Lecture Notes in Mathematics

Türker Bıyıkoğlu Josef Leydold
Peter F. Stadler

Laplacian Eigenvectors of Graphs

Perron-Frobenius and Faber-Krahn Type Theorems

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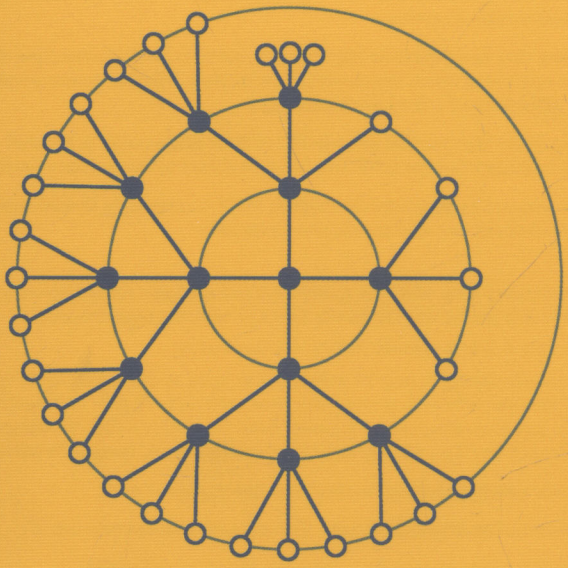

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Preface

Eigenvectors of graph Laplacians are a rather esoteric topic for a book. In fact, we are not aware of even a single review or survey article dedicated to this topic. We have, however, two excuses: (1) There are fascinating subtle differences between the properties of solutions of Schrödinger equations on manifolds on the one hand, and their discrete analogs on graphs. (2) "Geometric" properties of (cost) functions defined on the vertex sets of graphs are of practical interest for heuristic optimization algorithms. Lov Grover's observation that the cost functions of quite a few of the well-studied combinatorial optimization problems are eigenvector of associated graph Laplacians prompted us to investigate such eigenvectors more systematically.

The book in essence covers two topics: Nodal domain theorems which give bounds on the number of connected subgraphs on which an eigenvector does not change sign, and Faber-Krahn-type inequalities which are concerned with the shape of domains (i.e., graphs in our setting) with fixed volume that minimize the first Dirichlet eigenvalue. The connecting theme between these two topics is focus on local and global properties of the eigenvectors (rather than eigenvalues) and convenience of the Rayleigh quotient in the proofs.

The mindful reader will find that more often than not a simple star graph already provides a counterexample for "obvious" conjectures. In fact, we used the Petersen graph just because it seems against tradition to write about graph theory without using the Petersen graph as a counterexample at least once. The simplicity of the counterexamples highlights how little we know about the universe of graph Laplacian eigenvectors (and fitness landscapes in general), and how misguided an intuition trained on well-behaved manifolds can be in this realm: even small moves frequently causes a broken nose caused by some unexpected wall.

The history of this monograph goes back more than a decade and has its roots in the interdisciplinary research environment at the Department of Theoretical Chemistry at the University of Vienna, Austria. A collaboration with Brian Davies during his stay at the Erwin Schrödinger Institute in Vienna in 1995 stimulated our interest in Laplacian eigenvectors and eventually

resulted in a research grant from the Austrian *Fonds zur Förderung der Wissenschaftlichen Forschung* (project no. 14094-MAT) to investigate this topic in a more systematic way. Over the years, many colleagues contributed through helpful discussions, among them Wim Hordijk, Jürgen Jost, Bojan Mohar, Tomaž Pisanski, Dan Rockmore, and Gerhard Wöginger. We also thank the Max Planck Institute for Mathematics in the Sciences in Leipzig for their hospitality and for providing a fruitful scientific working for one of us (TB).

