The Graph-Simplex Correspondence and its Algorithmic Foundations

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A dissertation presented to the faculty in the department of mathematics in candidacy for the degree of *Master of Science.*

September, 2019

Abstract

Lay Summary

Acknowledgements

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Nomenclature[2]

Simplex Geometry

$\mathcal{T}$	General simplex	Section 2.5
$\mathcal{T}^*$	Dual simplex to $\mathcal{T}$	Section 2.5.1
$\mathbf{\Sigma}(\mathcal{T})$	Vertex matrix of simplex $\mathcal{T}$	
$\mathcal{S}_G$ $(\widehat{\mathcal{S}}_G)$	(Normalized) Simplex of G	Section 3.2.1
$\mathcal{S}_G^+$ $(\widehat{\mathcal{S}}_G^+)$	Inverse simplex of $\mathcal{S}_G$ $(\widehat{\mathcal{S}}_G)$	Section 3.2.2
$\mathcal{T}\restriction_U, \mathcal{T}_U, \mathcal{T}[U]$	Face of simplex $\mathcal{T}$ restricted to U	Equation (2.23)
$\mathbf{\Sigma}_G$ $(\widehat{\mathbf{\Sigma}}_G)$	Vertex matrix of the simplex $\mathcal{S}_G$ $(\widehat{\mathcal{S}}_G)$	Section 3.2
$\mathbf{\Sigma}_G^+$ $(\widehat{\mathbf{\Sigma}}_G^+)$	Vertex matrix of the simplex $\mathcal{S}_G^+$ $(\widehat{\mathcal{S}}_G^+)$	
$\{\boldsymbol{\sigma}_i\}$ $(\{\widehat{\boldsymbol{\sigma}}_i\})$	Vertex vectors of (normalized) simplex	
$\boldsymbol{a}(\mathcal{T}_U)$	Altitude vector from $\mathcal{T}_U$ to $\mathcal{T}_{U^c}$	Section 2.5
$\boldsymbol{c}(\mathcal{T}_U)$	Centroid of simplex $\mathcal{T}_U$	Equation (2.25)
$\mathcal{E}(\mathcal{T})$	Steiner circumscribed ellipsoid of $\mathcal{T}$	Definition 4.1
$\bar{d}$	Avg. squared distance in a simplex	Equation (4.1)
$\boldsymbol{\xi}$	Avg. squared distance of vertices minus $\bar{d}$	Equation (4.1)
$\boldsymbol{x}_{U^c}$	Barycentric coordinate for face $\mathcal{T}_U$	
$\mathcal{S}_0$	Canonical/Centred Simplex of $\mathcal{S}$	Definition 2.5
$\cong, \cong^{\circlearrowleft}$	Congruency between simplices	Section 2.5
$[\mathcal{T}], [\mathcal{T}]^{\circlearrowleft}$	Congruence classes of simplices	Equation (2.24)

Graph Theory

$G = (V, E, w)$	Undirected, connected, and weighted graph	Section 2.3
$V(G)$, $E(G)$	Vertex set and edge set of graph G	
$\boldsymbol{A}_G$	Adjacency matrix of graph G	
$\boldsymbol{W}_G$	Weight matrix of graph G	
$w_G(i, j)$	Weight of edge (i, j) in G	
$\delta_G(i)$	Set of neighbours of i in G	Equation (2.6)
$\delta_G U$	Cut set of U in G	

[2]The subscript G and paranthetical (G) is often dropped from relevant symbols.

$w_G(i)$	Weight of vertex $i \in V(G)$	
$\mathrm{vol}_G(U)$	Volume of set U, i.e., $\sum_{i\in U} w(i)$	Equation (2.7)
Γ_G	Total weight of all spanning trees in G	Equation (2.18)
$r_G^{\mathrm{eff}}(i,j)$	Effective resistance between i and j	Definition 2.2
$\boldsymbol{R}_G$	Effective resistance matrix	Section 2.4
$\mathcal{R}_G$	Effective Polytope of G	Equation (4.18)

Linear Algebra & Spectral Graph Theory

$\boldsymbol{L}_G$	Combinatorial Laplacian Matrix of G	Equation (2.8)
$\widehat{\boldsymbol{L}}_G$	Normalized Laplacian Matrix of G	Equation (2.13)
$\mathcal{L}_G$	Quadratic form associated with $\boldsymbol{L}_G$	Equation (2.12)
$\widehat{\mathcal{L}}_G$	Quadratic form associated with $\widehat{\boldsymbol{L}}_G$	Equation (2.15)
$\{\lambda_i(G)\}$ $(\{\lambda_i(G)\})$	Eigenvalues of $\boldsymbol{L}_G$ $(\widehat{\boldsymbol{L}}_G)$	Section 2.3.2
$\boldsymbol{\Lambda}_G$ $(\widehat{\boldsymbol{\Lambda}}_G)$	Diagonal Eigenvalue matrix of $\boldsymbol{L}_G$ $(\widehat{\boldsymbol{L}}_G)$	
$\{\boldsymbol{\varphi}_i(G)\}$ $(\{\widehat{\boldsymbol{\varphi}}_i(G)\})$	Eigenvectors of $\boldsymbol{L}_G$ $(\widehat{\boldsymbol{L}}_G)$	
$\boldsymbol{\Phi}_G$ $(\widehat{\boldsymbol{\Phi}}_G)$	Eigenvector matrix of $\boldsymbol{L}_G$ $(\widehat{\boldsymbol{L}}_G)$	
$\boldsymbol{Q}^+$	Pseudoinverse of matrix $\boldsymbol{Q}$	Section 2.2.1
$\dim \boldsymbol{Q}$	Dimension of space spanned by columns of $\boldsymbol{Q}$	
range Q	Range of $\boldsymbol{Q}$	
$\ker \boldsymbol{Q}$	Kernel of $\boldsymbol{Q}$	
$\lVert\cdot\rVert_p$	p-norm in $\mathbb{R}^d$	Equation (2.1)

Miscellaneous

$\mathbb{R}$	Real numbers	Section 2.1
$\mathbb{Q}$	Rational numbers	
$\mathbb{C}$	Complex numbers	
$\mathbb{N}$	Natural numbers	
δ_{ij}	Kronecker delta function	
χ_U	Indicator for event U	
$\boldsymbol{\chi}_U$	Indicator vector for set U	
$\boldsymbol{D}(\mathcal{X})$	Squared distance matrix of set of points $\mathcal{X}$	
$\mathrm{conv}(\mathcal{X})$	Convex hull of set of points $\mathcal{X}$	Equation (2.2)

Chapter 1

Introduction

This thesis is concerned with uniting two fundamental and hitherto mostly unrelated objects: the graph and the simplex. A graph is fundamentally a *combinatorial* object—by which we mean lacking inherent geometry. That is, it be described by two finite lists: a list of its *nodes* or *vertices* and a second of the connections between these vertices. No underlying geometric space need be defined. The fact that we often picture graphs as being embedded in the plane is merely demonstrates that we often like to reason visually, and does not reflect any underlying geometry of the graph. Indeed, the same graph may be embedded in infinitely many ways in the plane. Conversely, simplices—best thought of as high dimensional triangles—are inherently geometric. Any complete description of a simplex must include, for example, the distance between two of its vertices.

A deep connection between graphs and simplices might seem unlikely a priori, and it is precisely this fact which makes such a connection worth studying. Such a connection was unknown until Miroslav Fiedler made the connection in his 1993 paper entitled "A geometric approach to the Laplacian matrix of a graph" [Fie93]. Here he introduced what we will henceforth refer to as the *graph-simplex correspondence*, proving the existence of a bijection between graphs and hyperacute simplices.

§1.1. Prior Work

Steinitz's theorem which investigates the relationship between undirected graphs arising from convex polyhedra in $\mathbb{R}^3$ [Ste22]. Sharpe [Sha67] said something about something which should probably be cited, but not exactly sure what it is yet.

§1.2. Contribution

We view our main contribution as providing a self contained treatise of the what we are calling the graph-simplex correspondence. We include Fiedler's main results on the topic, as well those newly discovered results of Devriendt and Van Mieghem [DVM18]. We also expand on these results in several ways.

We state these contributions below, but let us first remark upon the presentation of the aspects in this thesis which do not contain new results.

First, in his original paper on the correspondence and subsequent book on simplex geometry more generally [Fie11], Fiedler investigated the correspondence by means of a (somewhat complicated) block matrix relationship involving the Gramian matrix of the outer normals of the simplex and its distance matrix. Devriendt and Van Mieghem demonstrate that the correspondence can be stated more simply (in the author's opinion) in terms of the graph's Laplacian matrix, but investigate only the simplex associated to a given graph, and are less concerned with the graph associated to a simplex. Combining these two approaches, we also investigate the correspondence by means of the Laplacian, but

- First, although at first seemingly unrelated to the correspondence itself, we provide a novel mathematical treatment of what we call the "dual simplex" of a given simplex. This object was remarked upon by Fiedler in his 2011 book [Fie11], but he did not investigate its properties. We present several general properties of the dual simplex and use it to frame graph-simplex correspondence, especially of the normalized Laplacian.

- While Fiedler (implicitly) and Devriendt and Van Mieghem (explicitly) studied the correspondence by means of the combinatorial Laplacian of a graph, we expand the correspondence to the "normalized" Laplacian. This matrix also describes the complete structure of the graph, but is more intimately related to several of its features, such as describing random walk dynamics [CG97]. We introduce this new mapping along with the original in Section 3.2. We then study the properties of the simplex associated to the normalized Laplacian—which we term the "normalized" simplex

- With regards to the normalized simplex, in Section 3.5 we investigate its mathematical properties. This proves a more challenging task than in the case of the combinatorial simplex because, as we will show, the inverse normalized simplex is *not* the dual of the normalized simplex in general.

- We also uncover a link between the simplex of a graph and a geometric object related to the effective resistance of the graph, which we call the "effective polytope". It seems that the existence of this object has been previously acknowledged (e.g., [Gha15]), but never rigorously studied. This material appears in Section 4.4.

- Perhaps most significantly, we initiate the study of the algorithmic foundations of the correspondence (Chapter 5). This entails three distinct aspects.

  1. We explore several consequences for computational complexity. Owing to the ubiquity of graphs in theory and application, the complexity classes of many graph-theoretic problems are well established (e.g., computing maximum-cuts and independent sets are "hard", while spanning trees are "easy", etc.) If, via the correspondence, such problems have analogues in the simplex then this has implications concerning the difficulty of these geometric problems. Moreover, while the analogues problems in the simplex domain may have known to be easy or hard in general convex polytopes, understanding the complexity in (hyperacute) simplices may yield an improved understanding of the hardness "threshold" for such problems.

2. We then explore the natural question of whether various aspects of the correspondence can be computed efficiently. For example, given G how quickly can we compute $\mathcal{S}_G$ or $\mathcal{S}_G^+$ efficiently? What about computing $\mathcal{S}_G$ given $\mathcal{S}_G^+$, or vice versa? Our results in this space are mostly negative; transitioning between many of these objects require time no less than that required to perform an eigendecomposition of a Laplacian matrix. This is perhaps to be expected given that the mapping is based on the eigendecomposition of the Laplacian matrix. However, we emphasize is it not immediate; while the mapping relies on the eigendecomposition, it uses the relations between the eigenvalues and eigenvectors. It is a priori feasible that the relationships are computable more quickly than the eigenvalues and eigenvectors themselves.
3. Finally, we explore several approximations. Given that the simplex of a graph with n vertices lives in $\mathbb{R}^{n-1}$—a high dimensional space—we might hope that we can "approximately" embed it in lower dimensions. We explore this possibility in Section 5.4.1. Owing to the lower bounds achieved on the "precise" mappings between various objects mentioned above, we might hope that we can approximate several of these mappings. This is explored in Section 5.4. Instead of purely geometric approximations, we might also wonder what happens to the correspondence when we approximate the Laplacian with another.

§1.3. Organization

The rest of the thesis will be organized as follows. Section 2 will present the relevant background material in the areas of linear algebra, spectral graph theory, and simplex geometry. Here we will also define and make some preliminary explorations of the dual simplex. The background material of Sections 2.1, 2.2, and 2.3.1 is quite standard; the reader familiar with these subject areas should be able to skip them without too much trouble. We encourage all readers to peruse Section!2.5 because, for one, the field of simplex geometry is less well studied in general than the others and secondly, as stated above, we provide a novel treatment of the dual simplex.

§1.4. Ideas and TODOs

- Next sections to think more about:
  1. Inequalities (Section 4.2)
  2. Low Rank Approximations of $\boldsymbol{L}_G$ (Section 5.4.3)
  3. Could include more of Fiedler's results in Section 4.1. Also should see if we can obtain similar results vis-a-vis the normalized simplex .
  4. Keep thinking about the normalized simplex.
- Most promising new ideas:
  1. Use algorithms and known results concerning effective results and translate them to simplex results.

- Less promising new ideas:
  1. In [Fie98], Fielder gives some sort of correspondence involving “ultrametric matrices”. Look this up and understand it—could be interesting.
  2. Applications of Schur Complement?

Chapter 2

Background and Fundamentals

This chapter is devoted to introducing the pre-requisite knowledge necessary to grapple with the material in subsequent sections. The subject matter of this dissertation lies at the intersection of several mathematical topics, ensuring that any treatment of the material will give rise to notational challenges. Nevertheless, we have strived—courageously, in the author's unbiased opinion—to use standard notation wherever possible in the hopes that readers familiar with spectral graph theory may skip this background material without losing the plot.

§2.1. General Notation

We use the standard notation for sets of numbers: $\mathbb{R}$ (reals), $\mathbb{N}$ (naturals), $\mathbb{Z}$ (integers), $\mathbb{C}$ (complex). We use the subscript ≥ 0 (resp., > 0) to restrict a relevant set to its non-negative (resp., positive) elements ($\mathbb{R}_{\geq 0}$, for example). We will often introduce new notation or definitions by using the notation $\overset{\text{def}}{=}$. The complement of a set U (with respect to what will be clear from context) is denoted U^c. Given a set of scalars K, we let $K^{n\times m}$ denote the set of $n \times m$ matrices (n rows and m columns) with elements in K. Matrices will typically be denoted by uppercase letters in boldface, e.g., $\boldsymbol{Q} \in K^{n\times m}$. Matrices will also often be referred to as linear transformations and written, for example, as $\boldsymbol{Q} : K^m \to K^n$. We let $\boldsymbol{Q}(i, \cdot)$ (resp., $\boldsymbol{Q}(\cdot, i)$) denote the i-th row (resp., column) of the matrix $\boldsymbol{Q}$. For a set U, K^U denotes the set of all functions from U to K. Elements of K^U are also called vectors. For any $n \in \mathbb{N}$, set $[n] \overset{\text{def}}{=} \{1, 2, \ldots, n\}$. As usual, we let $K^n = K^{[n]}$. Vectors will typically be denoted by lowercase boldcase letters. Lowercase greek letters will often be used for scalars. It will often be intuitively useful to identity vectors with their endpoints, rather than the traditional "arrow" originating from the origin. When this is the case, we will often use the word point instead of vector. We emphasize that they are formally the same object.

For $n \in \mathbb{N}$, let $\mathbf{0}_n \in \mathbb{R}^n$ and $\mathbf{1}_n \in \mathbb{R}^n$ be the vectors of all zeroes and all ones. Let $\mathbf{I}_n$ and $\mathbf{J}_n$ refer to the $n \times n$ identity matrix and all-ones matrix respectively (so $\mathbf{J}_n = \mathbf{1}_n\mathbf{1}_n^t$). When the dimension n is understood from context, will typically omit it as a subscript. We use $\chi(E)$ or χ_E as the indicator of an event E, i.e., $\chi(E) = 1$ if E occurs, and 0 otherwise. For example, $\chi(i \in U) = 1$ if $i \in U$, and 0 if $i \in U^c$. Similarly, for $U \subseteq K$, $\boldsymbol{\chi}_U \in \mathbb{R}^K$ is the indicator vector of the set U, so $\boldsymbol{\chi}_U(i) = \chi(i \in U)$. By $\operatorname{diag}(x_1, x_2, \ldots, x_n)$ we mean the $n \times n$ matrix $\boldsymbol{Q}$ entries $\boldsymbol{Q}(i, i) = x_i$ and $\boldsymbol{Q}(i, j) = 0$ for $i \neq j$. Given vectors $\mathbf{v}_1, \ldots, \mathbf{v}_n$, we will often denote by $(\mathbf{v}_1, \ldots, \mathbf{v}_n)$ the matrix whose i-th column is $\mathbf{v}_i$. The i-th coordinate of a vector $\boldsymbol{x}$ will be denoted either by $\boldsymbol{x}(i)$ or simply $x(i)$. We trust this will not be overly confusing. For $1 \leq p < \infty$, the *p-norm* of $\boldsymbol{x} \in \mathbb{R}^d$ is

$$\|\boldsymbol{x}\|_p = \left(\sum_{i=1}^{d} x_i^p \right)^{1/p}, \tag{2.1}$$

while the *0-norm* of $\boldsymbol{x}$ is the number of non-zero entries of $\boldsymbol{x}$, and is denoted by $\|\boldsymbol{x}\|_0$. Given a vector or matrix, we use the superscript t to denote it's transpose, i.e.,, given $\boldsymbol{Q}$, $\boldsymbol{Q}^t$ is defined as $\boldsymbol{Q}^t(i,j) = \boldsymbol{Q}(j,i)$. The standard inner product on $\mathbb{R}^d$ is denoted as $\langle \cdot, \cdot \rangle$, that is, $\langle \boldsymbol{x}, \boldsymbol{y} \rangle = \sum_i x(i)y(i)$. Elementary properties of the inner product will often be used without justification, such as its bilinearity: $\langle \boldsymbol{x}, \alpha \boldsymbol{y}_1 + \boldsymbol{y}_2 \rangle = \langle \boldsymbol{x}, \alpha \boldsymbol{y}_1 \rangle + \langle \boldsymbol{x}, \boldsymbol{y}_2 \rangle$ for $\alpha \in \mathbb{R}$. We will sometimes use the notation $\perp$ to mean "orthogonal to", so $\boldsymbol{x} \perp \boldsymbol{y}$ iff $\langle \boldsymbol{x}, \boldsymbol{y} \rangle = 0$. We will often use the shorthand "iff" to mean "if and only if". We use δ_{ij} to denote the Kronecker delta function, i.e., $\delta_{ij} = 1$ if $i = j$ and 0 otherwise. We may sometimes include a comma and write $\delta_{i,j}$.

A set $\mathcal{X} \subseteq \mathbb{R}^m$ is *convex* if for all $\boldsymbol{x}, \boldsymbol{y} \in \mathcal{X}$ and $\lambda \in (0,1)$, $\lambda \boldsymbol{x} + (1-\lambda)\boldsymbol{y} \in \mathcal{X}$. The *convex hull* of a finite set of points $X = \{\boldsymbol{x}_1, \ldots, \boldsymbol{x}_k\} \subseteq \mathbb{R}^n$ is

$$\operatorname{conv}(\mathcal{X}) \stackrel{\text{def}}{=} \left\{ \sum_{\ell} \alpha_i \boldsymbol{x}_i : \sum_{\ell} \alpha_i = 1, \ \alpha_i \geq 0 \right\}, \tag{2.2}$$

or equivalently, the smallest convex set containing X [GKPS67]. We will often denote the *squared distance matrix of* $\mathcal{X}$ by $\boldsymbol{D}(\mathcal{X}) \in \mathbb{R}^{|\mathcal{X}| \times |\mathcal{X}|}$, whose entries are given by $\boldsymbol{D}(\boldsymbol{x}, \boldsymbol{y}) = \|\boldsymbol{x} - \boldsymbol{y}\|_2^2$.

§2.2. Linear Algebra

We assume familiarity with the basic linear algebraic notions—similarity, dimension, range, etc. All relevant background material can be found in a standard reference, e.g. [Axl97]. We begin by stating a well-known but substantial result first proved by Cauchy (see [Haw75] for the relevant history), which initiated the systematic study of the spectrum of matrices and which underpins the results in this dissertation.

Theorem 2.1 (Spectral Theorem for real matrices). *Every real, symmetric $n \times n$ matrix has a set of n orthogonal eigenvectors and real eigenvalues.*

Next we state a result which will underpin our construction of the "dual simplex" in Section 2.5.1.

Lemma 2.1. *Let $\mathbf{v}_1, \ldots, \mathbf{v}_k$ be a set of linearly independent vectors in $\mathbb{R}^n$. There exists a set of vectors, $\mathbf{u}_1, \ldots, \mathbf{u}_k$ such that $\langle \mathbf{v}_i, \mathbf{u}_j \rangle = \delta_{ij}$ for all $i, j \in [k]$. The collections $\{\mathbf{v}_i\}$ and $\{\mathbf{u}_i\}$ are called* biorthogonal *or* dual bases.

Given the set $\{\mathbf{v}_i\}$ of linearly independent vectors, the complementary set $\{\mathbf{u}_i\}$ given by Lemma 2.1 is called the *sister* or *dual set to* $\{\mathbf{v}_i\}$. If $\{\mathbf{v}_i\}$ constitutes a basis of the underlying space, then we might call $\{\mathbf{u}_i\}$ the *sister* or *dual basis*. We present a simple observation which will be useful in later sections.

OBSERVATION 2.1. *Let $\{\mathbf{v}_1, \ldots, \mathbf{v}_n\} \subseteq \mathbb{R}^n$ be a set of linearly independent vectors. The sister basis given by Lemma 2.1 is unique.*

Proof. Suppose $\{\mathbf{u}_i\}$ and $\{\boldsymbol{w}_i\}$ are biorthogonal bases. Fix $i \in [n]$. By independence, $\text{span}(\mathbf{v}_1, \ldots, \mathbf{v}_{i-1}, \mathbf{v}_{i+1}, \ldots, \mathbf{v}_n)$ is a hyperplane—that is,

$$\dim \text{span}(\mathbf{v}_1, \ldots, \mathbf{v}_{i-1}, \mathbf{v}_{i+1}, \ldots, \mathbf{v}_n)^\perp = 1.$$

Both $\mathbf{u}_i$ and $\boldsymbol{w}_i$ are orthogonal to this hyperplane (since they orthogonal to $\mathbf{v}_j$ for all $j \neq i$), thus are either parallel or anti-parallel. Therefore, there exists some $\alpha \in \mathbb{R}$ such that $\mathbf{v}_i = \alpha \boldsymbol{w}_i$. By definition, $\langle \mathbf{v}_i, \mathbf{u}_i \rangle = \langle \mathbf{v}_i, \boldsymbol{w}_i \rangle = 1$, hence $\langle \mathbf{v}_i, \alpha \boldsymbol{w}_i \rangle = \langle \mathbf{v}_i, \boldsymbol{w}_i \rangle$ implying that $\alpha = 1$. This demonstrates that $\mathbf{u}_i = \boldsymbol{w}_i$ for all i. ⊠

Let $\boldsymbol{M} \in \mathbb{R}^{n \times n}$ matrix. We recall that a vector $\boldsymbol{\varphi}$ satisfying $\boldsymbol{M}\boldsymbol{\varphi} = \lambda \boldsymbol{\varphi}$ is an *eigenvector* of $\boldsymbol{M}$, and call λ the associated *eigenvalue*. It's clear that if $\boldsymbol{\varphi}$ is an eigenvector then so it $c\boldsymbol{\varphi}$ for any constant $c \in \mathbb{R}$. If $\boldsymbol{M}$ is real and symmetric, then the Spectral theorem dictates that there exists an orthonormal basis consisting of eigenvectors $\{\boldsymbol{\varphi}_1, \boldsymbol{\varphi}_2, \ldots, \boldsymbol{\varphi}_n\}$ of $\boldsymbol{M}$ whose corresponding eigenvalues $\{\lambda_1, \ldots, \lambda_n\}$ are all real. Let $\boldsymbol{\Phi} = (\boldsymbol{\varphi}_1, \boldsymbol{\varphi}_2, \ldots, \boldsymbol{\varphi}_n)$ be the matrix whose i-th column is the i-th eigenvector of $\boldsymbol{M}$, and set $\boldsymbol{\Lambda} = \text{diag}(\lambda_1, \ldots, \lambda_n)$. Observe that

$$\boldsymbol{M}\boldsymbol{\Phi} = \boldsymbol{M}(\boldsymbol{\varphi}_1, \ldots, \boldsymbol{\varphi}_n) = (\boldsymbol{M}\boldsymbol{\varphi}_1, \ldots, \boldsymbol{M}\boldsymbol{\varphi}_n) = (\lambda_1\boldsymbol{\varphi}_1, \ldots, \lambda_n\boldsymbol{\varphi}_n) = \boldsymbol{\Phi}\boldsymbol{\Lambda}. \tag{2.3}$$

Moreover, if $\{\boldsymbol{\varphi}_i\}_i$ are assumed to be orthonormal then $\boldsymbol{\Lambda}\boldsymbol{\Lambda}^\intercal = \mathbf{I}$ from which it follows from (2.3) that

$$\boldsymbol{M} = \boldsymbol{\Phi}\boldsymbol{\Lambda}\boldsymbol{\Phi}^t = \sum_{i \in [n]} \lambda_i \boldsymbol{\varphi}_i \boldsymbol{\varphi}_i^t, \tag{2.4}$$

which is called the *eigendecomposition* of $\boldsymbol{M}$.

