	**# chips**	**extra chips**	L^*	U^*	U **violation**
LP	3146	0.00%	0.054025	0.108112	0.01%
Fill Game, $l = 1$	3718	18.18%	0.054052	0.110566	2.28%
$l = 10$	3700	17.61%	0.054052	0.110657	2.36%
$l = 50$	3170	0.76%	0.054052	0.112689	4.24%
$l = 100$	3162	0.51%	0.054052	0.111080	2.75%

Trial 2	**# chips**	**extra chips**	L^*	U^*	U **violation**
LP	8523	0.00%	0.081034	0.108103	0.00%
Fill Game, $l = 1$	9482	11.25%	0.081083	0.119603	10.64%
$l = 10$	9500	11.46%	0.081083	0.121325	12.23%
$l = 50$	9794	14.91%	0.081078	0.128606	18.97%
$l = 100$	9845	15.51%	0.081078	0.128945	19.28%

Trial 3	**# chips**	**extra chips**	L^*	U^*	U **violation**
LP	12954	0.00%	0.097242	0.108226	0.11%
Fill Game, $l = 1$	13861	7.00%	0.097293	0.129171	19.49%
$l = 10$	13825	6.72%	0.097294	0.131090	21.26%
$l = 50$	14007	8.13%	0.097293	0.135747	25.57%
$l = 100$	14081	8.70%	0.097293	0.137609	27.29%

a smaller unit of fill. Also, since U is taken to be the maximum window density of the layout file before fill is added, adding any chips at all to tiles in this most dense window will violate U. This can be ameliorated by letting U be somewhat above the maximum window density in the original layout.

A significant amount of refinement is necessary for the fill game to be of practical use to the VLSI design community, but the fundamental soundness of the concept of adding side constraints to the Dirichlet game in order to approximate a solution to the Min Fill objective for layout density control is born out by the experimental data.

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