Leipzig, *Türker Bıyıkoğlu*
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May 2006 *Peter F. Stadler*

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Introduction

The foundations of spectral graph theory were laid in the fifties and sixties of the 20th century. The eigenvalues of graphs, most often defined as the eigenvalues of the adjacency matrix, have since then received much attention as a means of characterizing classes of graphs and for obtaining bounds on properties such as the diameter, girth, chromatic number, connectivity [14, 17, 45, 46, 83, 85]. The interest has since then shifted somewhat from the adjacency spectrum to the spectrum of the closely related *graph Laplacian* [14, 35, 41, 85, 88, 137, 139]. In particular, Laplacian graph spectra are being investigated as a means of characterizing large "small world networks" and random graphs, see e.g. [33, 34, 119] for a few examples. For the most part, the theory is still concerned with the eigenvalues.

The *eigenvectors* of graphs, on the other hand, have received only sporadic attention on their own, e.g. [134]. Even the book *Eigenspaces of Graphs* by Cvetković et al. [47] contains only a few pages on the geometric properties of the eigenvectors which are mostly used as a convenient proof technique.

In this book we will focus on mostly geometric properties of the eigenvectors themselves. The motivation for this topic is twofold. As we shall see in this first introductory chapter, these objects arise in very diverse applications, from mathematical biology to combinatorial optimization. The Laplacian eigenvectors are used as tools in heuristics to solve combinatorial problems on given graphs, usually without a thorough understanding why they work so well. From a more formal point of view, Laplacian eigenvectors are the natural discretization of eigenfunctions of Laplace-Beltrami operators on manifolds. Surprisingly, some of their properties in the discrete case are reminiscent of corresponding results in the continuous setting, but often there are subtle differences which we found interesting enough to explore in some detail.

We should, at this point, warn the reader: this book collects a number of interesting facets of our topic, enough as we hope to stimulate further research, but it cannot provide a coherent theoretical framework or a powerful machinery to tackle the properties of Laplacian eigenfunctions in generality.

1.1 Matrix Representations of a Graph

There are two obvious ways of specifying a simple[1] graph $G(V, E)$ with vertex set $V = \{1, \ldots, n\}$ and edge set E by means of a matrix: the adjacency matrix and the incidence matrix. The *adjacency matrix* $\mathbf{A}$ has entries $A_{xy} = 1$ if $xy \in E$ and $A_{xy} = 0$ otherwise: In order to specify the incidence matrix $\boldsymbol{\nabla}$ we need an arbitrary but fixed orientation (direction) for each edge $e = xy$. Then $\boldsymbol{\nabla}$ is a $(|E| \times |V|)$ matrix and has entries $\nabla_{ex} = -1$ if x is the initial vertex of edge e, $\nabla_{ex} = 1$ if x is the terminal vertex of edge e, and $\nabla_{ex} = 0$ otherwise, i.e., if x is not in e.

Let us now consider a real-valued function f over V, $f\colon V \to \mathbb{R}$. This is simply a vector indexed by the vertices of G. In this book we prefer to use a "functional" notation that emphasizes the similarities between the situation of graphs and manifolds. Obviously the set of such functions forms a vector space which is isomorphic to $\mathbb{R}^n$ (and thus we will — by abuse of notation — simply denote this vector space by $\mathbb{R}^n$). Similarly there exists a set of real-valued functions over E. The map $f \mapsto \boldsymbol{\nabla} f$ is known as the *co-boundary mapping* of the graph G. Its value $(\boldsymbol{\nabla} f)(e)$ at a given edge e is the difference of the values of f at the two end-points of the edge e (considering orientation). Therefore the incidence matrix $\boldsymbol{\nabla}$ is a kind of difference or "discrete differential" operator on G.

Let us now consider an Eulerian graph G. Recall that G is Eulerian if and only if G is connected and all vertices have even degree. Let C be an (arbitrary) Eulerian cycle in G (i.e., a closed walk that traverses each edge exactly once) and fix an orientation of G such that C is properly oriented in the sense that all edge point "forward" along C. The cycle C may pass through each vertex x multiple times; the incoming edge of the i-th pass is $e'_i = (y'_i, x)$, the outgoing edge is $e''_i = (x, y''_i)$. We can now define "2nd derivatives" along C:

$$\begin{aligned}(\partial^2_{C;i} f)(x) :&= (\boldsymbol{\nabla} f)(e'') - (\boldsymbol{\nabla} f)(e') \\ &= [f(y''_i) - f(x)] - [f(x) - f(y'_i)] \\ &= f(y'_i) + f(y''_i) - 2f(x)\ .\end{aligned}$$