A symmetric matrix $\boldsymbol{Q} \in \mathbb{R}^{n \times n}$ is *positive semidefinite (PSD)* if $\boldsymbol{x}^t \boldsymbol{Q} \boldsymbol{x} \geq 0$ for all $\boldsymbol{x} \in \mathbb{R}^n$. If $\boldsymbol{Q}$ is PSD, then we define

$$\boldsymbol{Q}^{1/2} \stackrel{\text{def}}{=} \boldsymbol{\Phi}\boldsymbol{\Lambda}^{1/2}\boldsymbol{\Phi}^t = \sum_{i \in [n]} \sqrt{\lambda_i} \boldsymbol{\varphi}_i \boldsymbol{\varphi}_i^t.$$

The following basic result will be useful for us.

LEMMA 2.2. *For any $\boldsymbol{Q} : \mathbb{R}^n \to \mathbb{R}^m$, $\text{rank}(\boldsymbol{Q}) = \text{rank}(\boldsymbol{Q}^t\boldsymbol{Q})$.*

Proof. It suffices to show that $\dim \ker \boldsymbol{Q} = \dim \ker \boldsymbol{Q}^t \boldsymbol{Q}$, by rank-nullity. Clearly $\ker \boldsymbol{Q} \subseteq \ker \boldsymbol{Q}^t \boldsymbol{Q}$ since $\boldsymbol{Q}\boldsymbol{f} = \mathbf{0}$ implies $\boldsymbol{Q}^t\boldsymbol{Q}\boldsymbol{f} = \mathbf{0}$. Conversely, if $\boldsymbol{Q}^t\boldsymbol{Q}\boldsymbol{f} = \mathbf{0}$ then $0 = \boldsymbol{f}^t\boldsymbol{Q}^t\boldsymbol{Q}\boldsymbol{f} = \|\boldsymbol{Q}\boldsymbol{f}\|_2^2$, implying that $\boldsymbol{Q}\boldsymbol{f} = \mathbf{0}$. ⊠

2.2.1. Pseudoinverse

If $\boldsymbol{M}$ is a singular matrix, a natural question to ask is whether there exists a matrix whose relationship to $\boldsymbol{M}$ "approximates", in some relevant sense, the relationship between a matrix and its inverse. This question was asked and answered, on separate occasions, by both Elikam Moore and Sir Roger Penrose. Both discovered—originally Moore in 1921 and later Penrose in the 1950's—what is now known as the *Moore-Penrose pseudoinverse* of a matrix [Moo20, Pen55, Pen56]. It is defined as follows.

Definition 2.1 (Moore-Penrose pseudoinverse [BH12]). Let $\boldsymbol{M} \in \mathbb{C}^{n\times m}$ for some $n, m \in \mathbb{N}$. We call a matrix $\boldsymbol{M}^+ \in \mathbb{C}^{m\times n}$ satisfying both

(i). $\boldsymbol{M}\boldsymbol{M}^+\boldsymbol{M} = \boldsymbol{M}$ and $\boldsymbol{M}^+\boldsymbol{M}\boldsymbol{M}^+ = \boldsymbol{M}^+$;

(ii). $\boldsymbol{M}\boldsymbol{M}^+$ and $\boldsymbol{M}^+\boldsymbol{M}$ are hermitian, i.e., $\boldsymbol{M}\boldsymbol{M}^+ = (\boldsymbol{M}\boldsymbol{M}^+)^t$, $\boldsymbol{M}^+\boldsymbol{M} = (\boldsymbol{M}^+\boldsymbol{M})^t$;

the *Moore-Penrose Pseudoinverse* of $\boldsymbol{M}$.

We will often drop the identifier "Moore-Penrose" and simply write that $\boldsymbol{M}^+$ is the pseudoinverse of $\boldsymbol{M}$. It's not immediate from the definition, but the pseudoinverse of $\boldsymbol{M}$ has several desirable properties: When $\boldsymbol{M}$ is real, so is $\boldsymbol{M}^+$; $(\boldsymbol{M}^+)^+ = \boldsymbol{M}$; $(\boldsymbol{M}^+\boldsymbol{M})^t = \boldsymbol{M}^+\boldsymbol{M}$. Importantly, when $\boldsymbol{M}$ is invertible, then $\boldsymbol{M}^+ = \boldsymbol{M}^{-1}$. Moreover, the pseudoinverse always exists:

Lemma 2.3 ([BH12]). *Let $\boldsymbol{M} \in \mathbb{C}^{n\times m}$. The pseudoinverse $\boldsymbol{M}^+$ of $\boldsymbol{M}$ exists and is unique. Moreover, the following properties hold:*

(i). $\boldsymbol{M}\boldsymbol{M}^+$ is an orthogonal projector obeying $\mathrm{range}(\boldsymbol{M}\boldsymbol{M}^+) = \mathrm{range}(\boldsymbol{M})$; and

(ii). $\boldsymbol{M}^+\boldsymbol{M}$ is an orthogonal projector obeying $\mathrm{range}(\boldsymbol{M}^+\boldsymbol{M}) = \mathrm{range}(\boldsymbol{M}^+)$.

Together, Definition 2.1 and Lemma 2.3 do not necessarily yield a way to obtain the pseudoinverse of a matrix $\boldsymbol{M}$. We next demonstrate that when the eigendecomposition is known, we can give a precise expression for the pseudoinverse.

Lemma 2.4. *Suppose $\boldsymbol{M} \in \mathbb{C}^{m\times m}$ admits the eigendecomposition*

$$\boldsymbol{M} = \sum_{i=1}^{k} \lambda_i \boldsymbol{\varphi}_i \boldsymbol{\varphi}_i^t,$$

where λ_i, $1 \le i \le k$ are the non-zero eigenvalues of $\boldsymbol{M}$ with corresponding orthornomal eigenvectors $\boldsymbol{\varphi}_1, \ldots, \boldsymbol{\varphi}_k$. Then the pseudoinverse of $\boldsymbol{M}$ is

$$\boldsymbol{M}^+ = \sum_{i=1}^{k} \frac{1}{\lambda_i} \boldsymbol{\varphi}_i \boldsymbol{\varphi}_i^t. \tag{2.5}$$

Proof. Put $\mathbf{Q} = \sum_{i=1}^{k} \lambda_i^{-1} \boldsymbol{\varphi}_i \boldsymbol{\varphi}_I^t$. Since the pseudoinverse is unique, it suffices to show that $\mathbf{Q}$ satisfies the condition of Definition 2.1. Since the eigenvectors are orthonormal by assumption, $\boldsymbol{\varphi}_i^t \boldsymbol{\varphi}_j = \delta_{i,j}$ for all i, j. Hence,

$$\begin{aligned} \boldsymbol{M}\mathbf{Q} &= \sum_{i=1}^k \lambda_i \boldsymbol{\varphi}_i \boldsymbol{\varphi}_i^t \sum_{j=1}^k \lambda_j^{-1} \boldsymbol{\varphi}_j \boldsymbol{\varphi}_j^t = \sum_{i,j=1}^k \lambda_i \lambda_j^{-1} \boldsymbol{\varphi}_i \boldsymbol{\varphi}_i^t \boldsymbol{\varphi}_j \boldsymbol{\varphi}_j^t \\ &= \sum_{i=1}^k \lambda_i \lambda_i^{-1} \boldsymbol{\varphi}_i \boldsymbol{\varphi}_i^t \boldsymbol{\varphi}_i \boldsymbol{\varphi}_i^t = \sum_{i=1}^k \boldsymbol{\varphi}_i \boldsymbol{\varphi}_i^t = \mathbf{Q}\boldsymbol{M}. \end{aligned}$$

Performing a similar computation then demonstrates that

$$\boldsymbol{M}\mathbf{Q}\boldsymbol{M} = \sum_{i=1}^k \boldsymbol{\varphi}_i \boldsymbol{\varphi}_i^t \sum_{j=1}^k \lambda_j \boldsymbol{\varphi}_j \boldsymbol{\varphi}_j^t = \sum_{i,j=1} \lambda_i \boldsymbol{\varphi}_i \boldsymbol{\varphi}_i^t \boldsymbol{\varphi}_j \boldsymbol{\varphi}_j^t = \sum_{i=1}^k \lambda_i \boldsymbol{\varphi}_i \boldsymbol{\varphi}_i^t = \boldsymbol{M},$$

and similarly, $\mathbf{Q}\boldsymbol{M}\mathbf{Q} = \mathbf{Q}$. Moreover, $\boldsymbol{\varphi}_i \boldsymbol{\varphi}_i^t(k,\ell) = \boldsymbol{\varphi}_i(k)\boldsymbol{\varphi}_i(\ell) = \boldsymbol{\varphi}_i(\ell)\boldsymbol{\varphi}_i(k) = (\boldsymbol{\varphi}_i \boldsymbol{\varphi}_i^t)^t(k,\ell)$ implying that $\boldsymbol{\varphi}_i \boldsymbol{\varphi}_i^t = (\boldsymbol{\varphi}_i \boldsymbol{\varphi}_i^t)^t$, so

$$(\mathbf{Q}\boldsymbol{M})^t = (\boldsymbol{M}\mathbf{Q})^t = \left(\sum_{i=1}^k \boldsymbol{\varphi}_i \boldsymbol{\varphi}_i^t)\right)^t = \sum_{i=1}^k (\boldsymbol{\varphi}_i \boldsymbol{\varphi}_i^t)^t = \sum_{i=1}^k \boldsymbol{\varphi}_i \boldsymbol{\varphi}_i^t = \boldsymbol{M}\mathbf{Q} = \mathbf{Q}\boldsymbol{M},$$

so both required conditions hold, and we conclude that $\mathbf{Q} = \boldsymbol{M}^+$. ⊠

§2.3. Spectral Graph Theory

Similarly to Section 2.2, the results in this section can be found in any self-contained reference on (spectral) graph theory (see e.g., [Spi09, CG97]).

We begin with basic graph theory. We denote a *graph* by a triple $G = (V, E, w)$ where V is the *vertex set*, $E \subseteq V \times V$ is the *edge set* and $w : V \times V \to \mathbb{R}_{\geq 0}$ (the non-negative reals) a *weight function*. We let the domain of w be $V \times V$ for convenience; for $(i, j) \notin E$ we have $w((i, j)) = 0$. We call G *unweighted* if $w((i, j)) = \chi_{(i,j)\in E}$ for all i, j. In this case, we may omit the weight function and simply write $G = (V, E)$. Unless otherwise stated, G will be undirected (edges do not have directions) and connected (each vertex is reachable from every other vertex). We will typically take $V = [n]$ for simplicity. For a vertex $i \in V$, we denote the set of its neighbours by

$$\delta_G(i) \stackrel{\text{def}}{=} \{j \in V : w(i, j) > 0\}, \tag{2.6}$$

a set we call that *neighbourhood* of i. The *degree of* i if $\deg(i) \stackrel{\text{def}}{=} |\delta(i)|$. The *weight of* i if $w(i) \stackrel{\text{def}}{=} \sum_{j\in\delta(i)} w(i, j)$. Note that if G is unweighted, then $w(i) = \deg(i)$. If the degree of each vertex in G is equal to k, we call G a *k-regular graph*. We call G *regular* if it is k-regular for some k. If $U \subseteq V$ contains only vertices with the same degree (resp., weight), we call it *degree (resp., weight) homogeneous*. For a set of subset of vertices U, the *volume of* U is

$$\mathrm{vol}_G(U) \stackrel{\text{def}}{=} \sum_{i\in U} w(i), \tag{2.7}$$

and the volume of G is $\text{vol}(G) \stackrel{\text{def}}{=} \text{vol}_G(V(G))$. As usual, we will drop the subscript if the graph is clear from context. Owing to possible mental lapses and above average caffeine intake, we may sometimes abuse notation and extend the weight function w to sets of edges or vertices by setting $w(A) = \sum_{a\in A} w(a)$. Thus, for instance, $w(U) = \text{vol}(U)$, for $U \subseteq V$. (The more notation the better, right?)

Given a subset $U \subseteq V$, we write $G[U]$ to be the graph induced by U, i.e., $V(G[U]) = V \cap U$ and $E(G[U]) = E \cap U \times U$. If a graph is connected and acyclic (i.e., there is a unique path between each pair of vertices) we call it a *tree*. It's well known that a tree on n nodes has $n-1$ edges.

As mentioned above, we will typically work with undirected graphs. In this case, we identify each tuple (i,j) with its sister pair (j,i). This implies, for example, that when summing over all edges $(i,j) \in E$ we are *not* summing over all vertices and their neighbours. Indeed, this latter summation double counts the edges: $\sum_{(i,j)\in E} = \frac{1}{2}\sum_i \sum_{j\in\delta(i)}$. We will often write $i \sim j$ to denote an edge (i,j); so, for example, $\sum_{i\sim j} = \sum_{(i,j)\in E}$.

We will also appeal to so-called "handshaking lemma" for unweighted graphs, which states that $\sum_i \deg_G(i) = 2|E(G)|$; easily verified with a counting argument.

2.3.1. Laplacian Matrices

Here we introduce various matrices of graphs, including the Laplacian. For a useful survey of Laplacian see [Mer94].

Let $G = (V, E, w)$ be a graph, with $V = [n]$ and $|E| = m$. Let $\boldsymbol{W}$ be the *weight matrix* of G, i.e., $\boldsymbol{W} = \text{diag}(w(1), w(2), \ldots, w(n))$. The *degree matrix* of G is

$$\text{diag}(\deg(1), \deg(2), \ldots, \deg(n)).$$

The *adjacency matrix* of G encodes the edge relations, namely, $\boldsymbol{A}_G(i,j) = w((i,j))$ for all $i \neq j$, and $\boldsymbol{A}_G(i,i) = 0$ for all i. Notice that (for undirected graphs) $\boldsymbol{A}_G$ is symmetric. Note that if G is unweighted, then $\boldsymbol{W}_G$ and the degree matrix are equivalent. The *combinatorial Laplacian* of G is the matrix

$$\boldsymbol{L}_G \stackrel{\text{def}}{=} \boldsymbol{W}_G - \boldsymbol{A}_G. \tag{2.8}$$

There are several useful representations of the Laplacian. Let $\boldsymbol{L}_{i,j} = w(i,j)(\chi_i - \chi_j)(\chi_i - \chi_j)^t \in \mathbb{R}^{V\times V}$, i.e.,

$$\boldsymbol{L}_{i,j}(a,b) = \begin{cases} w(i,j) & a = b \in \{i,j\}, \\ -w(i,j), & (a,b) = (i,j), \\ 0, & \text{otherwise.} \end{cases}$$

Then

$$\boldsymbol{L}_G = \sum_{i\sim j} \boldsymbol{L}_{i,j}. \tag{2.9}$$

Another representation comes via the *incidence matrix* of G, $\boldsymbol{B}_G \in \mathbb{R}^{E\times V}$, defined as follows. Place an arbitrary orientation on the edges of G (say, for example, (i,j) is directed from i to

j iff $i < j$), and for an edge e, let $e^- \in V$ denote the vertex at which e begins, and e^+ the vertex at which it ends. Set

$$\boldsymbol{B}_G(e,i) = \begin{cases} 1 & \text{if } i = e^-, \\ -1 & \text{if } i = e^+, \\ 0 & \text{otherwise}, \end{cases} \tag{2.10}$$

or, equivalently, $\boldsymbol{B}_G(e,i) = (\chi_{(i=e^-)} - \chi_{(i=e^+)})$. Then,

$$(\boldsymbol{B}_G^t \boldsymbol{W}_G \boldsymbol{B}_G)(i,j) = \sum_{e\in E} \boldsymbol{B}_G^t(i,e)\boldsymbol{B}_G(e,j) = \sum_{e\in E} w(e)(\chi_{i=e^-} - \chi_{i=e^+})(\chi_{j=e^-} - \chi_{j=e^+}).$$

Let $\alpha(e) = (\chi_{i=e^-} - \chi_{i=e^+})(\chi_{j=e^-} - \chi_{j=e^+})$. If $i = j$, then $\alpha(e) = 1$ iff e is incident to i, and 0 otherwise. If $i \neq j$, then $\alpha(e) = 1$ for $e = (i,j)$ and 0 otherwise, regardless of whether $i = e^-$ and $j = e^+$ or vice versa (this is what ensures that the orientation we chose for the edges is inconsequential). Consequently,

$$(\boldsymbol{B}_G^t \boldsymbol{W}_G \boldsymbol{B}_G)(i,j) = \begin{cases} \sum_{e\ni i} w(e), & \text{if } i = j, \\ -w((i,j)), & \text{otherwise}, \end{cases}$$

which is precisely $\boldsymbol{L}_G(i,j)$. That is, we have

$$\boldsymbol{L}_G = (\boldsymbol{W}_G^{1/2}\boldsymbol{B}_G)^t(\boldsymbol{W}_G^{1/2}\boldsymbol{B}_G). \tag{2.11}$$

We associate with $\boldsymbol{L}_G$ the quadratic form $\mathcal{L}_G : \mathbb{R}^V \to \mathbb{R}$ which acts on functions $\boldsymbol{f} : V \to \mathbb{R}$ as

$$f \xmapsto{\mathcal{L}_G} \boldsymbol{f}^t \boldsymbol{L}_G \boldsymbol{f}.$$

The Laplacian quadratic form will be crucial in our study of the geometry of graphs. Luckily for us then, its action on a vector is captured by an elegant closed-form formula. Computing

$$\boldsymbol{L}_{i,j}\boldsymbol{f} = w(i,j)(\boldsymbol{\chi}_i - \boldsymbol{\chi}_j)(\boldsymbol{\chi}_i - \boldsymbol{\chi}_j)^t\boldsymbol{f} = w(i,j)(\boldsymbol{f}(i) - \boldsymbol{f}(j))(\boldsymbol{\chi}_i - \boldsymbol{\chi}_j).$$

we find that

$$\boldsymbol{f}^t\boldsymbol{L}_{i,j}\boldsymbol{f} = w(i,j)(\boldsymbol{f}(i) - \boldsymbol{f}(j))^2.$$

Therefore, applying Equation 2.9 yields

$$\mathcal{L}_G(\boldsymbol{f}) = \boldsymbol{f}^t\left(\sum_{i\sim j}\boldsymbol{L}_{i,j}\right)\boldsymbol{f} = \sum_{i\sim j}\boldsymbol{f}^t\boldsymbol{L}_{i,j}\boldsymbol{f} = \sum_{i\sim j} w(i,j)(\boldsymbol{f}(i) - \boldsymbol{f}(j))^2. \tag{2.12}$$

Another Laplacian matrix associated with G is the *normalized Laplacian*, given by

$$\widehat{\boldsymbol{L}}_G = \boldsymbol{W}_G^{-1/2}\boldsymbol{L}_G\boldsymbol{W}_G^{-1/2} = \mathbf{I} - \boldsymbol{W}_G^{-1/2}\boldsymbol{A}_G\boldsymbol{W}_G^{-1/2}. \tag{2.13}$$

The normalized Laplacian is intimately related to various phenomena, most notable random walks on the graph [CZ07, CG97]. To investigate $\widehat{\boldsymbol{L}}_G$ we may carry out a similar procedure to above. In particular, if we define $\widehat{\boldsymbol{L}}_{i,j} = \boldsymbol{W}_G^{-1/2}\boldsymbol{L}_{i,j}\boldsymbol{W}_G^{-1/2}$ then we obtain the equivalent of Equation 2.9 for the normalized Laplacian:

$$\widehat{\boldsymbol{L}}_G = \sum_{i\sim j}\widehat{\boldsymbol{L}}_{i,j}. \tag{2.14}$$

Likewise,

$$\boldsymbol{W}_G^{-1/2}\widehat{\boldsymbol{B}}_G^t\boldsymbol{W}_G\widehat{\boldsymbol{B}}_G\boldsymbol{W}_G^{-1/2} = \boldsymbol{W}_G^{-1/2}\boldsymbol{L}_G\boldsymbol{W}_G^{-1/2} = \widehat{\boldsymbol{L}}_G$$

As we've done here, we will typically emphasize the associate of elements associated to the normalized Laplacian with a hat. Using Equation (2.14), we see that the quadratic form $\widehat{\mathcal{L}}_G$ associated with $\widehat{\boldsymbol{L}}_G$ acts as

$$\widehat{\mathcal{L}}_G(\boldsymbol{f}) = \sum_{i\sim j} w(i,j)\left(\frac{\boldsymbol{f}(i)}{\sqrt{w(i)}} - \frac{\boldsymbol{f}(j)}{\sqrt{w(j)}}\right)^2. \tag{2.15}$$

<u>*2.3.2. The Laplacian Spectrum*</u>

Both the combinatorial and normalized Laplacian of an undirected graph G are real, symmetric matrices. By the spectral theorem therefore, they both admit a basis of orthonormal eigenfunctions corresponding to real eigenvalues. Focus for the moment on the combinatorial Laplacian $\boldsymbol{L}_G$, with eigenvalues $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ and corresponding orthonormal eigenfunctions $\boldsymbol{\varphi}_1, \ldots, \boldsymbol{\varphi}_n$. A straightforward consequence of Equation 2.11 is that all eigenvalues of $\boldsymbol{L}_G$ are non-negative. Let λ be an eigenvalue with (unit) eigenvector $\boldsymbol{\varphi}$. Then,

$$\lambda = \lambda\langle\boldsymbol{\varphi},\boldsymbol{\varphi}\rangle = \langle\lambda\boldsymbol{\varphi},\boldsymbol{\varphi}\rangle = \langle\boldsymbol{L}_G\boldsymbol{\varphi},\boldsymbol{\varphi}\rangle = \langle\boldsymbol{B}_G^t\boldsymbol{B}_G\boldsymbol{\varphi},\boldsymbol{\varphi}\rangle = \langle\boldsymbol{B}_G\boldsymbol{\varphi},\boldsymbol{B}_G\boldsymbol{\varphi}\rangle = \|\boldsymbol{B}_G\boldsymbol{\varphi}\|_2^2 \geq 0.$$

Let $V_1, \ldots, V_k \subseteq V$, $V_i \cap V_j = \emptyset$ for $i \neq j$ be the disjoint vertex sets of the distinct connected components of G. (If G is connected then $k = 1$.) The quadratic form satisfies

$$\mathcal{L}_G(f) = \sum_{\ell=1}^k \sum_{i\sim j, i,j\in V_\ell} w(i,j)(f(i)-f(j))^2.$$

Suppose $\boldsymbol{L}\boldsymbol{\varphi} = \boldsymbol{0}$. Then $\boldsymbol{\varphi}^t\boldsymbol{L}\boldsymbol{\varphi} = \mathcal{L}(\boldsymbol{\varphi}) = 0$, which implies that $\boldsymbol{\varphi}(i) = \boldsymbol{\varphi}(j)$ for all $i, j \in V_\ell$. We can immediately see k orthonormal vectors which satisfy this condition, namely

$$\frac{1}{\sqrt{|V_1|}}\boldsymbol{\chi}_{V_1}, \ldots, \frac{1}{\sqrt{|V_k|}}\boldsymbol{\chi}_{V_k}.$$

On the other hand, consider a non-zero vector $\boldsymbol{\varphi}$ which is orthogonal to all of the above vectors. Then

$$0 = \sum_{i=1}^k \langle\boldsymbol{\varphi},\boldsymbol{\chi}_{V_i}\rangle = \langle\boldsymbol{\varphi},\boldsymbol{1}\rangle = \sum_{i=1}^k \boldsymbol{\varphi}(i),$$

implying that there exists $\ell \in [k]$ such that $\boldsymbol{\varphi}(i) \neq \boldsymbol{\varphi}(j)$ for some $i, j \in V_\ell$. Hence, $\mathcal{L}(\boldsymbol{\varphi}) > 0$ and so $\boldsymbol{L}\boldsymbol{\varphi} \neq 0$. Therefore, there are no other linearly independent eigenfunctions corresponding to the zero eigenvalue. We have thus shown that 0 is an eigenvalue of $\boldsymbol{L}$ with multiplicity equal to the number of connected components and

$$\ker(\boldsymbol{L}) = \operatorname{span}(\{\boldsymbol{\chi}_{V_1}, \ldots, \boldsymbol{\chi}_{V_k}\}).$$

For the most part this thesis will deal with connected graphs, in which case $\ker(\boldsymbol{L}) = \operatorname{span}(\{\mathbf{1}\})$.

A similar analysis holds for the normalized Laplacian. Using the same argument but replacing $\boldsymbol{B}$ with $\widehat{\boldsymbol{B}}$ demonstrates that its eigenvalues are non-negative. Its kernel can be determined as follows. For any eigenfunction $\boldsymbol{\varphi}$ of $\boldsymbol{L}$ corresponding to the zero eigenvalue, observe that

$$\widehat{\boldsymbol{L}}\boldsymbol{W}^{1/2}\boldsymbol{\varphi} = \boldsymbol{W}^{-1/2}\boldsymbol{L}\boldsymbol{W}^{-1/2}\boldsymbol{W}^{1/2}\boldsymbol{\varphi} = \boldsymbol{W}^{-1/2}\boldsymbol{L}\boldsymbol{\varphi} = \mathbf{0},$$

so $\boldsymbol{W}^{1/2}\boldsymbol{\chi}_{V_1}, \ldots, \boldsymbol{W}^{1/2}\boldsymbol{\chi}_{V_k}$ lie in the kernel of $\widehat{\boldsymbol{L}}$. Conversely, if $\boldsymbol{\varphi} \in \ker(\widehat{\boldsymbol{L}})$, define vp' such that $\boldsymbol{\varphi} = \boldsymbol{W}^{1/2}\boldsymbol{\varphi}'$ (this is possible because $\boldsymbol{W}^{1/2}$ is diagonal—we simply factor out $\sqrt{w(i)}$ from $\boldsymbol{\varphi}(i)$ to obtain $\boldsymbol{\varphi}'(i)$). Then

$$\mathbf{0} = \widehat{\boldsymbol{L}}\boldsymbol{\varphi}' = \boldsymbol{W}^{-1/2}\boldsymbol{L}\boldsymbol{W}^{-1/2}\boldsymbol{W}^{1/2}\boldsymbol{\varphi} = \boldsymbol{W}^{-1/2}\boldsymbol{L}\boldsymbol{\varphi},$$

so $\boldsymbol{L}\boldsymbol{\varphi} = \mathbf{0}$ (since $w(i) > 0$ for all i). That is, each element in the kernel of $\widehat{\boldsymbol{L}}$ takes the form $\boldsymbol{W}^{1/2}\boldsymbol{\varphi}$ for $\boldsymbol{\varphi} \in \ker(\boldsymbol{L})$. We conclude that

$$\ker(\widehat{\boldsymbol{L}}) = \operatorname{span}(\{\boldsymbol{W}^{1/2}\boldsymbol{\chi}_{V_1}, \ldots, \boldsymbol{W}^{1/2}\boldsymbol{\chi}_{V_k}\}).$$

We end this section by discussing two properties of graph Laplacians. The first is their pseudoinverse relationships, and the second is the remarkable link between the eigenvalues of the combinatorial Laplacian and spanning trees of the graph.