Note that $(\partial^2_{C;i} f)(x)$ is independent of the orientation on G. Interpreting each pass of C through x as a different "dimension" it seems natural to consider the sum over these "2nd derivatives" as a "Laplace-Beltrami operator"

$$\begin{aligned}(\boldsymbol{\Delta} f)(x) &= \sum_{\text{passes } i \text{ of } C \text{ through } x} (\partial^2_{C;i} f)(x) \\ &= \sum_{i=1}^{d(x)/2} [f(y'_i) + f(y''_i) - 2f(x)] = \sum_{y \sim x} [f(y) - f(x)]\end{aligned}$$

[1] For basic definitions and results the reader is referred to Appendix A.

which is independent of the choice of the Eulerian cycle C and the orientation on G. Naturally, one generalizes this definition of $\mathbf{\Delta}$ to arbitrary graphs.

In the graph theory literature, however, it is customary to define the Laplacian operator (map) $\mathcal{L}\colon \mathbb{R}^{|V|} \to \mathbb{R}^{|V|}$ with the opposite sign:

$$(\mathcal{L}f)(x) = (-\mathbf{\Delta}f)(x) = \sum_{y\sim x} [f(x) - f(y)] \,. \tag{1.1}$$

From an algebraic point of view it appears more natural to define

$$\mathbf{L} = \mathbf{\nabla}^{\mathsf{T}} \mathbf{\nabla} \tag{1.2}$$

which is known as the *Laplacian (matrix)* of G. We have

$$L_{xy} = \sum_{e\in E} \nabla_{ex} \nabla_{ey} = \begin{cases} -1 & \text{if } xy \in E, \\ d(x) & \text{if } x = y, \\ 0 & \text{otherwise,} \end{cases} \tag{1.3}$$

where $d(x) = |\{e \in E | x \in e\}|$ is the *degree* of the vertex x. It is important to note that L_{xy} in (1.3) is independent of the orientation of the edges. Clearly, we have the identity $(\mathcal{L}f)(x) = (\mathbf{L}f)(x)$.

Defining the diagonal matrix $\mathbf{D}$ with entries $D_{xx} = d(x)$, called the *degree matrix*, we obtain a simple connection between the Laplacian and the adjacency matrix of a graph,

$$\mathbf{L} = \mathbf{D} - \mathbf{A} \,. \tag{1.4}$$

The Laplacian $\mathbf{L}$ therefore uniquely determines its graph through its off-diagonal entries.

The close relation between $\mathbf{\nabla}$ and $\mathbf{L}$ on the one hand, and their differential operator counterparts on the other hand, is exemplified by the following discrete version of *Green's formula*, which is easily verified by direct computation [159]:

Proposition 1.1. *Let $f\colon V \to \mathbb{R}$ and $g : V \to \mathbb{R}$ be two arbitrary functions. Then*

$$\sum_{x\in V} f(x)\,(\mathbf{L}g)(x) = \sum_{x\in V} g(x)\,(\mathbf{L}f)(x) = \sum_{e\in E} (\mathbf{\nabla}f)(e)\,(\mathbf{\nabla}g)(e) \,.$$

Using angular brackets $\langle \cdot, \cdot \rangle$ to denote the usual scalar product of two vectors in $\mathbb{R}^n$ and the symbol $-\mathbf{\Delta}$ for $\mathbf{L}$ we can formulate Green's formula in a more familiar form as

$$-\langle f, \mathbf{\Delta}g \rangle = -\langle \mathbf{\Delta}f, g \rangle = \langle \mathbf{\nabla}f, \mathbf{\nabla}g \rangle \,.$$

The Laplacian $\mathbf{L}$ can thus be viewed as a proper discretization of the usual Laplace-Beltrami differential operator.

1.2 Finite Differences

Partial elliptic differential equations play an important rôle in mathematical physics. Examples are the Poisson equation

$$\Delta u = f \quad \text{on } \Omega$$

with given domain $\Omega \subseteq \mathbb{R}^s$ and $f \in \mathcal{C}^0(\Omega)$, the eigenvalue problem

$$-\Delta u = \lambda u \quad \text{on } \Omega$$

or Schrödinger's equation. Here Δ denotes the classical Laplace operator given as $\Delta u = \sum_{i=1}^{s} u_{x_i x_i}$.

Computing solutions of such differential equations is a challenging task in numerical mathematics. An old and popular method is based on *finite differences*: A grid or mesh is used to divide $\mathbb{R}^s$ into small hyper-rectangles or simplices. At the nodes of the grid the Laplace operator Δ is approximated by a difference operator. For $\Omega \subseteq \mathbb{R}^2$ and a square mesh of width h we get the so called *Five-Point Formula*

$$\Delta_h u(x,y) = [u(x+h,y)+u(x,y+h)+u(x-h,y)+u(x,y-h)-4\,u(x,y)]/h^2\,.$$

From a graph theoretical point of view the square mesh is the Cartesian product of two paths of proper lengths, $P_{k_1} \Box P_{k_2} \subset \mathbb{Z}^2$, and Δ_h is the graph Laplacian $\mathbf{L}(P_{k_1} \Box P_{k_2})$ times the constant $-1/h^2$. Thus the graph Laplacian arises in a quite natural way. For details about finite differences (and other methods for solving elliptic partial differential equations) the interested reader is referred to [92], or to [120] for the special case of Laplacian eigenvalues.

1.3 Landscapes on Graphs

Maybe the most direct interest in the structure of the *eigenfunctions* of graph Laplacians comes from the theory of *fitness landscapes*, see [149] for a review. Evolution theory has as its cornerstone the concept of *fitness*. Fitness is traditionally defined as the relative reproductive success of a genotype as measured by survival, fecundity or other life history parameters [27, 96, 165]. The key principle of Darwinian evolutionary theory is that natural selection acts so as to (locally) maximize the fitness of a species or population. The concept of a *fitness landscape* originated in the 1930s in theoretical biology [177, 178] as a means of visualizing this kind evolutionary adaptation: A fitness landscape is a kind of "potential function" on which a population moves uphill due to the combined effects of mutation and selection. Thus, natural selection can be viewed as a type of "hill climbing" on the topography implied by the fitness function.

Models of disordered systems, in particular spin glasses, naturally led to the notion of landscapes [18, 135]: Each spin configuration is assigned an

energy by virtue of the Hamiltonian that specifies the model. In the simplest case so-called Ising spins are considered, which can only take two values: *up* ($\sigma = +1$) and *down* ($\sigma = -1$). The Hamiltonian of the system typically considers the interactions between neighboring spins, in the simplest case

$$f(\boldsymbol{\sigma}) = \sum_{\text{neighbors } i,\, j} \sigma_i \sigma_j \ .$$

There is also a close conceptual similarity of the landscapes in biology and spin glass physics with the *potential energy surfaces* (PES) of theoretical chemistry [95, 136].

In combinatorial optimization the fitness function f is usually referred to as the *cost function* on a *search space* X [80]. The Traveling Salesman Problem (TSP) is probably the most frequently studied combinatorial optimization problem. The ingredients of the TSP are simple enough: The configurations are the $n!$ permutations of the n locations, usually called a "tour". We write $\pi = (\pi(1), \ldots, \pi(n))$ for the order in which they are visited. Given the travel distance (or cost) C_{kl} from city l to city k we can write down the cost function in the form

$$f(\pi) = \sum_{i=1}^{n-1} C_{\pi(i+1),\pi(i)} + C_{\pi(1),\pi(n)} \ ,$$

where the last term describes returning to the point of origin.

In formal terms, a *landscape* is a triple $(X, \mathcal{X}, f)$ consisting of:

1. A set X of configurations,
2. a notion $\mathcal{X}$ of neighborhood, nearness, distance, or accessibility on X, and
3. a fitness function $f\colon X \to \mathbb{R}$.