Pseudoinverse of $\boldsymbol{L}_G$ and $\widehat{\boldsymbol{L}}_G$. Since $\boldsymbol{L}_G$ and $\widehat{\boldsymbol{L}}_G$ are both symmetric, $\operatorname{range}(\boldsymbol{L}^t) = \operatorname{range}(\boldsymbol{L}) = \mathbb{R}^n \setminus \ker(\boldsymbol{L}) = \mathbb{R}^n \setminus \operatorname{span}(\{\mathbf{1}\})$, and $\operatorname{range}(\widehat{\boldsymbol{L}}^t) = \operatorname{range}(\widehat{\boldsymbol{L}}) = \mathbb{R}^n \setminus \ker(\widehat{\boldsymbol{L}}) = \mathbb{R}^n \setminus \operatorname{span}(\{\boldsymbol{W}^{1/2}\mathbf{1}\})$. It follows by Lemma 2.3 that the pseudoinverses of these two Laplacians satisfy

$$\boldsymbol{L}_G\boldsymbol{L}_G^+ = \boldsymbol{L}_G^+\boldsymbol{L}_G = \mathbf{I} - \frac{1}{n}\mathbf{1}\mathbf{1}^t, , \tag{2.16}$$

i.e., the projection onto $\operatorname{span}(\mathbf{1})^\perp$, and

$$\widehat{\boldsymbol{L}}_G\widehat{\boldsymbol{L}}_G^+ = \widehat{\boldsymbol{L}}_G^+\widehat{\boldsymbol{L}}_G = \mathbf{I} - \frac{1}{\operatorname{vol}(G)}\boldsymbol{W}_G^{1/2}\mathbf{1}(\boldsymbol{W}_G^{1/2}\mathbf{1})^t = \mathbf{I} - \frac{1}{\operatorname{vol}(G)}\sqrt{\boldsymbol{w}}\sqrt{\boldsymbol{w}}^t, \tag{2.17}$$

the projection onto $\operatorname{span}(\boldsymbol{w})^\perp$, where $\sqrt{\boldsymbol{w}} = (\sqrt{w(1)}, \ldots, \sqrt{w(n)})$. Note that the denominator in (2.17) is $\operatorname{vol}(G)$ instead of n to ensure the result is a projection matrix. Put $\mathbf{P} = \mathbf{I} - \frac{1}{\operatorname{vol}(G)}\sqrt{\boldsymbol{w}}\sqrt{\boldsymbol{w}}^t$. Then

$$\mathbf{P}^2 = \mathbf{I} - \frac{2}{\operatorname{vol}(G)}\sqrt{\boldsymbol{w}}\sqrt{\boldsymbol{w}}^t + \frac{1}{\operatorname{vol}(G)^2}\sqrt{\boldsymbol{w}}\sqrt{\boldsymbol{w}}^t\sqrt{\boldsymbol{w}}\sqrt{\boldsymbol{w}}^t = \mathbf{P},$$

since $\sqrt{\boldsymbol{w}}^t\sqrt{\boldsymbol{w}} = \mathrm{vol}(G)$.

Kirchoff's Theorem. A *spanning tree* of a graph G is a connected subgraph T of G with $V(T) = V(G)$ and $|E(T)| = |V(T)| - 1$. That is, T contains the minimum number of edges possible to connect all vertices of G. We will make use of the following Theorem, often called the *Kirchhoff Tree Theorem*, named after Gustav Kirchhoff for the work done in [Kir47]. It was first stated in its most familiar form by Maxwell [Max73]. We use the formulation found in [CK78].

THEOREM 2.2. *Let $G = (V, E, w)$ be a connected, weighted, and undirected graph. Let $\boldsymbol{L}$ be G's combinatorial Laplacian matrix. Then for all $i, j \in [n]$,*

$$\Gamma_G = (-1)^i(-1)^j \det(\boldsymbol{L}_{-i,-j}) = \frac{1}{n}\sum_{i=1}^{n-1} \lambda_i,$$

where $\lambda_1, \ldots, \lambda_{n-1}$ are the non-zero eigenvalues of G, $\boldsymbol{L}_{-i,-j}$ is the matrix obtained by removing the i-th row and j-th column of $\boldsymbol{L}$, and Γ_G is the weight of all spanning trees of G.

Remark 2.1. The $\mathfrak{T}$ be the set of all spanning trees of a graph G. By the "weight of all spanning trees", we mean that

$$\Gamma_G = \sum_{T\in\mathfrak{T}} \prod_{i\in V(T)} w_G(i). \tag{2.18}$$

Thus, for G unweighted, $\prod_{i\in V(T)} w_G(i) = 1$ so Γ_G simply counts the number of spanning trees.

§2.4. Electrical Flows

Given an undirected, weighted graph $G = (V, E, w)$, orient the edges of G arbitrarily and encode this information in the matrix $\boldsymbol{B}$, as in Section 2.3.1, Equation (2.10). For an edge $e = (i, j)$ oriented from i to j, denote $e^+ = i$ and $e^- = j$. We will consider G as an electrical network. To do this, we imagine placing a resistor of resistance $1/w(e)$ on each edge e. Edges thus carry current between the nodes and, in general, higher weighted edges will carry more current. An *electrical flow* $\boldsymbol{f} : E \to \mathbb{R}_{\geq 0}$ on G assigns a current to each edge e and respects, roughly speaking, Kirchoff's current law and Ohm's law. More precisely, let $\boldsymbol{e}$ be a vector describing the amount of current injected at each node. By Kirchoff's law, the amount of current passing through a vertex i must be conserved. That is,

$$\sum_{e:i=e^+} f(e) - \sum_{e:i=e-} f(e) = e(i),$$

or, more succinctly,

$$\boldsymbol{B}^t\boldsymbol{f} = \boldsymbol{e}. \tag{2.19}$$

Note that this property is also called *flow conversation* in the network flow literature. By Ohm's law, the amount of flow across an edge is proportional to the difference of potential at its endpoints. The constant of proportionality is the inverse of the resistance of that edge, i.e., the weight of the edge. Let $\boldsymbol{\rho} : V \to \mathbb{R}_{\geq 0}$ describe the potential at each vertex. For $e = (i, j)$ with $i = e^+$, $j = e^-$, $\boldsymbol{\rho}$ is defined by the relationship

$$f(e) = w(e)(\rho(i) - \rho(j)) = w(e)(\boldsymbol{B}(e, i)\rho(i) + \boldsymbol{B}(e, j)\rho(j)),$$

so that

$$\boldsymbol{f} = \boldsymbol{W}\boldsymbol{B}\boldsymbol{\rho}. \tag{2.20}$$

Combining (2.19) and (2.20) we see that $\boldsymbol{e} = \boldsymbol{B}^t\boldsymbol{f} = \boldsymbol{B}^t\boldsymbol{W}\boldsymbol{B}\boldsymbol{\rho} = \boldsymbol{L}_G\boldsymbol{\rho}$, and so $\boldsymbol{\rho} = \boldsymbol{L}_G^+\boldsymbol{e}$ whenever $\langle \boldsymbol{e}, \mathbf{1}\rangle = \mathbf{0}$ (recall that $\boldsymbol{L}_G^+$ is the inverse of $\boldsymbol{L}_G$ in the space $\mathrm{span}(\mathbf{1})^t$).

The *effective resistance* of an edge $e = (i, j)$ is the potential difference induced across the edge when one unit of current is injected at i and extracted at j. That is, for $\boldsymbol{e} = \boldsymbol{\chi}_i - \boldsymbol{\chi}_j$, we want to measure $\rho(i) - \rho(j)$. We do this by noticing that

$$\rho(i) - \rho(j) = \langle \boldsymbol{\chi}_i, \boldsymbol{\rho}\rangle - \langle \boldsymbol{\chi}_j, \boldsymbol{\rho}\rangle = \langle \boldsymbol{\chi}_i - \boldsymbol{\chi}_j, \boldsymbol{L}_G^+\boldsymbol{e}\rangle = \mathcal{L}_G^+(\boldsymbol{\chi}_i - \boldsymbol{\chi}_j).$$

Note that here we've relied on the fact that $\boldsymbol{\chi}_i - \boldsymbol{\chi}_j \perp \mathbf{1}$. We cement the notion with a definition.

Definition 2.2. The *effective resistance* between nodes i and j is $r^{\text{eff}}(i, j) \stackrel{\text{def}}{=} \mathcal{L}_G^+(\boldsymbol{\chi}_i - \boldsymbol{\chi}_j)$.

We can relate the entries of the pseudoinverse Laplacian with the effective resistance as follows. First let us introduce the *effective resistance matrix of* G, denote $\boldsymbol{R}_G$, with entries $\boldsymbol{R}_G(i, j) = r^{\text{eff}}(i, j)$. Noting that

$$\boldsymbol{R}_G(i, j) = \boldsymbol{\chi}_i^t\boldsymbol{L}_G^+\boldsymbol{\chi}_i + \boldsymbol{\chi}_j^t\boldsymbol{L}_G^+\boldsymbol{\chi}_j - 2\boldsymbol{\chi}_i^t\boldsymbol{L}_G^+\boldsymbol{\chi}_j = \boldsymbol{L}_G^+(i, i) + \boldsymbol{L}_G^+(j, j) - 2\boldsymbol{L}_G^+(i, j),$$

we have

$$\boldsymbol{R}_G = \mathbf{1}\mathbf{u}^t + \mathbf{u}\mathbf{1}^t - 2\boldsymbol{L}_G^+,$$

where $\mathbf{u} = \mathrm{diag}(\boldsymbol{L}_G^+(i, i))$. From here we see that $\boldsymbol{x}^t\boldsymbol{R}_G\boldsymbol{x} = -2\boldsymbol{x}^t\boldsymbol{L}_G^+\boldsymbol{x}$ for any $\boldsymbol{x} \in \mathrm{span}(\mathbf{1})^\perp$. Therefore,

$$\begin{aligned}
\boldsymbol{L}_G^+(i, j) &= \boldsymbol{\chi}_i^t\boldsymbol{L}_G^+\boldsymbol{\chi}_j \\
&= \left(\boldsymbol{\chi}_i - \frac{1}{n}\mathbf{1}\right)^t \boldsymbol{L}_G^+\left(\boldsymbol{\chi}_j - \frac{1}{n}\mathbf{1}\right) \\
&= -\frac{1}{2}\left(\boldsymbol{\chi}_i - \frac{1}{n}\mathbf{1}\right)^t \boldsymbol{R}_G\left(\boldsymbol{\chi}_j - \frac{1}{n}\mathbf{1}\right) \\
&= \frac{1}{2n}\left(\sum_{k\in[n]} r^{\text{eff}}(i, k) + r^{\text{eff}}(j, k)\right) - \frac{1}{2}r^{\text{eff}}(i, j) - \frac{R_G}{n^2},
\end{aligned} \tag{2.21}$$

where R_G is the total effective resistance of the graph. For $i=j$, this becomes

$$\boldsymbol{L}_G^+(i,i) = \frac{1}{n}\sum_{k\in[n]} r^{\text{eff}}(i,k) - \frac{R_G}{n^2}. \tag{2.22}$$

§2.5. Simplices

Finally we reach what is our main object of study. We begin by describing a relationship among a set of vertices which, roughly speaking, generalizes the notion of "non-collinearity" to higher dimensions. We are then able to properly define a simplex and its dual. We end the section by briefly discussing several of the angles in a simplex.

Affine Independence. In order to properly define simplices, we need to define the notion of "affine independence" between points. In $\mathbb{R}^2$, for example, such a relationship characterizes the sets of three points which describe a triangle.

Definition 2.3. A set of points $\boldsymbol{x}_1,\dots,\boldsymbol{x}_k$ are said to be *affinely independent* if the only solution to $\sum_{i\in[n]}\alpha_i\boldsymbol{x}_i = \boldsymbol{0}$ with $\sum_{i\in[n]}\alpha_i = 0$ is $\alpha_1 = \cdots = \alpha_n = 0$.

Perhaps a more useful characterization of affine independence is the following.

Lemma 2.5. *The set $\{\boldsymbol{x}_1,\dots,\boldsymbol{x}_k\}$ is affinely independent iff for each j, $\{\boldsymbol{x}_j - \boldsymbol{x}_i\}_{i\neq j}$ is linearly independent.*

Proof. Suppose that $\{\boldsymbol{x}_j-\boldsymbol{x}_i\}_{i\neq j}$ is not linearly independent, and let $\{\beta_i\}$ (not all zero) be such that $\sum_{i\neq j}\beta_i(\boldsymbol{x}_j-\boldsymbol{x}_j)=\boldsymbol{0}$. Putting $\beta=\sum_i\beta_i$, we can write this as

$$\sum_{i\neq j}\frac{\beta_i}{\beta}\boldsymbol{x}_i - \boldsymbol{x}_j = \boldsymbol{0}.$$

But these coefficients sum to 0, i.e., $\sum_{i\neq j}\beta_i/\beta - 1 = 1-1-0$, so $\{\boldsymbol{x}_i\}$ are not affinely independent. Conversely, suppose that $\sum_i\alpha_i\boldsymbol{x}_i=\boldsymbol{0}$ where $\sum_i\alpha_i=0$ and $\alpha_k\neq 0$ for some k. Then,

$$\boldsymbol{0} = \sum_i\alpha_i\boldsymbol{x}_i = \sum_{i\neq j}\alpha_i\boldsymbol{x}_i + \alpha_j\boldsymbol{x}_j = \sum_{i\neq j}\alpha_i\boldsymbol{x}_i - \sum_{i\neq j}\alpha_i\boldsymbol{x}_j = \sum_{i\neq j}\alpha_i(\boldsymbol{x}_i-\boldsymbol{x}_j),$$

implying that $\{\boldsymbol{x}_j-\boldsymbol{x}_i\}_{i\neq j}$ is not linearly independent. ⊠

The following lemma demonstrates that if we form a matrix of size $n-1\times n$ from the column vectors of n affine independent vectors, then this matrix has full rank. Moreover, we may assume that the linear combination of the vectors is in fact an *affine combination*, in the following sense.

Lemma 2.6. *Let $\{\boldsymbol{x}_1,\dots,\boldsymbol{x}_n\}\subseteq\mathbb{R}^{n-1}$ be affinely independent, and let $\boldsymbol{y}\in\mathbb{R}^{n-1}$ be arbitrary. Then there exists coefficients $\{\alpha_i\}\subseteq\mathbb{R}$ obeying $\sum_{i\in[n]}\alpha_i=1$ such that $\boldsymbol{y}=\sum_{i\in[n]}\alpha_i\boldsymbol{x}_i$.*

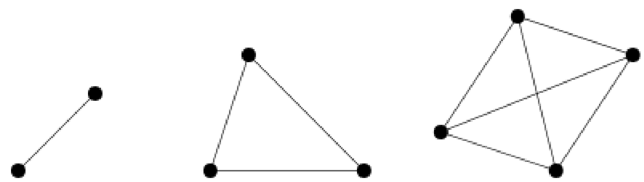


Figure 2.1: Simplices in dimensions one, two, and three. We wish the reader luck in visualizing a simplex (or anything really) in more than three dimensions.

Proof. By Lemma 2.5, the vectors $\boldsymbol{\zeta}_i = \boldsymbol{x}_i - \boldsymbol{x}_n$, $i < n$ are linearly independent and span $\mathbb{R}^{n-1}$. Therefore, there exist real numbers α_i, $i < n$ with $\boldsymbol{y} - \boldsymbol{x}_n = \sum_{i<n} \alpha_i \boldsymbol{\zeta}_i$. Putting $\alpha_n = 1 - \sum_{i<n} \alpha_i$, we have $\boldsymbol{y} = \sum_{i<n} \alpha_i \boldsymbol{\zeta}_i + x_n = \sum_{i<n} \alpha_i \boldsymbol{x}_i + (1 - \sum_{i<n} \alpha_i)\boldsymbol{x}_n = \sum_{i\in[n]} i\alpha_i \boldsymbol{x}_i$. It's immediate that $\sum_i \alpha_i = 1$. $\boxtimes$

The simplex. We jump straight into the definition.

Definition 2.4. A *simplex* $\mathcal{T}$ in $\mathbb{R}^{n-1}$ is the convex hull of n affinely independent vectors $\boldsymbol{\sigma}_1, \ldots, \boldsymbol{\sigma}_n$. That is, $\mathcal{S} = \operatorname{conv}(\boldsymbol{\sigma}_1, \ldots, \boldsymbol{\sigma}_n)$.

If we gather the vertices of the simplex $\mathcal{T}$ into the *vertex matrix* $\boldsymbol{\Sigma} = (\boldsymbol{\sigma}_1, \ldots, \boldsymbol{\sigma}_n)$ whose columns are the vertex vectors of $\mathcal{T}$, then we can write the simplex as

$$\mathcal{T} = \{\boldsymbol{\Sigma x} : \boldsymbol{x} \geq \boldsymbol{0},\ \|\boldsymbol{x}\|_1 = 1\}.$$

Given a point $\boldsymbol{p} = \boldsymbol{\Sigma x} \in \mathcal{S}$, $\boldsymbol{x}$ is called the *barycentric coordinate* of $\boldsymbol{p}$.

As is illustrated in two and three dimensions by the triangle and the tetrahedron, the projection of the simplex onto spaces spanned by subsets of its vertices yields simplices of lower dimensions. Let $U \subseteq [n]$. The *face of $\mathcal{T}$ corresponding to U* is

$$\mathcal{T} \restriction_U \stackrel{\text{def}}{=} \{\boldsymbol{\Sigma x} : \boldsymbol{x} \geq 0,\ \|\boldsymbol{x}\|_1 = 1,\ x(i) = 0 \text{ for all } i \in U^c\}. \tag{2.23}$$

The following observation demonstrates that $\mathcal{S} \restriction_U$ is a well-defined simplex.

Observation 2.2. *Any subset of an affinely independent set of vectors is again affinely independent.*

Proof. Let $\{v_i\}_{i\in[n]}$ be a set of vectors and let $U \subsetneq [n]$ be a proper subset of $[n]$. If $\{\mathbf{v}_i\}_{i\in U}$ is not affinely independent, then there exists $\{\alpha_i\}_{j\in U}$ not all zero such that $\sum_{i\in U} \alpha_i \mathbf{v}_i = \mathbf{0}$ and $\sum_i \alpha_i = 0$. Taking $\alpha_j = 0$ for $j \in U^c$ implies that $\sum_{i\in[n]} \alpha_i \mathbf{v}_i = \mathbf{0}$ while maintaining that $\sum_i \alpha_i = 0$. Hence $\{v_i\}_{i\in[n]}$ is not affinely independent. $\boxtimes$

Trusting the reader's capacity for variation, depending on the situation we may adopt different notation for the faces of a simplex. Oftentimes the vertical restriction symbol will be dropped and we will write only $\mathcal{S}_U$; other times we will write $\mathcal{S}[U]$, especially when the space reserved a subscript is being used for other purposes.

In our study of simplices we will be mainly concerned with their relative properties (e.g., volume, angles, shape, etc.) as opposed to their absolute positions in space. Thus, it will often be convenient to identity simplices which share the same relative properties, but are simply rotated and /or translated versions of one another. We will call such simplices *congruent*, or occasionally *isomorphic*. Unfortunately for notational simplicity, it will be required to sometimes differentiate between simplices which are congruent by translation only, and simplices which are congruent by translation *and* rotation. Let us call the former type of congruence *translational congruence*. We will continue to call the latter simply congruence. Thus, the set of translationally congruent simplices to a simplex $\mathcal{T}$ is a subset of those simplices which are congruent to $\mathcal{T}$. We use the symbol $\cong$ to denote translational congruency between simplices; so $\mathcal{T}_1 \cong \mathcal{T}_2$ iff $\boldsymbol{\Sigma}(\mathcal{S}_1) = \boldsymbol{\Sigma}(\mathcal{S}_2) + \boldsymbol{\alpha}\mathbf{1}^t$ for some $\boldsymbol{\alpha} \in \mathbb{R}^{n-1}$. We use $\cong^{\circlearrowleft}$ to denote general congruency; so $\mathcal{T}_1 \cong^{\circlearrowleft} \mathcal{T}_2$ iff $\boldsymbol{\Sigma}(\mathcal{T}_1) = \boldsymbol{Q}\boldsymbol{\Sigma}(\mathcal{T}_2) + \boldsymbol{\alpha}\mathbf{1}^t$ for some rotation matrix $\boldsymbol{Q}$ and $\boldsymbol{\alpha} \in \mathbb{R}^{n-1}$. We will also define two congruence classes of simplices. Put

$$[\mathcal{T}] \stackrel{\text{def}}{=} \{\mathcal{T}' : \mathcal{T}' \cong \mathcal{T}\}, \quad \text{and} \quad [\mathcal{T}]^{\circlearrowleft} \stackrel{\text{def}}{=} \{\mathcal{T}' : \mathcal{T}' \cong^{\circlearrowleft} \mathcal{T}\}. \tag{2.24}$$

.

A brief note now on nomenclature. We will typically use the symbol $\mathcal{T}$ to denote an arbitrary simplex. Later, we will use the symbol $\mathcal{S}$ to denote the simplex associated to a graph. In this way we hope to provide a clear separation between those statements which hold for general simplices and those which hold for simplices of a graph.

Centroids and altitudes. Two fundamental objects related to a simplex are its centroid and altitudes. The *centroid* of a simplex is the point

$$\boldsymbol{c}(\mathcal{T}) \stackrel{\text{def}}{=} \frac{1}{n}\boldsymbol{\Sigma}\mathbf{1} = \frac{1}{n}\sum_{i\in[n]} \boldsymbol{\sigma}_i. \tag{2.25}$$

The centroid of a simplex can be thought of as its centre of mass, assuming that weight is distributed evenly across its surface. The *altitude between faces $\mathcal{T}_U$ and $\mathcal{T}_{U^c}$* is a vector which lies in the orthogonal complement of both $\mathcal{S}_U$ and $\mathcal{S}_{U^c}$ and points from one face to the other. We denote the altitude pointing from $\mathcal{S}_{U^c}$ to $\mathcal{S}_U$ as $\boldsymbol{a}_(\mathcal{S}_U)$. We can write the altitude as $\boldsymbol{a}_U = \boldsymbol{p} - \boldsymbol{q}$ for some $\boldsymbol{p} \in \mathcal{S}_{U^c}$ and $\boldsymbol{q} \in \mathcal{S}_U$, and thus as $\boldsymbol{\Sigma}(\boldsymbol{x}_{U^c} - \boldsymbol{x}_U)$ where $\boldsymbol{x}_{U^c}$ and $\boldsymbol{x}_U$ are the barycentric coordinates of $\boldsymbol{p}$ and $\boldsymbol{q}$.

Nota Bene: While we conceptualize of the altitude $\boldsymbol{a}(\mathcal{T}_U)$ as pointing from $\mathcal{T}_U$ to $\mathcal{T}_{U^c}$, we remark that since we are working in $\mathbb{R}^{n-1}$ as a vector space, $\boldsymbol{a}(\mathcal{T}_U)$ still "begins" at the origin.

Centred simplex. In later sections it will be convenient to work with a translated copy of a given simplex which is centred at the origin. Accordingly, given any simplex $\mathcal{T}$ with vertices $\{\boldsymbol{\sigma}_i\}$, we let $\mathcal{T}_0$ denote the simplex with vertices $\{\boldsymbol{\sigma}_i - \boldsymbol{c}(\mathcal{T})\}$. Note that $\mathcal{T}_0 \in [\mathcal{T}]$.

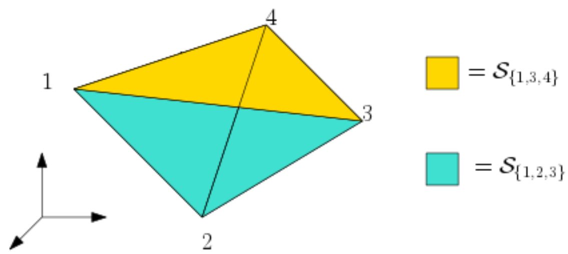


Figure 2.2:

It's clear that the centroid of $\mathcal{T}_0$ is the origin:

$$\begin{aligned}\boldsymbol{c}(\mathcal{T}_0) &= \frac{1}{n}(\boldsymbol{\sigma}_1 - \boldsymbol{c}(\mathcal{T}),\ \dots\ \boldsymbol{\sigma}_n - \boldsymbol{c}(\mathcal{T}))\mathbf{1} \\ &= \frac{1}{n}(\boldsymbol{\sigma}_1\ \dots\ \boldsymbol{\sigma}_n)\mathbf{1} - \frac{1}{n}(\boldsymbol{c}(\mathcal{T})\ \dots\ \boldsymbol{c}(\mathcal{T}))\mathbf{1} = \boldsymbol{c}(\mathcal{T}) - \boldsymbol{c}(\mathcal{T}) = \mathbf{0}.\end{aligned}$$

We solidify the concept with a definition.