The set X together with the "structure" $\mathcal{X}$ forms the configuration space. In the simplest case, $\mathcal{X}$ describes which configurations can be obtained from a given one by means of basic "moves" or transformations. Examples of such moves are the flipping of a single spin, the exchange of a single letter by another one in a genetic sequence, or the transposition of two cities along the salesman's tour. Usually the move-set is constructed in a symmetric way, so that the configuration space $(X, \mathcal{X})$ becomes an undirected finite graph G. More general classes of configuration spaces are discussed e.g. in [156].

Let us consider the function $\tilde{f}$ given by $\tilde{f}(x) = f(x) - \bar{f}$, where $\bar{f} = \frac{1}{|X|} \sum_{x \in X} f(x)$ is the average cost of an arbitrary configuration. Grover and others [37, 90, 157] observed that $\tilde{f}$ is in many cases an eigenfunction of the Laplacian $\mathbf{L}$ of the graph representing the configuration space $(X, \mathcal{X})$. These landscapes have been termed *elementary* in [157]. Some examples are collected in Table 1.1.

Lov Grover [90] showed that, if f is an elementary landscape, then

$$f(\hat{x}_{\min}) \leq \bar{f} \leq f(\hat{x}_{\max})$$

Table 1.1. Examples of Elementary Landscapes

Problem	Graph	degree	λ	Order	Reference
p-spin glass	$\mathcal{Q}_2^n$	n	$2p$	p	definition
NAES	$\mathcal{Q}_2^n$	n	4	2	[90]
Weight Partitioning	$\mathcal{Q}_2^n$	n	4	2	[90, 157]
GBP (constrained)	$\mathcal{Q}_2^n$	n	4	2	[2]
Max Cut	$\mathcal{Q}_2^n$	n	4	2	[2]
Graph α-Coloring	$\mathcal{Q}_\alpha^n$	$(\alpha-1)n$	2α	2	[157]
XY-spin glass	$\mathcal{Q}_\alpha^n$	$(\alpha-1)n$	2α	2	[79]
for $\alpha > 2$:	$\mathcal{C}_\alpha^n$	2	$8\sin^2(\pi/\alpha)$	2	[79]
Linear Assignment	$\Gamma(\mathsf{S}_n, \mathcal{T})$	n		1	[151]
TSP symmetric	$\Gamma(\mathsf{S}_n, \mathcal{T})$	$n(n-1)/2$	$2(n-1)$	2	[37, 90]
	$\Gamma(\mathsf{S}_n, \mathcal{J})$	$n(n-1)/2$	n	2	[37, 90]
antisymmetric	$\Gamma(\mathsf{S}_n, \mathcal{T})$	$n(n-1)/2$	$2n$	3	[11, 157]
	$\Gamma(\mathsf{S}_n, \mathcal{J})$	$n(n-1)/2$	$n(n+1)/2$	$\mathcal{O}(n)$	[11, 157]
Graph Matching	$\Gamma(\mathsf{S}_n, \mathcal{T})$	$n(n-1)/2$	$2(n-1)$	2	[157]
Graph Bipartitioning	$J(n, n/2)$	$n^2/4$	$2(n-1)$	2	[90, 161, 162]

Here $\mathcal{Q}_\alpha^n$ is a Hamming graphs, i.e., the n-fold Cartesian product of the complete graph K_α, $\Gamma(\mathsf{A}, \Omega)$ is the Cayley graph of the group A with generating set Ω, where S_n and A_n denotes the symmetric and alternating groups, resp., $\mathcal{T}$, $\mathcal{J}$, and $\mathcal{C}_3$ are the transpositions, reversals, and permutations defined by a cycle of length 3, resp. $J(p, q)$ is a Johnson graph. The order of eigenvalue λ is its position in the spectrum of $\mathbf{L}$ without counting multiplicities and defining the order of $\lambda = 0$ as 0.

where $\hat{x}_{\min}$ and $\hat{x}_{\max}$ are arbitrary local minima and maxima, respectively. This *maximum principle* shows that elementary landscapes are well-behaved: There are no local optima with worse than average fitness $\bar{f}$.

Many of the examples in Table 1.1 belong to the first few eigenvalues of $\mathbf{L}$. A simple relationship between λ and the autocorrelation function of f of $(X, \mathcal{X})$, see e.g. [157], suggests furthermore that the "ruggedness" [72, 173] of an elementary landscape, and hence its difficulty for evolutionary adaptation, should be related to its corresponding eigenvalue λ of $\mathbf{L}$. Furthermore, a Fourier-decomposition-like formalism was developed that decomposes arbitrary landscapes into their elementary components [98, 151, 174]:

$$f = a_0 + \sum_{k>0}^{n-1} a_k f_k \tag{1.5}$$

where the f_k form an orthonormal system of eigenfunction of the graph Laplacian, $\mathbf{L} f_k = \lambda_k f_k$, and $a_0 = \bar{f}$ is the average value of the function f. Let us denote the distinct eigenvalues of $\mathbf{L}$ by $\bar{\lambda}_p$, sorted in increasing order starting with $\bar{\lambda}_0 = \lambda_0 = 0$. We call p the *order* of the eigenvalue $\bar{\lambda}_p$. The *amplitude*

spectrum of $f: V \to \mathbb{R}$ is defined by

$$B_p = \sum_{k:\ \lambda_k = \bar{\lambda}_p} |a_k|^2 \Big/ \sum_{k>0} |a_k|^2 \,. \tag{1.6}$$

By definition, $B_p \geq 0$ and $\sum_p B_p = 1$. The amplitudes measures the relative contribution of the eigenspace of the eigenvalue with order p to the function f. Of course, a landscape is elementary if and only if $B_p = 1$ for a single order and 0 for all others.

1.4 Related Matrices

Let us briefly mention a few matrices that are closely related to $\mathbf{L}$. Sometimes a normalized version $\mathbf{L}^*$ representing the average difference between x and its neighbors is used:

$$(\mathbf{L}^* f)(x) = \frac{1}{d(x)} \sum_{y \sim x} [f(x) - f(y)] \,.$$

This definition is quite similar to (1.1). In fact for graphs without isolated vertices we have

$$\mathbf{L}^* = \mathbf{D}^{-1}\mathbf{L} = \mathbf{I} - \mathbf{D}^{-1}\mathbf{A} \,.$$

This version is used e.g. by Grover [90] and Barnes and coworkers [12, 155]. The first nontrivial eigenvalue of $\mathbf{L}^*$ plays an important role for synchronization in coupled map lattices [5, 105].

Chung [35] defined a general and normalized form of the Laplacian matrix, which is consistent with the eigenvalues in spectral geometry and in stochastic processes:

$$\tilde{L}_{xy} = \begin{cases} 1 & \text{if } x = y \text{ and } d(x) > 0, \\ -1/\sqrt{d(x)d(y)} & \text{if } xy \in E, \\ 0 & \text{otherwise.} \end{cases}$$

In matrix form we have $\tilde{\mathbf{L}} = \mathbf{D}^{-1/2}\mathbf{L}\mathbf{D}^{-1/2}$ for graphs without isolated vertices. $\tilde{\mathbf{L}}$ and $\mathbf{L}^*$ are similar for graphs without isolated vertices: $\mathbf{L}^* = \mathbf{D}^{-1/2}\tilde{\mathbf{L}}\mathbf{D}^{1/2}$.

Another associated matrix is the transition operator $\mathbf{T} = \mathbf{A}\mathbf{D}^{-1}$ of an unbiased random walk on G[2]. We have therefore

$$\mathbf{L}^* = \mathbf{I} - \mathbf{T}^{\mathsf{T}} \qquad \text{and hence} \qquad (\mathbf{L}^*)^{\mathsf{T}} = \mathbf{I} - \mathbf{T}$$

as the associated "Laplacian". This version is used e.g. in [164]. The matrices $\mathbf{L}^*$ and $\mathbf{T}$ are – in contrast to Chung's Laplacian $\tilde{\mathbf{L}}$ – not symmetric unless

[2] Contrary to the convention in the Markov chain literature we treat the distributions as column vectors here, i.e., a step of the Markov chains reads $p' = \mathbf{T}p$.

the graph G is regular; hence they do not belong to the class of operators that we will be concerned with in this book.