Definition 2.5. Given a simplex $\mathcal{T}$, the unique (up to rotation and translation) simplex with vertex matrix $\mathbf{\Sigma}(\mathcal{T}) - (\boldsymbol{c}(\mathcal{T})\ \dots\ \boldsymbol{c}(\mathcal{T}))$ centred at the origin is called the *canonical (or centred) simplex corresponding to* $\mathcal{T}$ and is denoted $\mathcal{T}_0$.

We may also refer to $\mathcal{T}_0$ as the *centred version of* $\mathcal{T}$ in order spare the author the agony induced by writing out the complete sentence "corresponding to the simplex $\mathcal{T}$".

2.5.1. Dual Simplex

Let $\mathbf{\Sigma} = (\boldsymbol{\sigma}_1, \dots, \boldsymbol{\sigma}_n) \in \mathbb{R}^{n-1\times n}$ be the vertex matrix of a simplex $\mathcal{T} \subseteq \mathbb{R}^{n-1}$. For each $i \in [n-1]$, put $\mathbf{v}_i = \boldsymbol{\sigma}_n - \boldsymbol{\sigma}_i$. Then $\{\mathbf{v}_1, \dots, \mathbf{v}_{n-1}\}$ is a linearly independent set, and thus admits a sister basis $\{\boldsymbol{\gamma}_1, \dots, \boldsymbol{\gamma}_{n-1}\}$ which together form biorthogonal bases of $\mathbb{R}^{n-1}$ (Lemma 2.1). Put $\boldsymbol{\gamma}_n = -\sum_{i=1}^{n-1} \boldsymbol{\gamma}_i$.

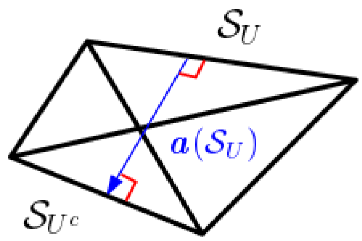
Claim 2.1. *The set* $\{\boldsymbol{\gamma}_1, \dots, \boldsymbol{\gamma}_n\}$ *is affinely independent.*

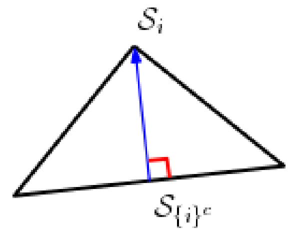
Proof. Suppose not and let $\{\beta_i\}$ be such that $\sum_i \beta_i \boldsymbol{\gamma}_i = \mathbf{0}$ with $\sum_i \beta_i = 0$. Then,

$$\mathbf{0} = \sum_i \beta_i \boldsymbol{\gamma}_i = \sum_{i=1}^{n-1} \beta_i \boldsymbol{\gamma}_i - \left(\sum_{i=1}^{n-1} \beta_i\right) \sum_{j=1}^{n-1} \boldsymbol{\gamma}_j = \sum_{i=1}^{n-1} \left(\beta_i - \sum_{j=1}^{n-1} \beta_j\right) \boldsymbol{\gamma}_i,$$

implying that $\{\boldsymbol{\gamma}_i\}_{i=1}^{n-1}$ is linearly dependent; a contradiction. ⊠

Therefore, the set $\{\boldsymbol{\gamma}_1, \dots, \boldsymbol{\gamma}_n\}$ determines a simplex, which we call the *dual simplex* of $\mathcal{T}$. Of course, it would highly suboptimal if the notion of a dual simplex depended on the labelling of the vertices of $\mathcal{T}$. More specifically, we defined the vertices of the dual simplex





$\boldsymbol{\gamma}_i$ with respect to the vectors $\boldsymbol{\sigma}_i - \boldsymbol{\sigma}_n$. It is not clear a priori whether the vertices of the dual simplex would change were we to relabel the indices of $\{\boldsymbol{\sigma}_i\}$. In fact, they do not—the demonstration of which is the purpose of the following lemma.

LEMMA 2.7. *Let $\{\boldsymbol{\sigma}_1, \ldots, \boldsymbol{\sigma}_n\}$ be a set of affinely independent vectors. Fix $k \in [n-1]$ and define $\mathbf{v}_i = \boldsymbol{\sigma}_i - \boldsymbol{\sigma}_n$ for $i \in [n-1]$ and $\mathbf{u}_i = \boldsymbol{\sigma}_i - \boldsymbol{\sigma}_k$ for $i \in [n] \setminus \{k\}$. If $\{\boldsymbol{\gamma}_1, \ldots, \boldsymbol{\gamma}_{n-1}\}$ is the sister basis to $\{\mathbf{v}_1, \ldots, \mathbf{v}_{n-1}\}$ and $\boldsymbol{\gamma}_n = -\sum_{i=1}^{n-1} \boldsymbol{\gamma}_i$, then $\{\boldsymbol{\gamma}_1, \ldots, \boldsymbol{\gamma}_{k-1}, \boldsymbol{\gamma}_{k+1}, \ldots, \boldsymbol{\gamma}_n\}$ is the sister basis to $\{\mathbf{u}_1, \ldots, \mathbf{u}_{k-1}, \mathbf{u}_{k+1}, \ldots, \mathbf{u}_n\}$.*

Proof. We need to show that $\langle \boldsymbol{\gamma}_i, \mathbf{u}_j \rangle = \delta_{ij}$ for all $i, j \neq k$. For $i \neq n$, we have

$$\begin{aligned} \langle \boldsymbol{\gamma}_i, \boldsymbol{\sigma}_j - \boldsymbol{\sigma}_k \rangle &= \langle \boldsymbol{\gamma}_i, \boldsymbol{\sigma}_j - \boldsymbol{\sigma}_n + \boldsymbol{\sigma}_n - \boldsymbol{\sigma}_k \rangle \\ &= \langle \boldsymbol{\gamma}_i, \boldsymbol{\sigma}_j - \boldsymbol{\sigma}_n \rangle - \langle \boldsymbol{\gamma}_i, \boldsymbol{\sigma}_k - \boldsymbol{\sigma}_n \rangle \\ &= \delta_{ij} - \delta_{ik} = \delta_{ij}, \end{aligned}$$

since $i \neq k$. For $i = n$ meanwhile,

$$\begin{aligned} \langle \boldsymbol{\gamma}_n, \boldsymbol{\sigma}_j - \boldsymbol{\sigma}_k \rangle &= -\sum_{\ell=1}^{n-1} \langle \boldsymbol{\gamma}_\ell, \boldsymbol{\sigma}_j - \boldsymbol{\sigma}_n + \boldsymbol{\sigma}_n - \boldsymbol{\sigma}_k \rangle \\ &= \sum_{\ell=1}^{n-1} \langle \boldsymbol{\gamma}_\ell, \boldsymbol{\sigma}_j - \boldsymbol{\sigma}_n \rangle - \sum_{\ell=1}^{n-1} \langle \boldsymbol{\gamma}_\ell, \boldsymbol{\sigma}_k - \boldsymbol{\sigma}_n \rangle = \sum_{\ell} \delta_{j\ell} - \delta_{k\ell} = 0. \end{aligned}$$

⊠

We also observe that, using the same notation as above,

$$-\sum_{i=1, i\neq k}^{n} \boldsymbol{\gamma}_i = -\Bigg(\sum_{i=1, i\neq k}^{n-1} \boldsymbol{\gamma}_i \Bigg) - \boldsymbol{\gamma}_n = -\sum_{i=1, i\neq k}^{n-1} \boldsymbol{\gamma}_i + \sum_{j=1}^{n-1} \boldsymbol{\gamma}_j = \boldsymbol{\gamma}_k,$$

hence had we set $\mathbf{v}_i = \boldsymbol{\sigma}_k - \boldsymbol{\sigma}_i$ and defined $\boldsymbol{\gamma}_k = -\sum_{i\neq k} \boldsymbol{\gamma}_i$ (as we did for $k = n$), Lemma 2.7 demonstrates that we would produce the same set of vectors for the dual simplex. We honour the fact that the dual simplex is independent of labelling, i.e., well-defined, with the following definition.

DEFINITION 2.6 (Dual Simplex). Given a simplex $\mathcal{T}_1 \subseteq \mathbb{R}^{n-1}$ with vertex set $\boldsymbol{\Sigma}(\mathcal{S}_1) = (\boldsymbol{\sigma}_1, \ldots, \boldsymbol{\sigma}_n)$, a simplex $\mathcal{T}_2 \subseteq \mathbb{R}^{n-1}$ with vertex vectors $\boldsymbol{\Sigma}(\mathcal{T}_2) = (\boldsymbol{\gamma}_1, \ldots, \boldsymbol{\gamma}_n)$ is called a *dual simplex* of $\mathcal{T}_1$ if for all $k \in [n]$, $\{\boldsymbol{\gamma}_i\}_{i\neq k}$ is the sister basis to $\{\boldsymbol{\sigma}_i - \boldsymbol{\sigma}_k\}_{i\neq k}$. We denote the dual of the simplex $\mathcal{T}$ as $\mathcal{T}^*$.

We remark that in light of the previous lemma that in order to determine whether the vertices $\{\boldsymbol{\gamma}_i\}$ are the dual vertices to $\{\boldsymbol{\sigma}_i\}$ it suffices to check whether $\langle \boldsymbol{\gamma}_i, \boldsymbol{\sigma}_j - \boldsymbol{\sigma}_k\rangle = \delta_{ij}$ for a single $k \neq i, j$, as opposed to all $k \in [n]$. This will be done henceforth and will not be further remarked upon. We also note that duality between simplices is not a relationship between individual simplices per se, but rather assigns to congruence class $[\mathcal{T}]$ a centred simplex. Indeed, let $\mathcal{T}_1 \in [\mathcal{T}]$ and let $\boldsymbol{\Sigma}(\mathcal{T}^*) = (\boldsymbol{\sigma}_1^*, \dots, \boldsymbol{\sigma}_n^*)$. We claim that the vertices $\boldsymbol{\Sigma}(\mathcal{T}^*)$ are also dual to $\boldsymbol{\Sigma}(\mathcal{T}_1^*) = (\boldsymbol{\gamma}_1, \dots, \boldsymbol{\gamma}_n)$. Let $\boldsymbol{\alpha} \in \mathbb{R}^{n-1}$ be such that $\boldsymbol{\gamma}_i = \boldsymbol{\sigma}_i + \boldsymbol{\alpha}\mathbf{1}^t$. Then,

$$\langle \boldsymbol{\sigma}_i^*, \boldsymbol{\gamma}_j - \boldsymbol{\gamma}_n\rangle = \langle \boldsymbol{\sigma}_i^*, (\boldsymbol{\sigma}_j + \boldsymbol{\alpha}) - (\boldsymbol{\sigma}_n + \boldsymbol{\alpha})\rangle = \langle \boldsymbol{\sigma}_i^*, \boldsymbol{\sigma}_j - \boldsymbol{\sigma}_n\rangle = \delta_{ij},$$

meaning that $\mathcal{T}^*$ is also dual to $\mathcal{T}_1$. We encapsulate this in an observation for easy recollection.

Observation 2.3. *A simplex $\mathcal{T}$ and corresponding centred simplex $\mathcal{T}_0$ share the same dual, i.e., $\mathcal{S}^* = \mathcal{T}_0^*$.*

Observe that the dual simplex is always centred by construction (since $\boldsymbol{\gamma}_n = -\sum_{i<n} \boldsymbol{\gamma}_i$). The following lemma demonstrates that, in the language of the preceding paragraph, if $\mathcal{T}^*$ is the dual of the congruence class $[\mathcal{T}]$, then the dual of $[\mathcal{T}^*]$ is the representative of $[\mathcal{T}]$ which is centred.

Lemma 2.8. *Let a simplex $\mathcal{T} \in \mathbb{R}^{n-1}$ have vertices $(\boldsymbol{\sigma}_i)$, $\mathcal{T}^*$ have vertices $(\boldsymbol{\sigma}_i^*)$ and $(\mathcal{T}^*)^*$ have vertices $(\boldsymbol{\gamma}_i)$. Then, after potential re-ordering of the indices, $\boldsymbol{\gamma}_i = \boldsymbol{\sigma}_i - \boldsymbol{\sigma}_n$ for $i < n$.*

Proof. We are given that $\langle \boldsymbol{\sigma}_i^*, \boldsymbol{\sigma}_j - \boldsymbol{\sigma}_n\rangle = \delta_{ij}$ and $\langle \boldsymbol{\gamma}_i, \boldsymbol{\sigma}_j^* - \boldsymbol{\sigma}_n^*\rangle = \delta_{ij}$. Since dual bases are unique, it suffices to show that $\boldsymbol{\sigma}_i - \boldsymbol{\sigma}_n$ satisfies the relationships of $\boldsymbol{\gamma}_i$, and indeed $\langle \boldsymbol{\sigma}_i - \boldsymbol{\sigma}_n, \boldsymbol{\sigma}_j^* - \boldsymbol{\sigma}_n^*\rangle = \langle \boldsymbol{\sigma}_i, \boldsymbol{\sigma}_j^* - \boldsymbol{\sigma}_n^*\rangle - \langle \boldsymbol{\sigma}_n, \boldsymbol{\sigma}_j^* - \boldsymbol{\sigma}_n^*\rangle = \delta_{ij} - \delta_{in} = \delta_{ij}$. ⊠

Remark 2.2. The notion of the dual simplex expounded here is the same as the object discovered by Fiedler in his book [Fie11, Chapter 5], which he calls the *inverse simplex*. In a covert attempt to confuse the reader, we will reserve the name inverse simplex for a (sometimes) distinct object. Fiedler defines the inverse simplex with respect to the centroid of the given simplex, finding vectors $\mathbf{u}_i$ such that $\langle \mathbf{u}_i, \boldsymbol{\sigma}_j - \boldsymbol{c}\rangle = \delta_{ij} - 1/n$, where $\boldsymbol{c} = \boldsymbol{c}(\mathcal{S})$. Such vectors then satisfy $\langle \mathbf{u}_i, \boldsymbol{\sigma}_j - \boldsymbol{\sigma}_k\rangle = \langle \mathbf{u}_i, \boldsymbol{\sigma}_j - \boldsymbol{c} - (\boldsymbol{\sigma}_k - \boldsymbol{c})\rangle = \delta_{ij} - \delta_{ik} = \delta_{ij}$ for $i, j \neq k$, hence are the (unique) dual vertices.

We summarize the discussion with the following theorem.

Theorem 2.3. *Each simplex has a unique dual simplex. Moreover, if $\mathcal{T}^*$ is the dual of $\mathcal{T}$, then $\mathcal{S}_0$ is the dual of $\mathcal{S}^*$, where $\mathcal{S}_0 \cong \mathcal{S}$ is centred.*

Proof. Existence follows from Lemma 2.1 using the construction above. Uniqueness follows from Observation 2.1 and Lemma 2.7. The second part of the statement follows from Lemma 2.8. ⊠

We end this section on dual simplices by giving a necessary condition of the relationship between a simplex and its dual.

Lemma 2.9. *Let $\mathcal{S}^*$ be the dual of the simplex $\mathcal{S} \in \mathbb{R}^{n-1}$. For all $U \subseteq [n]$, $\emptyset \neq U \neq [n]$, $\mathcal{S}_U$ is orthogonal to $\mathcal{S}^*_{U^c}$.*

Proof. Let $\mathbf{\Sigma}(\mathcal{S}) = (\boldsymbol{\sigma}_1, \dots, \boldsymbol{\sigma}_n)$ and $\mathbf{\Sigma}(\mathcal{S}^*) = (\boldsymbol{\sigma}_1^*, \dots, \boldsymbol{\sigma}_n^*)$. Let $\mathbf{\Sigma}\boldsymbol{x} \in \mathcal{S}_U$ and $\mathbf{\Sigma}^*\boldsymbol{y}_1, \mathbf{\Sigma}^*\boldsymbol{y}_2 \in \mathcal{S}^*_{U^c}$, where $\boldsymbol{y}_1$ and $\boldsymbol{y}_2$ are barycentric coordinates. Fix $k \in U^c$. We need to show that $\langle \mathbf{\Sigma}\boldsymbol{x}, \mathbf{\Sigma}^*\boldsymbol{y}_1 - \mathbf{\Sigma}^*\boldsymbol{y}_2 \rangle = 0$. First, using $\|\boldsymbol{y}_i\| = 1$, $i = 1, 2$, write

$$\begin{aligned}
\mathbf{\Sigma}^*\boldsymbol{y}_1 - \mathbf{\Sigma}^*\boldsymbol{y}_2 &= \sum_{j \in U^c} \boldsymbol{\sigma}_j^*(y_1(j) - y_2(j)) \\
&= \sum_{j \in U^c \setminus \{k\}} \boldsymbol{\sigma}_j^*(y_1(j) - y_2(j)) + \boldsymbol{\sigma}_k^*(y_1(k) - y_2(k)) \\
&= \sum_{j \in U^c \setminus \{k\}} \boldsymbol{\sigma}_j^*(y_1(j) - y_2(j)) - \boldsymbol{\sigma}_k^* \Bigg(\sum_{j \in U^c \setminus \{k\}} y_1(j) - y_2(j) \Bigg) \\
&= \sum_{j \in U^c \setminus \{k\}} (\boldsymbol{\sigma}_j^* - \boldsymbol{\sigma}_k^*)(y_1(j) - y_2(j)).
\end{aligned}$$

Now, by definition, $\langle \boldsymbol{\sigma}^i, \boldsymbol{\sigma}_j^* - \boldsymbol{\sigma}_k^* \rangle = \delta_{i,j}$ for $i, j \neq k$ so it follows that

$$\begin{aligned}
\langle \mathbf{\Sigma}\boldsymbol{x}, \mathbf{\Sigma}^*(\boldsymbol{y}_1 - \boldsymbol{y}_2) \rangle &= \sum_{i \in U} x(i) \langle \boldsymbol{\sigma}_i, \mathbf{\Sigma}^*(\boldsymbol{y}_1 - \boldsymbol{y}_2) \rangle \\
&= \sum_{i \in U} x(i) \sum_{j \in U^c \setminus \{k\}} \langle \boldsymbol{\sigma}_i, \boldsymbol{\sigma}_j^* - \boldsymbol{\sigma}_k^* \rangle (y_1(j) - y_2(j)) \\
&= \sum_{i \in U} x(i) \sum_{j \in U^c \setminus \{k\}} \delta_{ij}(y_1(j) - y_2(j)) = 0,
\end{aligned}$$

since $U^c \setminus \{k\} \cap \{i\} = \emptyset$. ⊠

2.5.2. Angles in a Simplex

There are several angles worth discussing in a simplex. For a simplex $\mathcal{T}$, let $\phi_{ij}(\mathcal{T})$ be the angle between the outer normals to $\mathcal{S}_{\{i\}^c}$ and $\mathcal{S}_{\{j\}^c}$. As usual, the paranthetical $(\mathcal{T})$ will typically be dropped when the simplex is understood from context. Using the notion of the dual simplex introduced in the previous section, we can write

$$\cos \phi_{ij}(\mathcal{T}) = \frac{\langle \gamma_i, \gamma_j \rangle}{\|\gamma_i\|_2 \cdot \|\gamma_j\|_2},$$

where $\{\gamma_i\}$ are the vertices of $\mathcal{T}^*$. Now, define $\theta_{ij}(\mathcal{T})$ to be the angle between $\mathcal{T}_{\{i\}^c}$ and $\mathcal{T}_{\{j\}^c}$. Appealing to elementary geometry, we see that the angles ϕ_{ij} and θ_{ij} are *supplementary*, i.e., their sum is π. Hence,

$$\cos \theta_{ij}(\mathcal{T}) = -\frac{\langle \gamma_i, \gamma_j \rangle}{\|\gamma_i\|_2 \cdot \|\gamma_j\|_2}, \tag{2.26}$$

where we've used that $\cos(\phi_{ij}) = \cos(\pi - \theta_{ij}) = -\cos(\theta_{ij})$.

Definition 2.7. We call the simplex $\mathcal{T} \subseteq \mathbb{R}^{n-1}$ *hyperacute* if $\theta_{ij}(\mathcal{T}) \leq \pi/2$ for all $i, j \in [n]$. If $\mathcal{T}$ is not hyperacute, it is called *obtuse*.

Chapter 3

The Graph-Simplex Correspondence

In this chapter we introduce the graph simplex correspondence and explore its mathematical foundations and properties. While the focus of this dissertation is the bijective relationship between graphs and simplices, we begin by introducing the more general relationship between matrices and convex polytopes. The correspondence between graphs and simplices will then follow as a consequence.

§3.1. Convex Polyhedra of Matrices

Here we introduce the (perhaps complex) convex polytope associated with a given matrix. Let $\boldsymbol{M} \in \mathbb{R}^{n\times n}$ be symmetric and admitting of the eigendecomposition $\boldsymbol{M} = \sum_{i=1}^{d} \lambda_i \boldsymbol{\varphi}_i \boldsymbol{\varphi}_i^t$ for some $d \leq n$ (i.e., $\boldsymbol{M}$ has eigenvalue zero with multiplicity $n-d$) where the eigenvectors $\{\boldsymbol{\varphi}_i\}_{i=1}^d$ are orthonormal. Writing out the eigendecomposition as

$$\boldsymbol{M} = \boldsymbol{\Phi}_M \boldsymbol{\Lambda}_M \boldsymbol{\Phi}_M^t = (\boldsymbol{\Phi}_M \boldsymbol{\Lambda}_M^{1/2})(\boldsymbol{\Phi}_M \boldsymbol{\Lambda}_M^{1/2})^t,$$

with $\boldsymbol{\Phi}_M = (\boldsymbol{\varphi}_1, \dots, \boldsymbol{\varphi}_d)$, $\boldsymbol{\Lambda}_M = \operatorname{diag}(\lambda_1, \dots, \lambda_d)$ (note the respective absences of $\boldsymbol{\varphi}_{d+1}, \dots, \boldsymbol{\varphi}_n$ and $\lambda_{d+1}, \dots, \lambda_n$), suggests that we might consider $\boldsymbol{\Lambda}_M^{1/2}\boldsymbol{\Phi}_M$ as a vertex matrix, thus $\boldsymbol{M}$ as a gram matrix. Inorexably compelled by this intuition, define the vertices $\boldsymbol{\sigma}_1, \dots, \boldsymbol{\sigma}_n$ given by the columns of $\boldsymbol{\Lambda}_M^{1/2}\boldsymbol{\Phi}_M^t$, i.e.,

$$\boldsymbol{\sigma}_i = (\boldsymbol{\Lambda}_M^{1/2}\boldsymbol{\Phi}_M^t)(\cdot, i) = (\boldsymbol{\varphi}_1(i)\lambda_1^{1/2}, \boldsymbol{\varphi}_2(i)\lambda_2^{1/2}, \dots, \boldsymbol{\varphi}_d(i)\lambda_d^{1/2})^t \in \mathbb{C}^d,$$

where we emphasize that the vertex vector will have complex entries if $\lambda_j < 0$ for any $j \in [d]$. We may now define the *polytope of the matrix* $\boldsymbol{M}$ as the polytope given by their convex hull:

$$\mathcal{P}_{\boldsymbol{M}} \stackrel{\text{def}}{=} \operatorname{conv}(\boldsymbol{\sigma}_1, \dots, \boldsymbol{\sigma}_n).$$

Letting $\boldsymbol{\Sigma} = \boldsymbol{\Sigma}(\mathcal{P}_{\boldsymbol{M}}) = (\boldsymbol{\sigma}_1, \dots, \boldsymbol{\sigma}_n) \in \mathbb{R}^{d\times n}$ be the matrix whose i-th column is the i-th vertex $\boldsymbol{\sigma}_i$—henceforth called the *vertex matrix of* $\mathcal{P}_M$—we see that $\boldsymbol{\Sigma} = \boldsymbol{\Lambda}_M^{1/2}\boldsymbol{\Phi}_M^t = (\boldsymbol{\Phi}_M\boldsymbol{\Lambda}^{1/2})^t$, and

$$\boldsymbol{\Sigma}^t\boldsymbol{\Sigma} = (\boldsymbol{\Phi}\boldsymbol{\Lambda}^{1/2})(\boldsymbol{\Phi}\boldsymbol{\Lambda}^{1/2})^t = \boldsymbol{\Phi}\boldsymbol{\Lambda}\boldsymbol{\Phi}^t = \boldsymbol{M}.$$

Observe that the polytope $\mathcal{S}(\boldsymbol{M})$ is d-dimensional, i.e., its vertices span a d-dimensional subspace,

$$\text{rank}(\boldsymbol{\Sigma}) = \text{rank}(\boldsymbol{\Sigma}^t\boldsymbol{\Sigma}) = \text{rank}(\boldsymbol{M}) = d,$$

where we've employed Lemma 2.2 and the fact that $\boldsymbol{M}$ has rank d due to its eigendecomposition. We thus conceptualize of $\mathcal{P}_M$ as a polytope in $\mathbb{R}^d$.