As an example for the application of the transition operator we briefly continue our discussion of fitness landscapes of the previous section. Let G be a D-regular graph and let $f\colon V \to \mathbb{R}$ be an arbitrary fitness function. Weinberger [173] suggested to characterize a fitness landscape by means of the autocorrelation function r of the values $f(x)$ sampled along a random walk on G. One easily verifies the following relation between $r(s)$ and the Laplacian spectrum [157]:

$$\begin{aligned} r(s) &= \frac{E[f(x_{t+s})f(x_t)] - E[f(x_{t+s})]E[f(x_t)]}{E[f(x_t)^2] - E[f(x_t)]^2} \\ &= \langle \tilde{f}, \mathbf{T}^s \tilde{f} \rangle / \langle \tilde{f}, \tilde{f} \rangle \\ &= \sum_{p>0} B_p \, (1 - \lambda_p/D)^s \end{aligned} \tag{1.7}$$

Here, the expectation $E[\,.\,]$ is taken over all random walks with transition matrix $\mathbf{T}$, all times t, and all initial conditions $x_0 \in V$. The autocorrelation function $r(s)$ is therefore a superposition of exponential functions. It decays more rapidly, when the amplitudes B_p with large Laplacian eigenvalues λ_p increase. A landscape is therefore elementary if and only if its autocorrelation function decays exponentially. The correlation length

$$\ell := \sum_{s=0}^{\infty} r(s) = D \sum_{p>0} B_p/\lambda_p \tag{1.8}$$

also reflects the fact that the "smoothness" or ruggedness of a fitness landscape is directly related to the amplitude spectrum. The correlation length of an elementary landscape is therefore determined by the order p of the associated Laplacian eigenvalue.

1.5 Graphs with a Boundary: The Discrete Dirichlet Problem

In 1966 Kac [106] asked whether it is possible to *hear the shape of a drum*. A mathematical drum is a domain D with a boundary ∂D in some $\mathbb{R}^n$ (or more generally in some manifold $\mathcal{M}$). If small vibrations are induced in the membrane, it is not unreasonable to expect a point on its surface to move only vertically. In the absence of damping the motion of the point is given by the wave equation

$$\Delta u + \lambda u = 0$$

with the constraint that $u(x) = 0$ for all $x \in \partial D$ (the so-called *Dirichlet boundary condition*). Here Δ denotes the Laplace-Beltrami operator. The solution of a Dirichlet problem involves a countable sequence of eigenvalues (in

this case the frequencies of the tones produced by the membrane). Kac's question thus can be rephrased in a more formal way: Can nonisometric drums D afford the same set of eigenvalues? The answer was given in 1992: We cannot hear the shape of a drum, i.e., there are nonisometric domains D that yield the same spectrum [86].

Fisher [70] considered the discrete analog to Kac's problem. In his model the membrane consists of a set of atoms which in the equilibrium state lie on the vertices of a regular lattice graph embedded in a plane. Each atom acts on its neighboring atoms by elastic forces. The discretization of the vibration of a membrane is the Laplacian matrix $\mathbf{L}$ of the graph G. The eigenvalues of $\mathbf{L}$ again correspond to the frequencies of the membrane. We also can't hear the discrete shape of a drum, because the eigenvalues of a graph do not determine the graph uniquely; see e.g. [45]. Nevertheless, in practice it is often possible to obtain at least good approximations of a graph (in terms of the cardinality of the symmetric difference between the true graph and its reconstruction) from its spectrum [103].

We need a notion of a graph with boundary for defining discrete analogs of Dirichlet boundary conditions. Of course, graphs do not have boundaries by themselves. Starting from a graph $G(V, E)$ we may, however, consider the induced subgraph $G[V^\circ]$ on a subset $V^\circ \subset V$, considering $V \setminus V^\circ$ as the boundary of $G[V^\circ]$ on which the constraint $u(x) = 0$ is enforced. We denote this boundary by ∂V. Formally we can define a *graph with boundary* as a graph $G(V^\circ \cup \partial V, E^\circ \cup \partial E)$ where V° denotes the set of *interior* vertices and ∂V the set of *boundary* vertices. The set of edges between interior vertices are called *interior* edges and denoted by E°; edges between V° and ∂V are called *boundary* edges and denoted by ∂E. Edges between boundary vertices do not make sense in our setting and are thus deleted. It must be noted here that a graph with boundary is called connected if the graph induced by its interior vertices, $G[V^\circ]$, is connected. The partition into interior and boundary vertices might be to some extend "arbitrary". In the case of drums, however, we might also choose to use a nail and fix the position of the membrane at an arbitrary point, thereby adding an additional point to the boundary of the domain of the corresponding Dirichlet problem. A more thorough discussion of Dirichlet problems on graphs will be given in Chap. 6.