Remark 3.1. The ordering of the non-zero eigenvalues did not enter our considerations when defining $\mathcal{P}_M$. Let us consider re-ordering the indices; take $\tau : [d] \to [d]$ to be any permutation and $\{\boldsymbol{\sigma}_i^\tau\}$ be the vertices as they would be defined under the ordering given by τ. Hence $\boldsymbol{\sigma}_i^\tau(j) = \boldsymbol{\varphi}_{\tau^{-1}(j)}(i)\lambda_{\tau^{-1}(j)}^{1/2}$. The pairwise distances between these vertices then obey

$$\|\boldsymbol{\sigma}_i^\tau - \boldsymbol{\sigma}_k^\tau\|_2^2 = \sum_{j=1}^d \lambda_{\tau^{-1}(j)}(\boldsymbol{\varphi}_{\tau^{-1}(j)}(i) - \boldsymbol{\varphi}_{\tau^{-1}(j)}(k))^2 = \sum_{j=1}^d \lambda_j(\boldsymbol{\varphi}_j(i) - \boldsymbol{\varphi}_j(k))^2 = \|\boldsymbol{\sigma}_i - \boldsymbol{\sigma}_j\|_2^2,$$

since τ is a bijection, hence summing over $\tau^{-1}(j)$ yields the same result as summing from 1 to d. Therefore, we see that the polytopes $\text{conv}(\boldsymbol{\sigma}_1^\tau, \ldots, \boldsymbol{\sigma}_n^\tau)$ and $\text{conv}(\boldsymbol{\sigma}_1, \ldots, \boldsymbol{\sigma}_n)$ are congruent. In fact, since they share the same centroid they are simply rotations of one another.

3.1.1. The Inverse Polytope

Given that we can associate a polytope with the matrix $\boldsymbol{M}$, it is natural to wonder about the relationship between this polytope and that associated to M^{-1} if $\boldsymbol{M}$ if invertible, or with its pseudoinverse $\boldsymbol{M}^+$ more generally. As illustrated in Section 2.2.1, with the eigendecompition of $\boldsymbol{M}$ as above, we can write the pseudoinverse as

$$\boldsymbol{M}^+ = \sum_{i=1}^d \lambda_i^{-1}\boldsymbol{\varphi}_i\boldsymbol{\varphi}_i^t = \boldsymbol{\Phi}_M\boldsymbol{\Lambda}_M^{-1/2}\boldsymbol{\Phi}_M.$$

We can thus associated with $\boldsymbol{M}^+$ a polytope $\mathcal{P}_{\boldsymbol{M}^+}$, which has as its vertex matrix $\boldsymbol{\Sigma}(\mathcal{P}_{\boldsymbol{M}^+}) = (\boldsymbol{\Phi}\boldsymbol{\Lambda}^{-1/2})^t$; that is, the vertices $\{\boldsymbol{\sigma}_i^+\}$ of $\mathcal{P}_{\boldsymbol{M}^+}$ are defined by $\boldsymbol{\sigma}_i^+(j) = \boldsymbol{\varphi}_j(i)/\lambda_j^{1/2}$. We call $\mathcal{P}_{\boldsymbol{M}^+}$ the *inverse polytope of* $\boldsymbol{M}$.

Let us observe several properties of the relationship between $\mathcal{P}_M$ and $\mathcal{P}_{M^+}$. In what follows we drop the subscript M from the eigenvalue and eigenvector matrix. Note that because of the orthogonality relationships among eigenvectors of $\boldsymbol{M}$,

$$\boldsymbol{\Phi}^t\boldsymbol{\Phi} = \begin{pmatrix} \langle\boldsymbol{\varphi}_1, \boldsymbol{\varphi}_1\rangle & \ldots & \langle\boldsymbol{\varphi}_1, \boldsymbol{\varphi}_d\rangle \\ \vdots & \ddots & \vdots \\ \langle\boldsymbol{\varphi}_d, \boldsymbol{\varphi}_1\rangle & \ldots & \langle\boldsymbol{\varphi}_d, \boldsymbol{\varphi}_d\rangle \end{pmatrix} = \mathbf{I}_d.$$

Consequently,

$$\boldsymbol{M}^+\boldsymbol{M} = \boldsymbol{\Phi}\boldsymbol{\Lambda}\boldsymbol{\Phi}^t\boldsymbol{\Phi}\boldsymbol{\Lambda}^{-1}\boldsymbol{\Phi}^t = \boldsymbol{\Phi}\boldsymbol{\Lambda}\boldsymbol{\Lambda}^{-1}\boldsymbol{\Phi}^t = \boldsymbol{\Phi}\boldsymbol{\Phi}^t,$$

and similarly $\boldsymbol{M}\boldsymbol{M}^+ = \boldsymbol{\Phi}\boldsymbol{\Phi}^t$. As it happens, the vertex matrices of $\mathcal{P}_M$ and $\mathcal{P}_M^+$ satisfy the same pseudoinverse relation:

$$\mathbf{\Sigma}^t\mathbf{\Sigma}^+ = \mathbf{\Phi}\mathbf{\Lambda}^{1/2}\mathbf{\Lambda}^{-1/2}\mathbf{\Phi}^t = \mathbf{\Phi}\mathbf{\Phi}^t,$$

and $(\mathbf{\Sigma}^+)^t\mathbf{\Sigma} = \mathbf{\Phi}\mathbf{\Phi}^t$. Using the properties of the relationship between a matrix and its pseudoinverse immediately yields the following result.

LEMMA 3.1. *Let $\mathbf{\Sigma} = \mathbf{\Sigma}(\boldsymbol{M})$ and $\mathbf{\Sigma}^+ = \mathbf{\Sigma}(\boldsymbol{M}^+)$ by the vertex matrices of $\mathcal{P}_M$ and $\mathcal{P}_{M^+}$ where $\boldsymbol{M}$ is a real and symmetric matrix. The matrices $\mathbf{\Sigma}^t\mathbf{\Sigma}^+$ and $(\mathbf{\Sigma}^+)^t\mathbf{\Sigma}$ are equal and moreover*

(i). act as the orthogonal projection onto $\mathrm{range}(\boldsymbol{M})$*;*

(ii). $(\mathbf{I} - \mathbf{\Sigma}^t\mathbf{\Sigma}^+)$ *acts as the orthogonal projection onto* $\ker(\boldsymbol{M})$.

Proof. Apply Lemma 2.3. ⊠

Further exploring the relationships between the vertex matrices and themselves, we find that

$$\mathbf{\Sigma}\mathbf{\Sigma}^t = \begin{pmatrix} \sum_i \boldsymbol{\sigma}_i(1)\boldsymbol{\sigma}_i(1) & \dots & \sum_i \boldsymbol{\sigma}_i(1)\boldsymbol{\sigma}_i(n) \\ \vdots & \ddots & \vdots \\ \sum_i \boldsymbol{\sigma}_i(n)\boldsymbol{\sigma}_i(1) & \dots & \sum_i \boldsymbol{\sigma}_i(n)\boldsymbol{\sigma}_i(n) \end{pmatrix}$$

$$= \begin{pmatrix} \lambda_1\langle\boldsymbol{\varphi}_1, \boldsymbol{\varphi}_1\rangle & \dots & \lambda_1^{1/2}\lambda_n^{1/2}\langle\boldsymbol{\varphi}_1, \boldsymbol{\varphi}_n\rangle \\ \vdots & \ddots & \dots \\ \lambda_1^{1/2}\lambda_n^{1/2}\langle\boldsymbol{\varphi}_n, \boldsymbol{\varphi}_1\rangle & \dots & \lambda_n\langle\boldsymbol{\varphi}_n, \boldsymbol{\varphi}_n\rangle \end{pmatrix} = \mathbf{\Lambda}, \tag{3.1}$$

and likewise,

$$\widehat{\mathbf{\Sigma}}^+(\widehat{\mathbf{\Sigma}}^+)^t = \mathbf{\Lambda}^{-1}. \tag{3.2}$$

In summary, any real symmetric $n \times n$ matrix of rank d yields a d-dimensional convex polytope $\mathcal{P}_M$ in $\mathbb{C}^{d\times d}$. If all eigenvalues are positive then the polytope sits in $\mathbb{R}^{d\times d}$. The vertex matrices of $\mathcal{P}_M$ and $\mathcal{P}_{M^+}$—the polytope of the pseudoinverse of M—when multiplied together are equal to and hence satisfy the projection properties of $\boldsymbol{M}^+\boldsymbol{M}$. In the next section we will explore how to apply this result to graphs.

§3.2. A Bijection Between Graphs and Simplices

This section introduces the graph-simplex correspondence—the core of which is a bijective mapping between the set of all (finite) connected, weighted, and undirected graphs and hyperacute simplices. We begin by exploring the polytopes—and in particular the simplices—associated with a given graph. The subsequent section will then demonstrate how to extract a graph from an arbitrary hyperacute simplex.

3.2.1. The Simplices of a Graph

Fix an undirected, connected and weighted graph $G = (V, E, w)$. By means of the graph's adjacency and Laplacian matrices, the previous section yields several polytopes corresponding to G. The adjacency matrix $\boldsymbol{A}_G$, for instance, yields a complex polytope of dimension $\operatorname{rank}(\boldsymbol{A}_G)$. However, while Theorem 2.1 dictates that $\boldsymbol{A}_G$ has real eigenvalues and a set of orthogonal eigenvectors, we do not in general know the rank of $\boldsymbol{A}_G$, nor much of the magnitudes of its eigenvalues. This makes it difficult to explore the structure of $\mathcal{P}_{\boldsymbol{A}_G}$.

We will instead focus on the polytopes generated by G's Laplacian matrices; $\mathcal{S}_G \overset{\text{def}}{=} \mathcal{P}_{\boldsymbol{L}_G}$ and $\widehat{\mathcal{S}}_G \overset{\text{def}}{=} \mathcal{P}_{\widehat{\boldsymbol{L}}_G}$ corresponding to the combinatorial and normalized Laplacians, respectively. (The reasoning behind the nomenclature will quickly become apparent.) We let $\boldsymbol{\Sigma}_G = \boldsymbol{\Sigma}(\mathcal{P}_{\boldsymbol{L}_G}) = (\boldsymbol{\sigma}_1, \ldots, \boldsymbol{\sigma}_n)$ and $\widehat{\boldsymbol{\Sigma}}_G = \boldsymbol{\Sigma}(\mathcal{P}_{\widehat{\boldsymbol{L}}_G}) = (\widehat{\boldsymbol{\sigma}}_1, \ldots, \widehat{\boldsymbol{\sigma}}_n)$ denote the vertices of $\mathcal{S}_G$ and $\widehat{\mathcal{S}}_G$, respectively. We recall that $\boldsymbol{\Sigma} = \boldsymbol{\Lambda}^{1/2}\boldsymbol{\Phi}^t$ (resp., $\widehat{\boldsymbol{\Sigma}} = \widehat{\boldsymbol{\Lambda}}^{1/2}\widehat{\boldsymbol{\Phi}}^t$)) where $\boldsymbol{\Lambda}$ (resp., $\widehat{\boldsymbol{\Lambda}}$) is the diagonal matrix containing the non-zero eigenvalues of $\boldsymbol{L}_G$ (resp., $\widehat{\boldsymbol{L}}_G$) and $\boldsymbol{\Phi}$ (resp., $\widehat{\boldsymbol{\Phi}}$) is the matrix of the corresponding (normalized) eigenvectors. Since $\operatorname{rank}(\boldsymbol{L}_G) = \operatorname{rank}(\widehat{\boldsymbol{L}}_G) = n-1$, the polytopes $\mathcal{S}_G$ and $\widehat{\mathcal{S}}_G$ are simplices—a fact which is demonstrated more directly by the following Lemma.

LEMMA 3.2. *The vertices $\{\boldsymbol{\sigma}_i\}$ and $\{\widehat{\boldsymbol{\sigma}}_i\}$ are affinely independent.*

Proof. We provide the proof in the case of $\{\boldsymbol{\sigma}_i\}$ only. Suppose $\boldsymbol{\alpha} = (\alpha_1, \ldots, \alpha_n)$ is such that $\sum_{i=1}^n \alpha_i \boldsymbol{\sigma}_i = \boldsymbol{0}$, i.e., $\boldsymbol{\alpha} \in \ker(\boldsymbol{\Sigma})$. Since $\ker(\boldsymbol{\Sigma}) = \ker(\boldsymbol{\Sigma}^t\boldsymbol{\Sigma}) = \ker(\boldsymbol{L}) = \operatorname{span}(\{\boldsymbol{1}\})$, there exists some $k \in \mathbb{R}$ such that $\boldsymbol{\alpha} = k\boldsymbol{1}$. If $\langle \boldsymbol{\alpha}, \boldsymbol{1}\rangle = \langle k\boldsymbol{1}, \boldsymbol{1}\rangle = kn = 0$ however, then we must have $k = 0$, demonstrating that $\alpha_i = 0$ for all i. Hence the vectors $\{\boldsymbol{\sigma}_i\}$ are affinely independent. Likewise, if $\boldsymbol{\alpha} \in \ker(\widehat{\boldsymbol{\Sigma}}) = \ker(\widehat{\boldsymbol{L}}) = \operatorname{span}(\{\sqrt{\boldsymbol{w}}\})$, then $\boldsymbol{\alpha} = k\sqrt{\boldsymbol{w}}$. But $\langle k\sqrt{\boldsymbol{w}}, \boldsymbol{1}\rangle = k\sum_i w(i) = 0$, so $\boldsymbol{\alpha} = \boldsymbol{0}$. ⊠

Consequently, we will often refer to $\mathcal{S}_G$ as the *combinatorial simplex of* G or simply the *simplex of* G, and to $\widehat{\mathcal{S}}_G$ as the *normalized simplex of* G. If G is clear from context we will often drop it from the subscript. As per Section 3.1.1, we also introduce the *inverse simplex* and *inverse normalized simplex of* G, which have respective vertex matrices

$$\boldsymbol{\Sigma}^+ = \boldsymbol{\Lambda}^{-1/2}\boldsymbol{\Phi}^t, \qquad \text{and} \qquad \widehat{\boldsymbol{\Sigma}}^+ = \widehat{\boldsymbol{\Lambda}}^{-1/2}\widehat{\boldsymbol{\Phi}}^t.$$

We will often refer to the pair $\mathcal{S}_G$ and $\mathcal{S}_G^+$ as the *combinatorial simplices of* G, and the pair $\widehat{\mathcal{S}}_G$ and $\widehat{\mathcal{S}}_G^+$ as the *normalized simplices of* G, to avoid the tedious task of constantly referring to, say, the combinatorial simplex and its inverse.

As illustrated by the discussion at the end of Section 3.1.1, the vertex matrices of the polytope of a matrix and its inverse share the same relationship as the matrix and its pseudoinverse (Lemma 3.1). Since this relationship is well understood for the Laplacian and its pseudoinverse, we may explicit compute the relationships between $\boldsymbol{\Sigma}, \boldsymbol{\Sigma}^+$ and $\widehat{\boldsymbol{\Sigma}}, \widehat{\boldsymbol{\Sigma}}^+$.

Let $\widetilde{\boldsymbol{\Phi}}$ be the matrix containing all eigenvectors of $\boldsymbol{L}_G$ (i.e., also containing $\boldsymbol{1}/\sqrt{n}$). It is well known that $\widetilde{\boldsymbol{\Phi}}$ is an orthogonal matrix (see e.g., [VM13]), i.e., $\widetilde{\boldsymbol{\Phi}}^t\widetilde{\boldsymbol{\Phi}} = \widetilde{\boldsymbol{\Phi}}\widetilde{\boldsymbol{\Phi}}^t = \mathbf{I}$, a property which is also called *double orthogonality*. When expanded, this second equality implies that

$$\delta_{i,j} = \sum_{k=1}^{n} \boldsymbol{\varphi}_k(i)\boldsymbol{\varphi}_k(j) = \sum_{k=1}^{n-1} \boldsymbol{\varphi}_k(i)\boldsymbol{\varphi}_k(j) + 1/n. \tag{3.3}$$

From this, it follows that

$$\langle \sigma_i^+, \sigma_j \rangle = \delta_{i,j} - \frac{1}{n},$$

hence,

$$\boldsymbol{\Sigma}^t\boldsymbol{\Sigma}^+ = (\boldsymbol{\Sigma}^+)^t\boldsymbol{\Sigma} = \mathbf{I} - \frac{\mathbf{J}}{n}. \tag{3.4}$$

Beyond simply exemplifying an elegant relationship between $\boldsymbol{\Sigma}$ and $\boldsymbol{\Sigma}^+$, this also demonstrates the following important result.

Observation 3.1. *The dual simplex of $\mathcal{S}_G$ is equal to the inverse simplex $\mathcal{S}_G^+$.*

Proof. Recall that the dual simplex is the unique simplex with vertices $\boldsymbol{\sigma}_i^*$ obeying $\langle \boldsymbol{\sigma}_i^*, \boldsymbol{\sigma}_j - \boldsymbol{\sigma}_k \rangle = \delta ij$ for $i, j \neq k$. The vertices $\boldsymbol{\sigma}_i^+$ satisfy this property: $\langle \boldsymbol{\sigma}_i^+, \boldsymbol{\sigma}_j - \boldsymbol{\sigma}_k \rangle = (\delta_{ij} - 1/n) - (\delta_{ik} - 1/n) = \delta_{ij}$ since $i \neq k$. ⊠

Let θ_{ij}^+ be the interior angle between $\mathcal{S}^+_{\{i\}^c}$ and $\mathcal{S}^+_{\{j\}^c}$. Since $\mathcal{S}^+$ is dual to $\mathcal{S}$, Equation 2.26 gives

$$\cos\theta_{ij}^+ = -\frac{\langle \boldsymbol{\sigma}_i, \boldsymbol{\sigma}_j \rangle}{\|\boldsymbol{\sigma}_i\|_2\|\boldsymbol{\sigma}_j\|_2} = \frac{w(i,j)}{\sqrt{w(i)w(j)}} \in [0,1],$$

hence $\theta_{ij}^+ \in [0, \pi/2]$, which proves the following observation.

Observation 3.2. *The inverse combinatorial simplex of a graph is hyperacute.*

We turn out attention now to the normalized simplex. Double orthogonality also holds for the eigenvectors of the normalized Laplacian and so, recalling that $\boldsymbol{\varphi}_n \in \operatorname{span}(\boldsymbol{W}_G^{1/2}\mathbf{1})$, (Section 2.3.2) we can write

$$\boldsymbol{\varphi}_n = \frac{\sqrt{\boldsymbol{w}}}{(\operatorname{vol}(G))^{1/2}},$$

where we recall that $\operatorname{vol}(G) = \sum_{i\in[n]} w(i)$. Therefore, $\widehat{\boldsymbol{\varphi}}_n(i)\widehat{\boldsymbol{\varphi}}_n(j) = \sqrt{w(i)w(j)}/\operatorname{vol}(G)$, implying that

$$\delta_{i,j} = \sum_{k=1}^{n} \widehat{\boldsymbol{\varphi}}_k(i)\widehat{\boldsymbol{\varphi}}_k(j) = \sum_{k=1}^{n-1} \widehat{\boldsymbol{\varphi}}_k(i)\widehat{\boldsymbol{\varphi}}_k(j) + \frac{\sqrt{w(i)w(j)}}{\operatorname{vol}(G)},$$

and so

$$\widehat{\boldsymbol{\Sigma}}^t\widehat{\boldsymbol{\Sigma}}^+ = (\widehat{\boldsymbol{\Sigma}}^+)^t\widehat{\boldsymbol{\Sigma}} = \mathbf{I} - \frac{\sqrt{\boldsymbol{w}}\sqrt{\boldsymbol{w}}^t}{\operatorname{vol}(G)}. \tag{3.5}$$

It is worth emphasizing the fact that this inverse relationship is a function of the weights of the graph for the normalized simplex, while it is constant for the combinatorial simplex. As we will see, this dependency on $\boldsymbol{w}$ will severely complicate the relationship between $\widehat{\mathcal{S}}_G$ and $\widehat{\mathcal{S}}_G^+$, making their study more complicated than that of $\mathcal{S}_G$ and $\mathcal{S}_G^+$.

3.2.2. The Graph of a Simplex

We now proceed to demonstrating that each hyperacute simplex is the inverse simplex of a graph G. This will constitute the second half of the bijective relationship between graphs and simplices.

LEMMA 3.3. *Given a simplex $\mathcal{T} \subseteq \mathbb{R}^{n-1}$ centered at the origin, let $\{\mathbf{u}_i\}$ be vectors describing its outer normal directions, though with no particular length. Let $\boldsymbol{Q}$ be their Gram matrix; i.e., $\boldsymbol{Q}(i,j) = \langle \mathbf{u}_i, \mathbf{u}_j \rangle$. If $\boldsymbol{Q}_1 \in \mathbb{R}^{n\times n}$ is the diagonal matrix containing the norms of the outer normals,*

$$\boldsymbol{Q}_1 = diag\Big(\|\mathbf{u}_1\|_2, \dots, \|\mathbf{u}_n\|_2 \Big),$$

and $\boldsymbol{Q}_2 \in \mathbb{R}^{n\times n}$ describes the angles in the simplex,

$$\boldsymbol{Q}_2(i,j) = \begin{cases} 1, & \text{if } i = j, \\ -\cos\theta_{i,j}, & \text{otherwise,} \end{cases}$$

where $\theta_{i,j}$ is the (interior) angle between $\mathcal{T}_{\{i\}^c}$ and $\mathcal{T}_{\{j\}^c}$, then

$$\boldsymbol{Q} = \boldsymbol{Q}_1 \boldsymbol{Q}_2 \boldsymbol{Q}_1.$$

Proof. Using Equation 2.26 from the discussion in Section 2.5.2, we can write the entries of $\boldsymbol{Q}_2$ as

$$\frac{\langle \boldsymbol{\gamma}_i, \boldsymbol{\gamma}_j \rangle}{\|\boldsymbol{\gamma}_i\|_2 \|\boldsymbol{\gamma}_j\|_2},$$

where $\{\boldsymbol{\gamma}_i\}$ are the vertices of $\mathcal{T}^*$ (note that this holds for $i = j$ as well). Lemma 2.9 implies that these vertices are parallel to the outer normals of $\mathcal{T}$, hence $\boldsymbol{\gamma}_i = \kappa_i \mathbf{u}_i$ where $\kappa_i \in \mathbb{R}_{>0}$. Therefore,

$$(\boldsymbol{Q}_1\boldsymbol{Q}_2\boldsymbol{Q}_1)(i,j) = \|\mathbf{u}_i\|_2 \frac{\langle \kappa_i \mathbf{u}_i, \kappa_j \mathbf{u}_j \rangle}{\|\kappa_i \mathbf{u}_i\|_2 \|\kappa_j \mathbf{u}_j\|_2} \|\mathbf{u}_j\|_2 = \frac{\kappa_i \kappa_j}{|\kappa_i||\kappa_j|} \langle \mathbf{u}_i, \mathbf{u}_j \rangle = \langle \mathbf{u}_i, \mathbf{u}_j \rangle = \boldsymbol{Q}(i,j). \quad \boxtimes$$

Let $\mathcal{T}$ be a hyperacute simplex, and $\mathcal{T}^*$ its dual. The vertex matrix $\boldsymbol{\Sigma}^*$ of $\mathcal{T}^*$ contains the outer normals of $\mathcal{T}$ (see discussion on dual simplex in Section 2.5.1). Hence, taking $\boldsymbol{Q} = (\boldsymbol{\Sigma}^*)^t \boldsymbol{\Sigma}^*$ in the above Lemma applied to the simplex $\mathcal{T}$, we obtain explicit entries for this Gram matrix:

$$((\boldsymbol{\Sigma}^*)^t \boldsymbol{\Sigma}^*)(i,j) = \begin{cases} \|\boldsymbol{\sigma}_i^*\|_2^2, & \text{if } i = j, \\ -\cos\theta_{i,j} \|\boldsymbol{\sigma}_i^*\|_2 \cdot \left\|\boldsymbol{\sigma}_j^*\right\|_2, & \text{if } i \neq j. \end{cases}$$

We claim that $\boldsymbol{Q}$ is the Laplacian matrix of some graph G. First, the matrix is symmetric. Second, for each i, $\boldsymbol{Q}(i,i) = \|\boldsymbol{\sigma}_i^*\|_2^2 > 0$, and for $i \neq j$, $\boldsymbol{Q}(i,j) \le 0$ since $\theta_{i,j} \le \pi/2$ by assumption (note therefore the importance that $\mathcal{T}$ is hyperacute). Finally, denote $\boldsymbol{\Sigma}^* = (\boldsymbol{\sigma}_1^*, \dots, \boldsymbol{\sigma}_n^*)$, and recall from the construction of the dual simplex in Section 2.5.1 that

$\boldsymbol{\sigma}_n^* = -\sum_{i<n} \boldsymbol{\sigma}_i^*$. Therefore, for $i \neq n$,

$$\sum_{j=1}^{n} \boldsymbol{Q}(i,j) = \sum_{j=1}^{n-1} \langle \boldsymbol{\sigma}_i^*, \boldsymbol{\sigma}_j^* \rangle + \langle \boldsymbol{\sigma}_i^*, -\sum_{j<n} \boldsymbol{\sigma}_j^* \rangle = \sum_{j<n} \langle \boldsymbol{\sigma}_i^*, \boldsymbol{\sigma}_j^* \rangle - \sum_{j<n} \langle \boldsymbol{\sigma}_i^*, \boldsymbol{\sigma}_j^* \rangle = 0,$$

hence $\boldsymbol{Q}\mathbf{1} = \mathbf{0}$, meaning that

$$\boldsymbol{Q}(i,i) = -\sum_{j \neq i} \boldsymbol{Q}(i,j).$$

If we construct a weighted graph $G = (V, E, \boldsymbol{w})$ on n vertices with edge weights $\boldsymbol{w}(i,j) = -\boldsymbol{Q}(i,j)$, it then follows that $\boldsymbol{Q} = (\boldsymbol{\Sigma}^*)^t \boldsymbol{\Sigma}^* = \boldsymbol{L}_G$. Thus, the simplex $\mathcal{T}^*$ is congruent to the combinatorial simplex of G (by virtue of the fact that $\langle \boldsymbol{\sigma}_i^*, \boldsymbol{\sigma}_j^* \rangle = \boldsymbol{L}_G(i,j)$), and $\mathcal{T}$ is (congruent to) the dual of the combinatorial simplex of G.

Remark 3.2. All the faffing[1] about with congruence is, unfortunately, necessary. If G is the graph constructed from the simplex $\mathcal{T}$ as above, there is no reason that its inverse combinatorial simplex $\mathcal{S}_G^+$ as constructed in Section 3.2.1 will be precisely $\mathcal{T}$. In fact, this is highly unlikely. The construction of G from $\mathcal{T}$ and its dual $\mathcal{T}^*$ used only the magnitudes of the vectors of $\{\boldsymbol{\sigma}_i^*\}$ and not their absolute position. Thus, any rotation of $\mathcal{T}$ would produce the same graph. It is for this reason that the relationship between graphs and simplices must deal with congruence relationships.

We summarize the material in Sections 3.2.1 and 3.2.2 with the following theorem.

Theorem 3.1. *There exists a bijection between (the congruence classes of) hyperacute simplices in $\mathbb{R}^{n-1}$ and connected, weighted graphs on n vertices.*

Several observations are in order. First, the astute reader may wonder why it was necessary in this section to explore the relation between a given hyperacute simplex $\mathcal{T}$ and its corresponding graph by means of the dual simplex $\mathcal{T}^*$. A second, *more* astute reader will then question the sanity of the first, and point out that in order to demonstrate that $\mathcal{T}$ is congruent to the inverse simplex of G, one would have to have a firm grasp of the structure of $\boldsymbol{L}_G^+$, which is much more poorly understood in general than $\boldsymbol{L}_G$. For instance, would one have to argue that there exists a graph G such that $\boldsymbol{\Sigma}(\mathcal{T})^t \boldsymbol{\Sigma}(\mathcal{T}) = \boldsymbol{L}_G^+$. This seems difficult to do in general since, for example, even the sign of the entries of $\boldsymbol{L}_G^+$ aren't known.

Second, considering that Theorem 3.1 was proved using combinatorial simplices, one might wonder whether a similar relationship holds between "normalized" simplices and graphs. That is, given $\mathcal{T}$, when is $\mathcal{T}^*$ the normalized simplex of a graph? Since the vertices of the normalized simplex lie on the unit sphere, we would require that $\|\boldsymbol{\sigma}_i^*\|_2 = 1$, which is clearly only holds for a very restricted class of simplex. Assume this holds. We would then need to cosntruct a graph with weights obeying

$$\cos\theta_{ij} = \frac{1}{\sqrt{w(i)w(j)}},$$

[1] U.K. slang has obviously had its effect on me.

hence
$$\frac{1}{\sqrt{w(i)}} = \sum_{j\neq i} \cos\theta_{ij}\sqrt{w(j)}.$$
Think more about whether this system of equations has a solution.

§3.3. Examples & Simplices of Special Graphs

In this section we provide several of examples of simplices of graphs in order to give the reader a more intuitive feeling of the correspondence. Fix a connected and undirected graph $G=(V,E,w)$. We begin by considering the simplices generated by three special graphs relating to G—the complement graph G^c, an arbitrary subgraph of G, and the case in which G is a product graph. We then proceed to analyzing several concrete examples.

Simplex of complement graph, G^c. Suppose that G is unweighted; so $w(i,j)\in\{0,1\}$ for all i,j. The *complement graph of* G, denoted G^c, is the graph $G^c=(V,E^c)$ where $E^c=\{(i,j):(i,j)\notin E\}$. That is, it has edges where G has none and vice versa. Therefore, it has the adjacency matrix $\boldsymbol{A}^c \overset{\text{def}}{=} \boldsymbol{A}_{G^c} = \mathbf{1}\mathbf{1}^t - \mathbf{I} - \boldsymbol{A}_G$ and degree matrix $\boldsymbol{D}^c \overset{\text{def}}{=} \boldsymbol{D}_{G^c} = (n-1)\mathbf{I} - \boldsymbol{D}_G$ since $\deg(i)_{G^c} = n-1-\deg(i)_G$. The Laplacian of G^c thus reads as
$$\boldsymbol{L}^c = \boldsymbol{D}^c - \boldsymbol{A}^c = n\mathbf{I} - \boldsymbol{D}_G - \mathbf{1}\mathbf{1}^t + \boldsymbol{A}_G = n\mathbf{I} - \mathbf{1}\mathbf{1}^t - \boldsymbol{L}_G.$$
Of course, $\mathbf{1}$ is still an eigenfunction of $\boldsymbol{L}^c$ (G^c is, after all, a graph). For $\boldsymbol{\varphi}\perp\mathbf{1}$, we have
$$\boldsymbol{L}^c\boldsymbol{\varphi} = n\boldsymbol{\varphi} - \mathbf{1}\langle\mathbf{1},\boldsymbol{\varphi}\rangle - \boldsymbol{L}\boldsymbol{\varphi} = (n-\lambda)\boldsymbol{\varphi},$$
from which it follows that $\boldsymbol{L}^c$ shares the same eigenfunctions as $\boldsymbol{L}$, with corresponding eigenvalues $\{n-\lambda_i\}$. Consequently, the simplex corresponding to G^c, $\mathcal{S}^c$ has vertices given by
$$\sigma_i(j) = \boldsymbol{\varphi}_j(i)\sqrt{n-\lambda_j},$$
and the inverse simplex has vertices
$$\sigma_i^+(j) = \frac{\boldsymbol{\varphi}_j(i)}{\sqrt{n-\lambda_j}}.$$

Subgraphs. Let $H\subseteq G$, in the sense that $w_H(i,j)\leq w_G(i,j)$ for all $i,j\in[n]$ (we allow for G to be weighted once again). Then, for any $\boldsymbol{f}:V\to\mathbb{R}$ we see that
$$\mathcal{L}_G(\boldsymbol{f}) = \sum_{i\sim j} w_G(i,j)(\boldsymbol{f}(i)-\boldsymbol{f}(j))^2 \geq \sum_{i\sim j} w_H(i,j)(\boldsymbol{f}(i)-\boldsymbol{f}(j))^2 = \mathcal{L}_H(\boldsymbol{f}).$$
Therefore,
$$\|\boldsymbol{\Sigma}_H\boldsymbol{f}\|_2^2 \leq \|\boldsymbol{\Sigma}_G\boldsymbol{f}\|_2^2.$$

In particular, taking $\boldsymbol{f} = \boldsymbol{\chi}_i$ for any i, this yields $\|\boldsymbol{\sigma}_i(G)\|_2^2 \geq \|\boldsymbol{\sigma}_i(H)\|_2^2$, where $\{\boldsymbol{\sigma}_i(G)\}$ are the vertices of $\mathcal{S}_G$, and $\{\boldsymbol{\sigma}_i(H)\}$ those of $\mathcal{S}_H$. That is, the length of the vertex vectors of G is greater than those of H.

If G is a multiple of H such that $w_G(i,j) = c \cdot w_H(i,j)$ for all i,j, then we see that $\mathcal{L}_G(f) = c \cdot \mathcal{L}_H(f)$ so that $\|\boldsymbol{\sigma}_i(G)\|_2^2 = c \cdot \|\boldsymbol{\sigma}_i(H)\|_2^2$. This gives us a sense that volume of the simplex of the supergraph is greater than that of the subgraph. This notion will be made more precise in Section 4.1.

Meanwhile however, the normalized simplex is unaffected by the re-weighting:

$$\begin{aligned}
\widehat{\mathcal{L}}_G(\boldsymbol{f}) &= \sum_{i\sim j} w_G(i,j)\left(\frac{\boldsymbol{f}(i)}{\sqrt{w_G(i)}} - \frac{\boldsymbol{f}(j)}{\sqrt{w_G(j)}}\right)^2 \\
&= \sum_{i\sim j} c \cdot w_H(i,j)\left(\frac{\boldsymbol{f}(i)}{\sqrt{c\cdot w_H(i)}} - \frac{\boldsymbol{f}(j)}{\sqrt{c\cdot w_H(j)}}\right)^2 \\
&= \sum_{i\sim j} w_H(i,j)\left(\frac{\boldsymbol{f}(i)}{\sqrt{w_H(i)}} - \frac{\boldsymbol{f}(j)}{\sqrt{w_H(j)}}\right)^2 = \widehat{\mathcal{L}}_H(\boldsymbol{f}),
\end{aligned}$$

implying that $\|\widehat{\boldsymbol{\sigma}}_i(G)\|_2 = \|\widehat{\boldsymbol{\sigma}}_i(H)\|$.

Product graphs. We begin with the definition of a product graph.

Definition 3.1. Given two graphs $G = (V(G), E(G))$ and $H = (V(H), E(H))$, the *product graph of G and H* is the graph with vertex set $V(G) \times V(H)$ and edge set $\{((i_1,j),(i_2,j)) : (i_1,i_2) \in E(G), j \in V(H)\} \cup \{((i,j_1),(i,j_2)) : (j_1,j_2) \in E(H), i \in V(G)\}$. It is typically denoted $G \times H$.

In order to investigate the simplex of a product graph, we must better understand its eigenstructure. The following discussion demonstrates that the eigenstructure of $G \times H$ relates directly to that of G and H. Put $n = |V(G)|$ and $m = |V(H)|$. Suppose G has eigenvalues $\lambda_1 \geq \cdots \geq \lambda_n$ and corresponding eigenvectors $\boldsymbol{\varphi}_1, \ldots, \boldsymbol{\varphi}_n$, as usual. Let H have eigenvalues $\mu_1 \geq \cdots \geq \mu_m$ and corresponding eigenvectors $\boldsymbol{\psi}_1, \ldots, \boldsymbol{\psi}_m$. We claim that $G \times H$ has mn eigenvalues $\{\lambda_i + \mu_j\}_{(i,j)i\in[n]\times[m]}$ with eigenvectors $\{f_{i,j}\}_{(i,j)\in[n]\times[m]}$ given by

$$f_{i,j}(k,\ell) = \boldsymbol{\varphi}_i(k)\boldsymbol{\psi}_j(\ell).$$

Indeed:

$$\begin{aligned}
(\boldsymbol{L}_{G\times H} f_{uv})(ij) &= \deg_{G\times H}((i,j)) f_{uv}(ij) - \sum_{(k,\ell)\in\delta((i,j))} f_{uv}(k\ell) \\
&= (\deg_G(i) + \deg_H(j))\boldsymbol{\varphi}_u(i)\boldsymbol{\psi}_v(j) - \sum_{(k,\ell)\in\delta_{G\times H}((i,j))} \boldsymbol{\varphi}_u(i)\boldsymbol{\psi}_v(j) \\
&= (\deg_G(i) + \deg_H(j))\boldsymbol{\varphi}_u(i)\boldsymbol{\psi}_v(j) - \sum_{k\in\delta_G(i)} \boldsymbol{\varphi}_u(k)\boldsymbol{\psi}_v(j) - \sum_{\ell\in\delta_H(j)} \boldsymbol{\varphi}_u(i)\boldsymbol{\psi}_v(\ell)
\end{aligned}$$

$$
\begin{aligned}
&= \Bigg(\deg_G(i)\boldsymbol{\varphi}_u(i) - \sum_{k\in\delta_G(i)} \boldsymbol{\varphi}_u(k)\Bigg)\boldsymbol{\psi}(j) \\
&\qquad + \Bigg(\deg_H(j)\boldsymbol{\psi}_v(j) - \sum_{\ell\in\delta_H(j)} \boldsymbol{\psi}_v(\ell)\Bigg)\boldsymbol{\varphi}_u(i) \\
&= (\boldsymbol{L}_G\boldsymbol{\varphi}_u)(i)\cdot\boldsymbol{\psi}_v(j) + (\boldsymbol{L}_H\boldsymbol{\psi}_v)(j)\cdot\boldsymbol{\varphi}_u(i) \\
&= \lambda_u\boldsymbol{\varphi}_u(i)\boldsymbol{\psi}_v(j) + \mu_v\boldsymbol{\psi}_v(j)\boldsymbol{\varphi}_u(i) \\
&= (\lambda_u+\mu_v)\boldsymbol{\varphi}_u(i)\boldsymbol{\psi}_v(j) = (\lambda_u+\mu_v)f_{uv}(ij),
\end{aligned}
$$

as desired. Consequently, the product graph yields a simplex $\mathcal{S}_{G\times H}\in\mathbb{R}^{mn-1}$ with vertices $\{\boldsymbol{\sigma}_{ij}\}_{(i,j)\in[n]\times[m]}$ given by

$$\boldsymbol{\sigma}_{ij}(k\ell) = f_{k\ell}(ij)(\lambda_k+\mu_\ell)^{1/2}.$$

3.3.1. Examples

We now move onto concrete examples of the simplices of particular graphs whose eigenstructures we can compute explicitly. We also compute the graph of perhaps the most well-known simplex: the probability simplex.

The complete graph, K_n. Let us consider the combinatorial simplex $\mathcal{S}=\mathcal{S}_{K_n}$. The Laplacian $\boldsymbol{L}_{K_n}$ has two eigenvalues: 0 with multiplicity 1 and n with multiplicity $n-1$. To see this, observe that for any $\boldsymbol{\varphi}$ perpendicular to $\mathbf{1}$, we have

$$
\begin{aligned}
\boldsymbol{L}_{K_n}\boldsymbol{\varphi} &= \Bigg(\boldsymbol{\varphi}(1)(n-1) - \sum_{i\neq 1}\boldsymbol{\varphi}(i),\dots,\boldsymbol{\varphi}(n)(n-1) - \sum_{i\neq n}\boldsymbol{\varphi}(i)\Bigg) \\
&= \Bigg(\boldsymbol{\varphi}(1)n - \sum_{i}\boldsymbol{\varphi}(i),\dots,\boldsymbol{\varphi}(n)n - \sum_{i}\boldsymbol{\varphi}(i)\Bigg) \\
&= (\boldsymbol{\varphi}(1)n,\dots,\boldsymbol{\varphi}(n)n) = n\boldsymbol{\varphi},
\end{aligned}
$$

since $\sum_i\boldsymbol{\varphi}(i) = \langle\boldsymbol{\varphi},\mathbf{1}\rangle = 0$. Let $\boldsymbol{Q}$ described the rotation matrix which rotates each vector by $\pi/4$ about each axis. Thus $\boldsymbol{Q}\boldsymbol{e}_1=\mathbf{1}$, and we can $n-1$ orthogonal eigenvectors $\boldsymbol{Q}\boldsymbol{e}_2,\dots,\boldsymbol{Q}\boldsymbol{e}_n$. The vertices of $\mathcal{S}$ are thus given by $\boldsymbol{\sigma}_i(j)=\sqrt{n}(\boldsymbol{Q}\boldsymbol{e}_{j+1})(i)$.

The Cycle graph, C_n. The cycle graph C_n has edge set $E=\{(i,j): j=i+1 \mod n\}$. We assume that n is even for this example. We leave it to the reader to verify by direct computation that the eigenvalues and eigenvectors of $\boldsymbol{L}_{C_n}$ are given by

$$\boldsymbol{\varphi}_i(j) = \cos\bigg(\frac{2\pi(i-1)j}{n}\bigg),\quad \lambda_i = 2-2\cos\bigg(\frac{2\pi(i-1)}{n}\bigg),$$

for $i = 1, \dots, n/2+1$, and

$$\boldsymbol{\varphi}_i(j) = \cos\left(\frac{2\pi(i-n/2-1)j}{n}\right), \quad \lambda_i = 2 - 2\cos\left(\frac{2\pi(i-n/2-1)}{n}\right),$$

for $i = n/2+2, \dots, n$. Therefore, the vertices of $\mathcal{S}_{C_n}$ are given by

$$\boldsymbol{\sigma}_i(j) = \begin{cases} \cos\left(\frac{2\pi(i-1)j}{n}\right)\left(2-\cos\left(\frac{2\pi(i-\chi(j>n/2+1)n/2-1)}{n}\right)\right), & i \leq n/2+1, \\ \sin\left(\frac{2\pi(i-n/2-1)j}{n}\right)\left(2-\cos\left(\frac{2\pi(i-\chi(j>n/2+1)n/2-1)}{n}\right)\right), & i > n/2+1. \end{cases}$$

The probability simplex. Fix $n \in \mathbb{N}$. The *probability simplex* is the simplex $\widetilde{\mathcal{S}}_p = \mathrm{conv}(\{\boldsymbol{\chi}_i\}_{i=1}^n \cup \{\mathbf{0}\})$. It is most likely the simplex of greatest familiarity to mathematicians and computer scientists, being used to reason geometrically about probability distributions. The probability simplex has centroid $\mathbf{1}/n \neq \mathbf{0}$ and we will consider its centred version

$$\mathcal{S}_p \stackrel{\text{def}}{=} \widetilde{\mathcal{S}}_p - \frac{\mathbf{1}}{n},$$

which has vertices $\boldsymbol{\sigma}_i = \boldsymbol{\chi}_i - \mathbf{1}/n$, $i < n$, and $\boldsymbol{\sigma}_n = -\mathbf{1}/n$. Note that $\boldsymbol{\sigma}_j - \boldsymbol{\sigma}_n = \boldsymbol{\chi}_j$ and so $\langle \boldsymbol{\chi}_i, \boldsymbol{\sigma}_j - \boldsymbol{\sigma}_n\rangle = \delta_{ij}$. Taking $\boldsymbol{\sigma}_i^* = \boldsymbol{\chi}_i$ and $\boldsymbol{\sigma}_n^* = -\sum_i \boldsymbol{\chi}_i = -\mathbf{1}$ thus gives us the dual vertices. The angles between the facets of $\mathcal{S}_p$ are thus defined by

$$\cos\theta_{ij}(\mathcal{S}_p) = -\langle \boldsymbol{\chi}_i, \boldsymbol{\chi}_j\rangle = -\delta_{ij},$$

for $i, j \in [n-1$ and

$$\cos\theta_{in}(\mathcal{S}_p) = \frac{\langle \boldsymbol{\chi}_i, \mathbf{1}\rangle}{\|1\|} = 1/\sqrt{n},$$

for all $i \in [n]$. This implies that $\theta_{ij}(\mathcal{S}_p) = 0$ for $i \neq j$, $i, j \neq n$ and $\theta_{in}(\mathcal{S}_p) \in= (0, \pi/2)$. Using the construction of Section 3.2.2, we associate to $\mathcal{S}_p$ the graph with Laplacian matrix $\mathbf{\Sigma}(\mathcal{S}_p^*)^{\rightarrow}\mathbf{\Sigma}(\mathcal{S}_p^*)$, where $\mathbf{\Sigma}(\mathcal{S}_p^*) = (\boldsymbol{\sigma}_1^*, \dots, \boldsymbol{\sigma}_n^*)$. This matrix has (i,j)-th entry 1 for $i = j$, 1 for $i = n$ or $j = n$, and 0 otherwise. This graph thus has each vertex connected to n, but to no others. That is, the graph of the probability simplex $\mathcal{S}_p$ is the star graph on n vertices.

§3.4. Properties of $\mathcal{S}_G$ and $\mathcal{S}_G^+$

We now embark on our voyage to understand the mathematical properties of the simplices of a graph. This section is devoted to the study of $\mathcal{S}_G$ and $\mathcal{S}_G^+$, while Section 3.5 is concerned with $\widehat{\mathcal{S}}_G$ and $\widehat{\mathcal{S}}_G^+$. For bibliographic purposes, we will encode many of the results as Lemmas even if they are relatively simple. There are many results, and this should enable easier accounting. We begin with three basic properties.

LEMMA 3.4. *The following three properties hold:*

1. *Both $\mathcal{S}_G$ and $\mathcal{S}_G^+$ are centred at the origin;*

2. *The squared distance between the vertices of $\mathcal{S}_G^+$ is equal to the effective resistance between the corresponding vertices of G;*

3. *For any non-empty $U \subsetneq V$, the faces $\mathcal{S}_U$ and $\mathcal{S}_{U^c}^+$ are orthogonal.*

Proof. For (i) we simply compute $\boldsymbol{c}(\mathcal{S}) = n^{-1}\boldsymbol{\Lambda}^{-1/2}\boldsymbol{\Phi}^t\mathbf{1} = \mathbf{0}$, since $\langle \boldsymbol{\varphi}_i, \mathbf{1}\rangle = 0$ for all $i < n$. Likewise, $\boldsymbol{c}(\mathcal{S}^+) = \mathbf{0}$. For (ii),

$$\left\|\boldsymbol{\sigma}_i^+ - \boldsymbol{\sigma}_j^+\right\|_2^2 = \|\boldsymbol{\sigma}_i^+\|_2^2 + \left\|\boldsymbol{\sigma}_j^+\right\|_2^2 - 2\langle\boldsymbol{\sigma}_i^+, \boldsymbol{\sigma}_j^+\rangle = \boldsymbol{L}_G^+(i,i) + \boldsymbol{L}_G^+(j,j) - 2\boldsymbol{L}_G^+(i,j) = r^{\text{eff}}(i,j).$$

Property three follows as a result of the fact that $\mathcal{S}_G^+$ is dual to $\mathcal{S}_G$ (Observation 3.1) and Lemma 2.9. ⊠

Property (ii) in the previous lemma was first noticed by Fielder [Fie11, Chapter 6], and was also remarked upon by Van Mieghem *et al.* [VMDC17] who used it in their study of best spreader nodes in electrical networks. We will return to this connection in later sections. We now turn our attention to properties of the angles of a simplex.

Lemma 3.5. *The combinatorial simplex $\mathcal{S}_G$ of a graph G is hyperacute iff $\boldsymbol{L}_G^+$ is a Laplacian.*

Proof. Using Equation 2.26 and the fact that $\mathcal{S}_G^+ = \mathcal{S}_G^*$ (Observation 3.1), we have

$$\cos\theta_{ij} = -\frac{\langle\boldsymbol{\sigma}_i^+, \boldsymbol{\sigma}_j^+\rangle}{\|\boldsymbol{\sigma}_i^+\|_2\left\|\boldsymbol{\sigma}_j^+\right\|_2},$$

where we recall that θ_{ij} is the angle between $\mathcal{S}_{\{i\}^c}$ and $\mathcal{S}_{\{j\}^c}$. Thus, $\mathcal{S}_G$ is hyperacute iff

$$-\langle\boldsymbol{\sigma}_i^+, \boldsymbol{\sigma}_j^+\rangle / \|\boldsymbol{\sigma}_i^+\|_2\left\|\boldsymbol{\sigma}_j^+\right\|_2 \in [0,1],$$

which occurs iff $\langle\boldsymbol{\sigma}_i^+, \boldsymbol{\sigma}_j^+\rangle \leq 0$. In this case $\boldsymbol{L}_G^+(i,j) \leq 0$, implying that $\boldsymbol{L}_G^+$ is a Laplacian (recall that it already satisfies the other required properties: $\boldsymbol{L}_G^+\mathbf{1} = \mathbf{0}$ and $\boldsymbol{L}_G^+(i,i) \geq 0$). ⊠

Corollary 3.1. *The combinatorial simplex of the complete graph, $\mathcal{S}_{K_n}$, is hyperacute.*

Proof. Let $\boldsymbol{L} = \boldsymbol{L}_{K_n}$. It suffices to show by the previous lemma that $\boldsymbol{L}^+ = \boldsymbol{L}_{K^n}^+$ is a Laplacian. We've already seen that $\boldsymbol{L}_G^+\mathbf{1} = \mathbf{0}$ for any G, so it remains only to show that $\boldsymbol{L}^+(k,k) > 0$ for all $k \in [n]$ and $\boldsymbol{L}^+(k,\ell) \leq 0$ for all $k \neq \ell$, i.e., that $\text{sign}(\boldsymbol{L}(k,\ell)) = \text{sign}(\boldsymbol{L}^+(k,\ell))$ for all k,ℓ. Recall from Section 3.3.1 that K_n has eigenvalue n with multiplicity $n-1$ and a single zero eigenvalue. Hence, $\boldsymbol{L} = n\sum_{i<n}\boldsymbol{\varphi}_i\boldsymbol{\varphi}_i^t$ and $\boldsymbol{L}^+ = n^{-1}\sum_{i<n}\boldsymbol{\varphi}_i\boldsymbol{\varphi}_i^t$. Therefore, $\text{sign}(\boldsymbol{L}(k,\ell)) = \text{sign}(n\sum_{i<n}\boldsymbol{\varphi}_i(k)\boldsymbol{\varphi}_i(\ell)) = \text{sign}(\sum_{i<n}\boldsymbol{\varphi}_i(k)\boldsymbol{\varphi}_i(\ell)) = \text{sign}(\boldsymbol{L}^+(k,\ell))$ which implies the result. ⊠

As Fiedler pointed out [Fie93], the correspondence also allows us to answer questions related to the distribution of angles of simplices. It is not, for example, a priori obvious that all distributions of angles are possible in a hyperacute simplex, in the following sense.