An interesting application of the first Dirichlet eigenvalue arises from a combinatorial game called *chip firing* [23]: Every vertex of a connected graph contains an integral number of chips. In each step of the game a vertex is selected that has at least as many chips as its degree and one chip is moved to each of its neighbors. The game can continue as long as there is a vertex with sufficiently many chips on it. The game terminates when no vertex can be selected. Chung and Ellis [32] considered a variant of this game, in which chips are removed from the game when they are moved across a boundary and gave an upper bound that depends on the first Dirichlet eigenvalue for the number of steps until such a game terminates.

If we restrict ourselves to solutions f of the Dirichlet problem on a graph $G(V^\circ \cup \partial V, E^\circ \cup \partial E)$ with boundary we have to look for a function f which vanishes on all boundary vertices, i.e. $f(x) = 0$ for $x \in \partial V$, and which satisfies for all interior vertices $x \in V^\circ$

$$(\mathbf{L}f)(x) = \sum_{y \sim x} [f(x) - f(y)] = \sum_{y \in V} L_{xy} f(y) = \sum_{y \in V^\circ} L_{xy} f(y) = \lambda f(x)$$

for some eigenvalue λ. Thus the Dirichlet problem can be reduced to a matrix eigenspace problem for $G[V^\circ]$. The corresponding *Dirichlet matrix* $\mathbf{L}^\circ(G)$ can be derived from the graph Laplacian $\mathbf{L}(G)$ simply by deleting all rows and columns that correspond to boundary vertices, i.e., by using the principal submatrix corresponding to interior vertices. Compared to the "free" graph Laplacian $\mathbf{L}(G[V^\circ])$ on the graph induced by its interior vertices, $G[V^\circ]$, the Dirichlet matrix differs just by an additional "potential" $p(x)$ in the diagonal elements:

$$\mathbf{L}^\circ(G) = \mathbf{L}(G[V^\circ]) + \mathbf{P} \tag{1.9}$$

where $\mathbf{P}$ is a diagonal matrix whose entries are $P_{xx} = p(x) = |\{y\colon yx \in \partial E\}|$. For a more "natural" motivation of this definition we refer the interested reader to [75] or Sect. 2.4.

1.6 Generalized Graph Laplacians

The Dirichlet operator and Chung's Normalized Laplacian motivate the definition of a more general class of matrices associated with a graph $G(V, E)$. We call a symmetric matrix $\mathbf{M}$ a *generalized Laplacian* or *discrete Schrödinger operator* of G if $M_{xy} < 0$ whenever xy is an edge of G and $M_{xy} = 0$ whenever x and y are distinct and not adjacent. There are no constraints on the diagonal entries of $\mathbf{M}$. Fiedler [67] and Roth [152] call such matrices *"essentially non-positive"*. The ordinary Laplacian $\mathbf{L}$ as well as the negative adjacency matrix $-\mathbf{A}$ are of course generalized Laplacians.

Such generalized graph Laplacians can be interpreted in two ways. First the off-diagonal entries can be seen as coefficient of a discrete analog of an elliptic operator which are used in mathematical physics to describe oscillation in nonhomogeneous matter. On the other hand it could be seen as "ordinary" Laplacian on a weighted graph. Then the weights w_{xy} on an edge xy has to taken into consideration. Thus we have a Hamiltonian operator $\mathcal{H}$ of the form

$$(\mathcal{H}f)(x) = \sum_{y \sim x} w_{xy} \, [f(x) - f(y)] + p(x) \, f(x) \; .$$

The first part of the right hand side then represents the kinetic part while $p(x)$ represents some potential. This is the analogous expression to (1.1) of some generalized Laplacian.