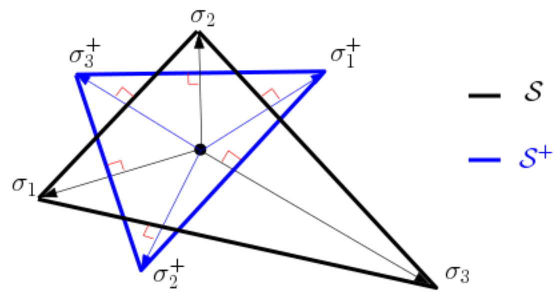


Figure 3.1: A simplex of a graph and its inverse.

LEMMA 3.6. *For every $n-1 \leq k \leq \binom{n}{2}$, there exists a hyperacute simplex on n vertices with k strictly acute interior angles.*

Proof. Fix k and consider a connected graph on n vertices with k edges (note the importance that $k \geq n-1$). The interior angles $\{\theta_{ij}^+\}_{i,j}$ of $\mathcal{S}_G^+$ obey $\cos\theta_{ij} = w(i,j)/\sqrt{w(i)w(j)}$, hence $\theta_{ij} = \pi/2$ whenever $w(i,j) = 0$, and $\theta_{ij} \in (0, \pi/2)$ for all $(i,j) \in E(G)$. Therefore, $\mathcal{S}_G^+$ meets the desired criteria. ⊠

The following lemma presents an alternate characterization of the simplex, and was first proved by Devriendt and Van Mieghem [DVM18]. As they notice, the following representation provides an easy way to check whether a given point lies inside the simplex.

LEMMA 3.7 ([DVM18]). *For a simplex $\mathcal{S}$ of a graph G,*

$$\mathcal{S} = \left\{ \boldsymbol{x} \in \mathbb{R}^{n-1} : \boldsymbol{x}^t \boldsymbol{\Sigma}^+ + \frac{\mathbf{1}^t}{n} \geq \mathbf{0}^t \right\}. \tag{3.6}$$

Proof. Put $E = \{\boldsymbol{x} \in \mathbb{R}^{n-1} : \boldsymbol{x}^t\boldsymbol{\Sigma}^+ + \mathbf{1}^t/n \geq \mathbf{0}^t\}$. First we show that $E \subseteq \mathcal{S}$. Since $\operatorname{rank}(\boldsymbol{\Sigma}) = n-1$, it follows that given any $\boldsymbol{x} \in E$ (indeed, any $\boldsymbol{x} \in \mathbb{R}^{n-1}$) we can write $\boldsymbol{x} = \boldsymbol{\Sigma}\boldsymbol{y}$ for some $\boldsymbol{y} \in \mathbb{R}^n$. Letting $\bar{y} = n^{-1}\sum_i y(i)$ be the mean of the vector $\boldsymbol{y}$, compute

$$\boldsymbol{x}^t\boldsymbol{\Sigma}^+ = \boldsymbol{y}^t\boldsymbol{\Sigma}^t\boldsymbol{\Sigma}^+ = \boldsymbol{y}^t(\mathbf{I} - \mathbf{1}\mathbf{1}^t/n) = \boldsymbol{y}^t - \bar{y}\mathbf{1}^t.$$

If $\boldsymbol{x} \in E$ the above implies that

$$\boldsymbol{y}^t - \bar{y}\mathbf{1}^t + \mathbf{1}^t/n \geq \mathbf{0}^t.$$

Moreover, since $\boldsymbol{\Sigma}\mathbf{1} = \mathbf{0}$, we have $\boldsymbol{x} = \boldsymbol{\Sigma}\boldsymbol{y} = \boldsymbol{\Sigma}(\boldsymbol{y} - \bar{y}\mathbf{1} + \mathbf{1}/n)$. Noticing that

$$\langle \boldsymbol{y} - \bar{y}\mathbf{1} + \mathbf{1}^t/n, \mathbf{1}\rangle = n\bar{y} - n\bar{y} + 1 = 1,$$

demonstrates that the vector $\widetilde{\boldsymbol{y}} = \boldsymbol{y} - \bar{y}\mathbf{1} + \mathbf{1}^t/n$ is a barycentric coordinate for $\boldsymbol{x}$, and so $\boldsymbol{x} \in \mathcal{S}$.

Conversely, for $\boldsymbol{x} \in \mathcal{S}$ let $\boldsymbol{y}$ be its barycentric coordinate. Then

$$\boldsymbol{x}^t \boldsymbol{\Sigma}^+ + \frac{\mathbf{1}^t}{n} = \boldsymbol{y}^t \left(\mathbf{I} - \frac{\mathbf{J}}{n} \right) + \frac{\mathbf{1}^t}{n} = \boldsymbol{y}^t - \frac{\mathbf{1}^t}{n} + \frac{\mathbf{1}^t}{n} = \boldsymbol{y}^t \geq \mathbf{0}^t,$$

hence $\mathcal{S} \subseteq E$. This completes the proof. ⊠

Just as each facet of a tetrahedron is contained in a plane and each edge is contained in an infinite line, each face $\mathcal{S}_U$ of a simplex U is contained in a *flat* of dimension $|U| - 1$. The following Lemma helps characterize these flats.

LEMMA 3.8. *Let $\mathcal{S}$ be the simplex of a graph $G = (V, E, w)$, and fix $U \subseteq V$. For any non-empty $E \subseteq U^c$,*

$$\mathcal{S}_U \subseteq \left\{ \boldsymbol{x} \in \mathbb{R}^{n-1} : \sum_{i \in E} \langle \boldsymbol{x}, \boldsymbol{\sigma}_i^+ \rangle + \frac{|E|}{n} = 0 \right\},$$

and

$$\mathcal{S}_U^+ \subseteq \left\{ \boldsymbol{x} \in \mathbb{R}^{n-1} : \sum_{i \in E} \langle \boldsymbol{x}, \boldsymbol{\sigma}_i \rangle + \frac{|E|}{n} = 0 \right\},$$

Proof. Let $\boldsymbol{x} \in \mathcal{S}_U$ be arbitrary. For any $i \in U^c$ we have $\langle \boldsymbol{x}, \boldsymbol{\sigma}_i^+ \rangle = -1/n$. Hence, for any $E \subseteq U^c$

$$\sum_{i \in E} \langle \boldsymbol{x}, \boldsymbol{\sigma}_i^+ \rangle + \frac{|E|}{n} = \sum_{i \in E} \left(\langle \boldsymbol{x}, \boldsymbol{\sigma}_i^+ \rangle + \frac{1}{n} \right) = \sum_{i \in E} \left(\frac{1}{n} - \frac{1}{n} \right) = 0,$$

implying that $\boldsymbol{x}$ is in the desired set. ⊠

Lemma 3.8 gives us an alternate way to prove Lemma 3.7. For any i, taking $U = N \setminus \{i\}$ and $E = \{i\}$, it implies that $\mathcal{S}_{\{i\}^c}$ is a subset of the hyperplane

$$\mathcal{H}_i \stackrel{\text{def}}{=} \{ \boldsymbol{x} \in \mathbb{R}^{n-1} : \langle \boldsymbol{x}, \boldsymbol{\sigma}_i^+ \rangle + 1/n = 0 \}.$$

All points in the simplex $\mathcal{S}$ lie to one side of $\mathcal{S}_{\{i\}^c}$, i.e., they lie in the halfspace

$$\mathcal{H}_i^{\geq} \stackrel{\text{def}}{=} \{ \boldsymbol{x} \in \mathbb{R}^{n-1} : \langle \boldsymbol{x}, \boldsymbol{\sigma}_i^+ \rangle + 1/n \geq 0 \}.$$

(We know it is this halfspace because $\mathbf{0} \in \mathcal{S} \cap \mathcal{H}_i^{\geq}$.) The simplex is the interior of the region defined by the intersection of the faces $\mathcal{S}_{\{i\}^c}$, i.e.,

$$\mathcal{S} = \bigcap_i \mathcal{H}_i^{\geq}. \tag{3.7}$$

Moreover, $\boldsymbol{x} \in \bigcap_i \mathcal{H}_i^{\geq}$ iff $\langle \boldsymbol{x}, \boldsymbol{\sigma}_i^+ \rangle + 1/n \geq 0$ for all i, i.e., $(\langle \boldsymbol{x}, \boldsymbol{\sigma}_1^+ \rangle, \ldots, \langle \boldsymbol{x}, \boldsymbol{\sigma}_n^+ \rangle) + \mathbf{1}/n \geq \mathbf{0}$, meaning $\boldsymbol{x}$ satisfies (3.6). We emphasize that a very similar discussion applies to $\mathcal{S}^+$, in which case one has

$$\mathcal{S}^+ = \bigcap_i (\mathcal{H}_i^+)^{\geq}, \tag{3.8}$$

for $(\mathcal{H}_i^+)^{\geq} \overset{\text{def}}{=} \{\boldsymbol{x} \in \mathbb{R}^{n-1} : \langle \boldsymbol{x}, \boldsymbol{\sigma}_i \rangle + 1/n \geq 0\}$.

Centroids and altitudes. We now turn to investigating the centroids and altitudes of the simplices, and how they relate to properties of the underlying graph. We begin by exploring the relationships between properties of the simplices themselves.

Recall that the altitude between $\mathcal{S}[U]$ and $\mathcal{S}[U^c]$ of a simplex $\mathcal{S}$ is denoted $\boldsymbol{a}(\mathcal{S}_U)$ and is the unique vector $\boldsymbol{p} - \boldsymbol{q}$ where $\boldsymbol{p} \in \mathcal{S}_{U^c}$ and $\boldsymbol{q} \in \mathcal{S}_U$ which lies in the orthogonal complement of both $\mathcal{S}_U$ and $\mathcal{S}_{U^c}$. One would thus expect that $\boldsymbol{a}(\mathcal{S}_U)$ and $\boldsymbol{a}(\mathcal{S}_{U^c})$ to be antiparallel; a fact verified by Lemma 3.9.

In what follows, we will often write $\boldsymbol{c}_U$ for $\boldsymbol{c}(\mathcal{S}_U)$ (resp., $\boldsymbol{c}_U^+$ for $\boldsymbol{c}(\mathcal{S}_U^+)$) and $\boldsymbol{a}_U$ for $\boldsymbol{a}(\mathcal{S}_U)$ (resp., $\boldsymbol{a}_U^+$ for $\boldsymbol{a}(\mathcal{S}_U^+)$).

Lemma 3.9 ([DVM18]). *Let $U \subseteq V$ be non-empty. Then the vectors $\boldsymbol{c}(\mathcal{S}_U)$ and $\boldsymbol{c}(\mathcal{S}_{U^c})$ are antiparallel. In particular, $(n - |U|)\boldsymbol{c}(\mathcal{S}_{U^c}) = |U|\boldsymbol{c}(\mathcal{S}_U)$ and*

$$\frac{\boldsymbol{c}(\mathcal{S}_U)}{\|\boldsymbol{c}(\mathcal{S}_U)\|_2} = -\frac{\boldsymbol{c}(\mathcal{S}_{U^c})}{\|\boldsymbol{c}(\mathcal{S}_{U^c})\|_2}.$$

Proof. This is a straightforward computation: Observing that $\boldsymbol{\chi}_U = \mathbf{1} - \boldsymbol{\chi}_{U^c}$ we have

$$\boldsymbol{c}_U = |U|^{-1}\boldsymbol{\Sigma}\boldsymbol{\chi}_U = |U|^{-1}\boldsymbol{\Sigma}(\mathbf{1} - \boldsymbol{\chi}_{U^c}) = -|U|^{-1}\boldsymbol{\Sigma}\boldsymbol{\chi}_{U^c} = -|U|^{-1}\frac{|U^c|}{|U^c|}\boldsymbol{\Sigma}\boldsymbol{\chi}_{U^c} = \frac{n-|U|}{|U|}\boldsymbol{c}_{U^c},$$

where we've used that $\boldsymbol{\Sigma}\mathbf{1} = \mathbf{0}$. This proves the first result; the second follows from normalizing the two vectors. ⊠

We would now like to examine the relationships between altitudes and centroids in the simplex and its inverse. We will demonstrate that centroids of opposing faces are antiparallel, and that the centroid of the face U is parallel to the altitude of originating from the face generated by U in its inverse. First however, we require the following technical result.

Lemma 3.10. *Any vector perpendicular to $\mathcal{S}_U$ can be written as $\boldsymbol{\Sigma}^+(\boldsymbol{f}_{U^c} + \alpha\boldsymbol{\chi}_U)$ for some $\alpha \in \mathbb{R}$ and vector $\boldsymbol{f}_{U^c}$ such that $\boldsymbol{f}(U) = \mathbf{0}$.*

Proof. Let $\boldsymbol{y} \in \mathbb{R}^{n-1}$ be orthogonal to $\mathcal{S}_U$. Since $\operatorname{rank}(\boldsymbol{\Sigma}^+) = n-1$, we can find some $\boldsymbol{z}$ such that $\boldsymbol{y} = \boldsymbol{\Sigma}^+\boldsymbol{z} = \sum_{i\in U^c}\boldsymbol{\sigma}_i^+ z(i) + \sum_{j\in U}\boldsymbol{\sigma}_j^+ z(j)$. Define $\boldsymbol{f}$ by $\boldsymbol{f}(U^c) = \boldsymbol{z}(U^c)$ and $\boldsymbol{f}(U) = \mathbf{0}$ and $\boldsymbol{z}_{U^c}$. We can then write $\boldsymbol{y}$ as $\boldsymbol{\Sigma}^+\boldsymbol{f} + \sum_{j\in U}\boldsymbol{\sigma}_j^+ z(j)$, so we must show that $\boldsymbol{z}(U)$ is a constant vector. The orthogonality of $\boldsymbol{y}$ to $\mathcal{S}_U$ implies that for every two barycentric coordinates $\boldsymbol{x}_U$ and $\boldsymbol{y}_U$ with $\boldsymbol{x}(U^c) = \boldsymbol{y}(U^c) = \mathbf{0}$,

$$\begin{aligned} 0 &= \langle \boldsymbol{y}, \boldsymbol{\Sigma}\boldsymbol{x}_U - \boldsymbol{\Sigma}\boldsymbol{y}_u \rangle \\ &= \sum_{i\in U^c} z(i)\langle \boldsymbol{\sigma}_i^+, \boldsymbol{\Sigma}(\boldsymbol{x}_U - \boldsymbol{y}_U)\rangle + \sum_{j\in U} z(j)\langle \boldsymbol{\sigma}_j^+, \boldsymbol{\Sigma}(\boldsymbol{x}_U - \boldsymbol{y}_U)\rangle \\ &= \sum_{j\in U} z(j)\langle \boldsymbol{\sigma}_j^+, \boldsymbol{\Sigma}(\boldsymbol{x}_U - \boldsymbol{y}_U)\rangle, \end{aligned} \tag{3.9}$$

where the final inequality follows because $\boldsymbol{\sigma}_i^+$ is orthogonal to $\mathcal{S}_U$ for $i \in U^c$ by Lemma 3.4. Now, for $j \in U$,

$$\langle \boldsymbol{\sigma}_j^+, \boldsymbol{\Sigma}(\boldsymbol{x}_U - \boldsymbol{y}_U)\rangle = \boldsymbol{\chi}_j^t \boldsymbol{\Sigma}^+ \boldsymbol{\Sigma}(\boldsymbol{x}_U - \boldsymbol{y}_U) = \boldsymbol{\chi}_j^t \left(\mathbf{I} - \frac{\mathbf{J}}{n}\right)(\boldsymbol{x}_U - \boldsymbol{y}_U) = \boldsymbol{\chi}_j^t(\boldsymbol{x}_U - \boldsymbol{y}_U). \tag{3.10}$$

Suppose for contradiction that $z(k) \neq z(j)$ for some $k, j \in U$. Put $\boldsymbol{x}_U = \boldsymbol{\chi}_k$ and $\boldsymbol{y}_U = \boldsymbol{\chi}_j$. Using Equation (3.10) write (3.9) as

$$z(k)\boldsymbol{\chi}_k^t(\boldsymbol{\chi}_k - \boldsymbol{\chi}_j) + z(j)\boldsymbol{\chi}_j^t(\boldsymbol{\chi}_k - \boldsymbol{\chi}_j) + \sum_{\ell \in U^c, \ell \neq j,k} z(\ell)\boldsymbol{\chi}_\ell^t(\boldsymbol{\chi}_k - \boldsymbol{\chi}_j) = z(k) - z(j) \neq 0,$$

a contradiction. ⊠

We can now proceed to the main result.

Lemma 3.11. *For a simplex $\mathcal{S}$ of a graph $G = (V, E)$ and any $U \subseteq V$, $U \neq \emptyset$,*

$$\frac{\boldsymbol{a}(\mathcal{S}_U)}{\|\boldsymbol{a}(\mathcal{S}_U)\|_2} = \frac{\boldsymbol{c}^+(\mathcal{S}_{U^c})}{\|\boldsymbol{c}^+(\mathcal{S}_{U^c})\|_2} = -\frac{\boldsymbol{c}^+(\mathcal{S}_U)}{\|\boldsymbol{c}^+(\mathcal{S}_U)\|_2}, \tag{3.11}$$

and

$$\frac{\boldsymbol{a}^+(\mathcal{S}_U)}{\|\boldsymbol{a}^+(\mathcal{S}_U)\|_2} = \frac{\boldsymbol{c}(\mathcal{S}_{U^c})}{\|\boldsymbol{c}(\mathcal{S}_{U^c})\|_2} = -\frac{\boldsymbol{c}(\mathcal{S}_U)}{\|\boldsymbol{c}(\mathcal{S}_U)\|_2}.$$

Proof. We prove the first set of equalities only; the second is obtained similarly. By definition, $\boldsymbol{a}_U$ is orthogonal to both $\mathcal{S}_U$ and $\mathcal{S}_{U^c}$. Lemma 3.10 then implies both that

$$\boldsymbol{a}_U = \boldsymbol{\Sigma}^+ \boldsymbol{f} + \alpha \boldsymbol{\Sigma}^+ \boldsymbol{\chi}_U,$$

and

$$\boldsymbol{a}_U = \boldsymbol{\Sigma}^+ \boldsymbol{g} + \beta \boldsymbol{\Sigma}^+ \boldsymbol{\chi}_{U^c},$$

for some $\alpha, \beta \in \mathbb{R}$, and vectors $\boldsymbol{f}, \boldsymbol{g}$ with $\boldsymbol{f}(U) = \mathbf{0}$ and $\boldsymbol{g}(U^c) = \mathbf{0}$. In particular then,

$$\frac{\boldsymbol{\Sigma}^+(\boldsymbol{f} + \alpha\boldsymbol{\chi}_U)}{\|\boldsymbol{\Sigma}^+(\boldsymbol{f} + \alpha\boldsymbol{\chi}_U)\|_2} = \frac{\boldsymbol{\Sigma}^+(\boldsymbol{g} + \beta\boldsymbol{\chi}_{U^c})}{\|\boldsymbol{\Sigma}^+(\boldsymbol{g} + \beta\boldsymbol{\chi}_{U^c})\|_2}. \tag{3.12}$$

By Lemma 3.9, taking $\boldsymbol{f} = \pm\boldsymbol{\chi}_{U^c}/|U^c|$, $\boldsymbol{g} = \mp\boldsymbol{\chi}_U/|U|$, and $\alpha = \beta = 0$ yield solutions to the above equation. We have thus obtained Equation (3.11) up to its sign; it remains to determine whether $\boldsymbol{a}(\mathcal{S}_U)$ is parallel to antiparallel to $\boldsymbol{c}(\mathcal{S}_U)$. Since it is one of the two, we have

$$\frac{\langle \boldsymbol{a}_U, \boldsymbol{c}_U^+\rangle}{\|\boldsymbol{a}_U\|_2 \|\boldsymbol{c}^+ U\|_2} \in \{1, -1\},$$

hence to see that they are antiparallel it suffices to show that $\langle \boldsymbol{a}_U, \boldsymbol{c}^+ U\rangle < 0$. Let $\boldsymbol{a}_U = \boldsymbol{\Sigma}\boldsymbol{y}_{U^c} - \boldsymbol{\Sigma}\boldsymbol{z}_U$ for barycentric coordinates $\boldsymbol{y}_{U^c}$ and $\boldsymbol{z}_U$ representing the faces $\mathcal{S}_{U^c}$ and $\mathcal{S}_U$. Then,

$$\langle \boldsymbol{a}_U, \boldsymbol{c}_U^+\rangle = \frac{1}{n}\langle \boldsymbol{\Sigma}(\boldsymbol{y}_{U^c} - \boldsymbol{z}_U), \boldsymbol{\Sigma}\boldsymbol{\chi}_U^+\rangle$$

$$
\begin{aligned}
&= \frac{1}{n}(\boldsymbol{y}_{U^c}^t - \boldsymbol{z}_U^t)\left(\mathbf{I} - \frac{\mathbf{J}}{n}\right)\boldsymbol{\chi}_U \\
&= -\frac{1}{n}\boldsymbol{z}_U^t\boldsymbol{\chi}_U - \frac{1}{n^2}(\boldsymbol{y}_{U^c}^t - \boldsymbol{z}_U^t)\mathbf{1}\mathbf{1}^t\boldsymbol{\chi}_U \\
&= -\frac{1}{n} < 0.
\end{aligned}
$$

Therefore, $\boldsymbol{a}_U$ is indeed antiparallel to $\boldsymbol{c}_U^+$, meaning that the correct signage is $\boldsymbol{f} = \boldsymbol{\chi}_{U^c}/|U^c|$ and $\boldsymbol{g} = -\boldsymbol{\chi}_U/|U|$. Thus,

$$
\frac{\boldsymbol{a}_U}{\|\boldsymbol{a}_U\|_2} = \frac{\boldsymbol{\Sigma}^+\boldsymbol{\chi}_{U^c}}{\left\|\boldsymbol{\Sigma}^+\boldsymbol{\chi}_{U^c}\right\|_2} = -\frac{\boldsymbol{\Sigma}^+\boldsymbol{\chi}_U}{\left\|\boldsymbol{\Sigma}^+\boldsymbol{\chi}_U\right\|_2},
$$

which is Equation (3.11). ⊠

Remark 3.3. We note that there are no other solutions, up to scaling, of the system of equations for $\boldsymbol{a}_U$ in the previous proof. Indeed, let $\boldsymbol{f}, \boldsymbol{g}, \alpha, \beta$ satisfy the equations. Then

$$
\boldsymbol{\Sigma}^+(\boldsymbol{f} - \beta\boldsymbol{\chi}_{U^c}) + \boldsymbol{\Sigma}^+(\alpha\boldsymbol{\chi}_U - \boldsymbol{g}) = \mathbf{0},
$$

so $f - \beta\boldsymbol{\chi}_{U^c} + \alpha\boldsymbol{\chi} - g \in \ker(\boldsymbol{\Sigma}^+) = \mathrm{span}(\mathbf{1})$, implying that $\boldsymbol{f} - \beta\boldsymbol{\chi}_{U^c} = k\boldsymbol{\chi}_{U^c}$ and $\alpha\boldsymbol{\chi}_U - g = k\boldsymbol{\chi}_U$ for some $k \in \mathbb{R}$, which yields the same solution as in the proof.

Whereas the previous few lemmas explored relationships among $\mathcal{S}_G$ and $\mathcal{S}_G^+$ only, we now begin to observe several connections between the geometry of the simplices and properties of the graph. We begin by recalling that given $U \subseteq V(G)$ the *cut-set* of U is

$$
\partial U \overset{\text{def}}{=} (U \times U^c) \cap E(G) = \{(i,j) \in E(G) : i \in U, j \in U^c\}.
$$

Noting that $|\boldsymbol{\chi}_U(i) - \boldsymbol{\chi}_U(j)| = \chi_{(i,j)\in\delta U}$, we see that

$$
w(\partial U) = \sum_{i,j\in E} w(i,j)|\boldsymbol{\chi}_U(i) - \boldsymbol{\chi}_U(j)| = \sum_{i,j\in E} w(i,j)(\boldsymbol{\chi}_U(i) - \boldsymbol{\chi}_U(j))^2 = \mathcal{L}(\boldsymbol{\chi}_U).
$$

Moreover, $\|\boldsymbol{c}(\mathcal{S}_U)\|_2^2 = \langle |U|^{-1}\boldsymbol{\Sigma}\boldsymbol{\chi}_U, |U|^{-1}\boldsymbol{\Sigma}\boldsymbol{\chi}_U\rangle = |U|^{-2}\mathcal{L}(\boldsymbol{\chi}_U)$ and so

$$
\|\boldsymbol{c}(\mathcal{S}_U)\|_2^2 = \frac{w(\partial U)}{|U|^2}. \tag{3.13}
$$

Via the same process we can also obtain an equivalent expression for the centroid of the inverse simplex:

$$
\left\|\boldsymbol{c}(\mathcal{S}_U^+)\right\|_2^2 = \frac{w(\partial^+ U)}{|U|^2}, \tag{3.14}
$$

where we follow the notation of [DVM18] and define $w(\partial^+ U) \overset{\text{def}}{=} \langle \boldsymbol{\Sigma}^+\chi_U, \boldsymbol{\Sigma}^+\chi_U\rangle = \langle \chi_U, \boldsymbol{L}^+\chi_U\rangle$. Equations (3.13) and (3.14) were also given in [DVM18]. As a sanity check, we note that the equations are consistent with the facts that $\|\boldsymbol{\sigma}_i\|_2^2 = w(i)$ and $\left\|\boldsymbol{\sigma}_i^+\right\|_2^2 = \boldsymbol{L}^+(i,i) = \widehat{\mathcal{L}}^+(\boldsymbol{\chi}_i)$. These equations allow us to give an interesting correspondence between the sizes of the altitudes and cut-sets of G.

LEMMA 3.12. *For any non-empty $U \subseteq V$, $\|\boldsymbol{a}_U^+\|_2^2 = 1/w(\partial U)$ and $\|\boldsymbol{a}_U\|_2^2 = 1/w(\partial^+ U)$.*

Proof. By definition of the altitude there exists barycentric coordinates $\boldsymbol{x}_U$ and $\boldsymbol{x}_{U^c}$ such that $a^+U = \boldsymbol{\Sigma}^+(\boldsymbol{x}_U - \boldsymbol{x}_{U^c})$. Combining this representation of a_U^+ with that given by Lemma 3.11, write

$$\|a_U^+\|_2 = \frac{\langle a_U^+, a_U^+\rangle}{\|a_U^+\|_2} = \frac{\langle \boldsymbol{\Sigma}^+(\boldsymbol{x}_{U^c} - \boldsymbol{x}_U), c_{U^c}\rangle}{\|c_{U^c}\|_2} = \frac{\langle \boldsymbol{\Sigma}^+(\boldsymbol{x}_{U^c} - \boldsymbol{x}_U), \boldsymbol{\Sigma}\boldsymbol{\chi}_{U^c}\rangle}{\sqrt{w(\delta U^c)}},$$

where the final equality comes from using the definition of the centroid in the numerator, and Equation 3.13 in the denominator. Recalling the relation between $\boldsymbol{\Sigma}$ and $\boldsymbol{\Sigma}^+$ given by Equation 3.4 and that $\boldsymbol{x}_U$ and $\boldsymbol{x}_{U^c}$ are barycentric coordinates, we can rewrite the above as

$$\frac{(\boldsymbol{x}_{U^c} - \boldsymbol{x}_U)^t(\mathbf{I} - \mathbf{1}\mathbf{1}^t/n)\boldsymbol{\chi}_{U^c}}{\sqrt{w(\delta U^c)}} = \frac{1}{\sqrt{w(\delta U^c)}}.$$

Squaring both sides while noting that $\delta U = \delta U^c$ completes the proof of the first equality. For the second, we proceed in precisely the same manner to obtain $\|a_U\|_2^2 = 1/w(\delta^+ U^c)$. However, it's not immediately obvious that $w(\delta^+ U^c) = w(\delta^+ U)$. To see this, first recall that $\boldsymbol{\Sigma}^+\mathbf{1} = \boldsymbol{\Lambda}^{-1/2}\boldsymbol{\Phi}^t\mathbf{1} = \mathbf{0}$, and so

$$\begin{aligned} w(\delta^+ U^c) &= \langle \boldsymbol{\Sigma}^+\boldsymbol{\chi}_{U^c}, \boldsymbol{\Sigma}^+\boldsymbol{\chi}_{U^c}\rangle \\ &= \langle \boldsymbol{\Sigma}^+(\mathbf{1} - \boldsymbol{\chi}_U), \boldsymbol{\Sigma}^+(\mathbf{1} - \boldsymbol{\chi}_U)\rangle \\ &= \langle \boldsymbol{\Sigma}^+\boldsymbol{\chi}_U, \boldsymbol{\Sigma}^+\boldsymbol{\chi}_U\rangle = w(\delta^+ U). \end{aligned}$$ ⊠

The aforementioned astute reader may have noticed that the above result implies something about the computational difficulty of determining the length of the minimum and maximum altitudes in hyperacute simplices. We tell this reader to "hold their horses"—this result and others like it will be presented in Chapter 5.

The next two lemmas were both proven by Devriendt and Van Mieghem [DVM18], extending work done by Fiedler. The following lemma gives an explicit expression for the altitudes in terms of graph properties and the inverse centroid.

LEMMA 3.13. *For any non-empty $U \subseteq V$,*

$$\boldsymbol{a}_U = \frac{n - |U|}{w(\delta^+ U)}\boldsymbol{c}_{U^c}^+, \quad \text{and} \quad \boldsymbol{a}_U^+ = \frac{n - |U|}{w(\delta U)}\boldsymbol{c}_{U^c}.$$

Proof. This is a consequence of identities (3.13) and (3.14) and Lemmas 3.11 and 3.12. Applying the latter and then the former, observe that

$$\boldsymbol{a}_U = \frac{\|\boldsymbol{a}_U\|_2}{\|\boldsymbol{c}_{U^c}^+\|_2}\boldsymbol{c}_{U^c}^+ = \left(\frac{1}{\sqrt{w(\delta^+ U^c)}} \Big/ \frac{\sqrt{w(\delta^+ U)}}{|U^c|}\right)\boldsymbol{c}_{U^c}^+ = \frac{n - |U|}{w(\delta^+ U)}c_{U^c}^+,$$

where we've once against used that $w(\delta^+ U^c) = w(\delta^+ U)$. A similar computation holds for $\boldsymbol{a}_U^+$. $\boxtimes$

Just as one generalizes the incidence of a vertex to the neighbourhood of a set of vertices, one can generalize an edge to the incidence between groups of vertices, as

$$\delta U_1 \cap \delta U_2 = \{(i,j) \in E(G), i \in U_1, j \in U_2\},$$

for $U_1, U_2 \subseteq V(G)$. The final lemma gives an expression for the weight (or size) of this set in terms of the altitudes and centroids of the simplices.

Lemma 3.14. *Let $U_1, U_2 \subseteq V$ with $U_1 \cap U_2 = \emptyset$. Then*

$$\langle \boldsymbol{c}(\mathcal{S}_{U_1}), \boldsymbol{c}(\mathcal{S}_{U_2})\rangle = -\frac{w(\delta U_1 \cap \delta U_2)}{|U_1||U_2|}, \quad \textit{and} \quad \langle \boldsymbol{a}_{U_1}^+, \boldsymbol{a}_{U_2}^+\rangle = -\frac{w(\delta U_1^c \cap \delta U_2^c)}{w(\delta U_1)w(\delta U_2)}.$$

Proof. For $i, j \in V$, $i \sim j$, observe that

$$\boldsymbol{\chi}_{U_1}^t \boldsymbol{L}_{i,j} \boldsymbol{\chi}_{U_2} = \begin{cases} -w(i,j), & i \in U_1, j \in U_2 \text{ or } i \in U_2, j \in U_1, \\ 0, & \text{otherwise.} \end{cases}$$

Therefore,

$$\begin{aligned} \langle \boldsymbol{c}_{U_1}, \boldsymbol{c}_{U_2}\rangle &= \langle |U_1|^{-1}\boldsymbol{\Sigma}\boldsymbol{\chi}_{U_1}, |U_2|^{-1}\boldsymbol{\Sigma}\boldsymbol{\chi}_{U_2}\rangle = |U_1|^{-1}|U_2|^{-1}\boldsymbol{\chi}_{U_1}^t \boldsymbol{L}_G \boldsymbol{\chi}_{U_2} \\ &= |U_1|^{-1}|U_2|^{-1}\sum_{i\sim j}\boldsymbol{\chi}_{U_1}^t \boldsymbol{L}_{(i,j)}\boldsymbol{\chi}_{U_2} = |U_1|^{-1}|U_2|^{-1}\sum_{(i,j)\in\delta U_1\cap\delta U_2} -w(i,j), \end{aligned}$$

which proves the first equality. The second is shown similarly by employing Lemma 3.13 and the previous identity:

$$\langle \boldsymbol{a}_{U_1}^+, \boldsymbol{a}_{U_2}^+\rangle = \frac{|U_1^c||U_2^c|}{w(\delta U_1)w(\delta U_2)}\langle \boldsymbol{c}_{U_1^c}, \boldsymbol{c}_{U_2^c}\rangle = -\frac{w(\delta U_1^c \cap \delta U_2^c)}{w(\delta U_1)w(\delta U_2)}.$$ $\boxtimes$

Given the number of—often related and interacting—results in this section, it may be worth providing a brief summary. The important takeaways are that (i) the geometry of the inverse simplex $\mathcal{S}^+$ is intimately related to the effective resistance of the graph (Lemma 3.4) and (ii) the lengths of the altitudes and centroids of $\mathcal{S}$ and $\mathcal{S}^+$ are proportional to the weights of cuts (Equations (3.13), (3.14), Lemmas 3.12, 3.13, 3.14). A less concrete but equally important takeaway is the idea of using

§3.5. Properties of $\widehat{\mathcal{S}}_G$ and $\widehat{\mathcal{S}}_G^+$

Here we study the normalized simplex $\widehat{\mathcal{S}}_G$ of the connected graph $G = (V, E, w)$—which we again fix throughout this section—a somewhat less accessible object than its unnormalized counterpart. The normalized simplex is, roughly speaking, distorted by the weights of the vertices. Consequently, many of the relationships between $\mathcal{S}_G$ and $\mathcal{S}_G^+$ are lost between $\widehat{\mathcal{S}}_G$

and $\widehat{\mathcal{S}}_G^+$. The first issue is that, in general, $\widehat{\mathcal{S}}_G$ and its inverse are not centred at the origin. Indeed, recall that the zero eigenvector $\widehat{\boldsymbol{\varphi}}_n$ of $\widehat{\boldsymbol{L}}_G$ sits in the space $\text{span}(\boldsymbol{W}_G^{1/2}\mathbf{1})$, which is distinct from $\text{span}(\mathbf{1})$ unless $\boldsymbol{W}_G^{1/2} = d\mathbf{I}$ for some d, in which case G is regular. If G is not regular, we thus have that $\boldsymbol{\varphi}_i \in \text{span}(\boldsymbol{W}_G^{1/2}\mathbf{1}) \subseteq \text{span}(\mathbf{1})^\perp$ for all $i < n$ implying that $\langle \boldsymbol{\varphi}_i, \mathbf{1}\rangle \neq 0$. In this case then,

$$\boldsymbol{c}(\widehat{\mathcal{S}}_G) = \frac{1}{n}\widehat{\boldsymbol{\Lambda}}^{1/2}\widehat{\boldsymbol{\Phi}}^t\mathbf{1} = \frac{1}{n}\begin{pmatrix} \sqrt{\lambda_1}\langle \boldsymbol{\varphi}_1, \mathbf{1}\rangle \\ \vdots \\ \sqrt{\lambda_{n-1}}\langle \boldsymbol{\varphi}_{n-1}, \mathbf{1}\rangle \end{pmatrix} \neq \mathbf{0}.$$

The above argument proves the following.

Lemma 3.15. *The centroid of $\widehat{\mathcal{S}}_G$ coincides with the origin of $\mathbb{R}^{n-1}$ iff G is regular.*

Given this, one might wonder whether the origin is even a point in the simplex $\widehat{\mathcal{S}}$. It is easily seen that it is, however. Consider the barycentric coordinate $\mathbf{u} = \sqrt{\boldsymbol{w}}/\left\|\sqrt{\boldsymbol{w}}\right\|_1$, where $\sqrt{\boldsymbol{w}} = (w(1)^{1/2}, \ldots, w(n)^{1/2})$. Since all eigenvectors $\widehat{\boldsymbol{\varphi}}_i$, $i < n$ are orthogonal to $\boldsymbol{\varphi}_n \in \text{span}(\boldsymbol{w}^{1/2})$ it follows that $\mathbf{0} = \widehat{\boldsymbol{\Sigma}}\mathbf{u} \in \widehat{\mathcal{S}}$.

The next set of properties which don't hold between $\widehat{\mathcal{S}}$ and $\widehat{\mathcal{S}}^+$ are the orthogonality relationships present between a simplex and its dual. That is, in general $\widehat{\mathcal{S}}_G^+$ is the not the dual of $\widehat{\mathcal{S}}_G$.

Lemma 3.16. *The inverse simplex $\widehat{\mathcal{S}}_G^+$ is the dual of $\widehat{\mathcal{S}}_G$ iff G is regular.*

Proof. For any $i, j, k \in \mathbb{N}$ write

$$\langle \widehat{\boldsymbol{\sigma}}_i^+, \widehat{\boldsymbol{\sigma}}_j - \widehat{\boldsymbol{\sigma}}_k\rangle = \delta_{ij} - \delta_{ik} + \frac{\sqrt{w(i)w(k)}}{n} - \frac{\sqrt{w(i)w(j)}}{n}. \tag{3.15}$$

First suppose that G is k-regular. Then for $i \neq k$, Equation (3.15) becomes $\langle \widehat{\boldsymbol{\sigma}}_i^+, \widehat{\boldsymbol{\sigma}}_j - \widehat{\boldsymbol{\sigma}}_k\rangle = \delta ij$. Since k was arbitrary, we see that $\{\widehat{\boldsymbol{\sigma}}_i^+\}$ is the sister pair of $\{\widehat{\boldsymbol{\sigma}}_j - \widehat{\boldsymbol{\sigma}}_k\}$. Conversely, suppose G is not regular and let i, k obey $0 \neq w(i) \neq w(k)$. Taking $i = j \neq k$ in (3.15) we see

$$\langle \widehat{\boldsymbol{\sigma}}_i^+, \widehat{\boldsymbol{\sigma}}_i - \widehat{\boldsymbol{\sigma}}_k\rangle = 1 - \frac{\sqrt{w(i)}}{n}(\sqrt{w(k)} - \sqrt{w(i)}) \neq 1,$$

so $\{\widehat{\boldsymbol{\sigma}}_i^+\}$ is not the sister set of $\{\widehat{\boldsymbol{\sigma}}_j - \widehat{\boldsymbol{\sigma}}_k\}$, completing the argument. ⊠

A consequence of the previous Lemma is that we can no longer apply Lemma 2.9 (regarding the orthogonality of $\mathcal{T}_U$ and $\mathcal{T}_{U^c}^*$) to obtain information concerning $\widehat{\mathcal{S}}_U$ and $\widehat{\mathcal{S}}_{U^c}^+$. The following two lemmas and corresponding corollary address the link between these faces, and—rather unfortunately—demonstrate that indeed, they are not orthogonal in general. The first gives sufficient conditions under which the faces are orthogonal, the second provides necessary conditions. Before we state the lemmas, recall from Section 2.3 that a subset of vertices is weight (or degree) homogenous if each vertex in the set has the same weight.

Lemma 3.17. *Let $U_1, U_2 \subseteq V(G)$ be two non-empty, weight homogenous subsets such that $U_1 \cap U_2 = \emptyset$. Then the faces $\widehat{\mathcal{S}}^+[U_1]$ and $\widehat{\mathcal{S}}[U_2]$ are orthogonal.*

Proof. Suppose $w(i) = w_1$ for all $i \in U_1$ and $w(i) = w_2$ for all $i \in U_2$. Let $\boldsymbol{x}_{U_1}$ be the barycentric coordinate of any point in $\widehat{\mathcal{S}}^+[U_1]$ and $\boldsymbol{x}_{U_2}$ that of any point in $\widehat{\mathcal{S}}[U_2]$.

$$\begin{aligned}\langle \widehat{\boldsymbol{\Sigma}}^+\boldsymbol{x}_{U_1}, \widehat{\boldsymbol{\Sigma}}\boldsymbol{x}_{U_2}\rangle &= \boldsymbol{x}_{U_1}^t\left(\mathbf{I} - \frac{\sqrt{\boldsymbol{w}}\sqrt{\boldsymbol{w}}^t}{\mathrm{vol}(G)}\right)\boldsymbol{x}_{U_2} \\ &= \boldsymbol{x}_{U_1}^t\boldsymbol{x}_{U_2} - \frac{1}{\mathrm{vol}(G)}\sum_{i\in U_1}\boldsymbol{x}_{U_1}(i)\sqrt{w(i)}\sum_{j\in U_2}\boldsymbol{x}_{U_2}(j)\sqrt{w(j)} \\ &= -\frac{1}{\mathrm{vol}(G)}\sqrt{w_1w_2}\sum_{i\in U_1}\boldsymbol{x}_{U_1}(i)\sum_{j\in U_2}\boldsymbol{x}_{U_2}(j) = -\frac{\sqrt{w_1w_2}}{\mathrm{vol}(G)},\end{aligned}$$

where the second equality is due to fact that $U_1 \cap U_2 = \emptyset$. This demonstrates that $\langle \widehat{\boldsymbol{\Sigma}}^+\boldsymbol{x}_{U_1}, \boldsymbol{p} - \boldsymbol{q}\rangle = 0$ for any $\boldsymbol{p}, \boldsymbol{q} \in \widehat{\mathcal{S}}[U_2]$, completing the proof. ⊠

LEMMA 3.18. *Suppose $U_1 \subseteq V(G)$ is not degree homogeneous. Then for all $U_2 \subseteq V(G)$ then faces $\widehat{\mathcal{S}}[U_1]$ (resp., $\widehat{\mathcal{S}}^+[U_1]$) and $\widehat{\mathcal{S}}^+[U_2]$ (resp., $\widehat{\mathcal{S}}[U_2]$) are not orthogonal.*

Proof. We show that $\widehat{\mathcal{S}}[U_1]$ and $\widehat{\mathcal{S}}^+[U_2]$ are not orthogonal; the other case is nearly identical. Let $i, j \in U_1$ be such that $w(i) \neq w(j)$ and consider the points $\boldsymbol{p} = \widehat{\boldsymbol{\Sigma}}\boldsymbol{\chi}_i, \boldsymbol{q} = \widehat{\boldsymbol{\Sigma}}\boldsymbol{\chi}_j \in \widehat{\mathcal{S}}[U_1]$. For any $\widehat{\boldsymbol{\Sigma}}^+\boldsymbol{x} \in \widehat{\mathcal{S}}^+[U_2]$, performing the usual arithmetic yields

$$\langle \widehat{\boldsymbol{\Sigma}}^+\boldsymbol{x}, \boldsymbol{p} - \boldsymbol{q}\rangle = \frac{1}{\mathrm{vol}(G)}\sum_{k\in U_2}\sqrt{w(k)}x(k)(\sqrt{w(j)} - \sqrt{w(j)}) \neq 0. \quad ⊠$$

We state a consequence of Lemmas 3.17 and 3.18 which exemplifies a clear contrast between the combinatorial simplices and the normalized simplices.

COROLLARY 3.2. *The vertex $\widehat{\boldsymbol{\sigma}}_i^+$ (resp., $\widehat{\boldsymbol{\sigma}}_i$) is orthogonal to $\widehat{\mathcal{S}}_{\{i\}^c}$ (resp., $\widehat{\mathcal{S}}^+_{\{i\}^c}$) iff $G[\{i\}^c] = G[V \setminus \{i\}]$ is regular.*

Proof. If $G[\{i\}^c]$ is regular then $\{i\}^c$ is weight homogenous. By Lemma 3.17 $\widehat{\mathcal{S}}[\{i\}] = \widehat{\boldsymbol{\sigma}}_i$ (resp., $\widehat{\mathcal{S}}^+[\{i\}] = \widehat{\boldsymbol{\sigma}}_i^+$) is orthogonal to $\widehat{\mathcal{S}}[\{i\}^c]$ (resp., $\widehat{\mathcal{S}}^+[\{i\}^c]$). (Note that the singleton $\{i\}$ is clearly degree homogeneous.) Conversely, if $G[\{i\}^c]$ is not regular then by Lemma 3.18 $\widehat{\boldsymbol{\sigma}}_i$ (resp., $\widehat{\boldsymbol{\sigma}}_i^+$) is not orthogonal to $\widehat{\mathcal{S}}[\{i\}^c]$ (resp., $\widehat{\mathcal{S}}^+[\{i\}^c]$). ⊠

Centroids and altitudes. Let us attempt to parallel the arguments given in Section 3.4 concerning the centroids and altitudes of $\mathcal{S}_G$ and $\mathcal{S}_G^+$. For the normalized Laplacian we have

$$\begin{aligned}\widehat{\mathcal{L}}(\boldsymbol{\chi}_U) &= \sum_{i\sim j} w(i,j)\left(\frac{\boldsymbol{\chi}_U(i)}{\sqrt{w(i)}} - \frac{\boldsymbol{\chi}_U(j)}{\sqrt{w(j)}}\right)^2 \\ &= \sum_{i\in U, j\in U^c} w(i,j)\left(\frac{\boldsymbol{\chi}_U(i)}{\sqrt{w(i)}} - \frac{\boldsymbol{\chi}_U(j)}{\sqrt{w(j)}}\right)^2 \\ &= \sum_{i\in U, j\in U^c} w(i,j)\frac{\boldsymbol{\chi}_U(i)}{w(i)}\end{aligned}$$

$$= \sum_{i\in U} \frac{1}{w(i)} \sum_{j\in\delta(i)\cap U^c} w(i,j)$$
$$= \sum_{i\in U} \frac{w_{G[i+U^c]}(i)}{w(i)}, \tag{3.16}$$

where we've used the shorthand $i + U^c = \{i\} \cup U^c$ and we recall that $G[I]$ is the graph restricted to the vertices in I. To interpret the above quantity, we might define

$$\gamma(i, B) \stackrel{\text{def}}{=} \frac{w_{G[i+B^c]}(i)}{w(i)},$$

as the *fractional weight of i in B*. Further defining $\gamma(A, B)$ as the *total fractional weight from A to B*:

$$\gamma(A, B) \stackrel{\text{def}}{=} \sum_{i\in A} \gamma(i, B),$$

we have

$$\widehat{\mathcal{L}}(\boldsymbol{\chi}_U) = \gamma(U, U^c),$$

and so the length of the centroid $c(\widehat{\mathcal{S}}_U)$ captures the total fraction of weight between U and U^c:

$$\left\| c(\widehat{\mathcal{S}}_U) \right\|_2^2 = \frac{1}{|U|^2} \langle \widehat{\mathbf{\Sigma}} \chi_U, \widehat{\mathbf{\Sigma}} \chi_U \rangle = \frac{1}{|U|^2} \widehat{\mathcal{L}}(\chi_U) = \frac{1}{|U|^2} \gamma(U, U^c), \tag{3.17}$$

which is the equivalent to Equation 3.13 for the normalized simplex. Performing a similar computation for $\boldsymbol{c}(\widehat{\mathcal{S}}_U^+)$ doesn't seem to yield anything overly insightful:

$$\left\| \boldsymbol{c}(\widehat{\mathcal{S}}_U^+) \right\|_2^2 = \frac{1}{|U|^2} \widehat{\mathcal{L}}^+(\boldsymbol{\chi}_U),$$

except perhaps to demonstrate that $\widehat{\mathcal{L}}^+(\boldsymbol{\chi}_U) \geq 0$ for all $U \subseteq V$.

Alternate descriptions and duals. As we did for the combinatorial simplices, we now try to formulate a hyperplane representation of the normalized simplices. As the reader will see, however, this is difficult due to the influence of the graph weights on their geometry. We begin with a lemma which is roughly the equivalent of Lemma 3.8 for the normalized simplex.

Lemma 3.19. *Let $U \subseteq V$ be non-empty and $F \subseteq U^c$. Setting*

$$\beta_i^S = \sqrt{w(i)} \frac{\max_{j\in S} \sqrt{w(j)}}{\text{vol}(G)},$$

for any set S, we have

$$\widehat{\mathcal{S}}_U \subseteq \widehat{\mathcal{H}}_F^{\geq} \stackrel{\text{def}}{=} \left\{ \boldsymbol{x} \in \mathbb{R}^{n-1} : \sum_{i\in F} (\langle \boldsymbol{x}, \widehat{\boldsymbol{\sigma}}_i^+ \rangle + \beta_i^{F^c}) \geq 0 \right\}.$$

Similarly,

$$\widehat{\mathcal{S}}_U^+ \subseteq (\widehat{\mathcal{H}}_F^+)^{\geq} \overset{def}{=} \left\{ \boldsymbol{x} \in \mathbb{R}^{n-1} : \sum_{i\in F}(\langle \boldsymbol{x}, \widehat{\boldsymbol{\sigma}}_i\rangle + \beta_i^{F^c}) \geq 0 \right\}.$$

Proof. Let $\boldsymbol{x} = \widehat{\boldsymbol{\Sigma}}\boldsymbol{y} \in \widehat{\mathcal{S}}_U$, where $\boldsymbol{y}$ is a barycentric coordinate with $\boldsymbol{y}(U^c) = \boldsymbol{0}$. For $i \in U^c$,

$$\langle \widehat{\boldsymbol{\Sigma}}\boldsymbol{y}, \widehat{\boldsymbol{\sigma}}_i^+\rangle = \boldsymbol{y}^t\widehat{\boldsymbol{\Sigma}}^t\widehat{\boldsymbol{\Sigma}}^+\boldsymbol{\chi}_i = \boldsymbol{y}^t\left(\mathbf{I} - \frac{\sqrt{\boldsymbol{w}}\sqrt{\boldsymbol{w}}^t}{\mathrm{vol}(G)}\right)\boldsymbol{\chi}_i = -\frac{1}{\mathrm{vol}(G)}\left(\sum_{j\in U} y(j)\sqrt{w(j)}\right)\sqrt{w(i)}.$$

Since $\|\boldsymbol{y}\|_1 = 1$, and $F^c \supseteq U$ (since $F \subseteq U^c$) it follows that

$$\sum_{j\in U} y(i)\sqrt{w(j)} \leq \max_{j\in U}\sqrt{w(j)} \leq \max_{j\in F^c}\sqrt{w(j)},$$

hence

$$\langle \widehat{\boldsymbol{\Sigma}}\boldsymbol{y}, \widehat{\boldsymbol{\sigma}}_i^+\rangle \geq -\frac{\sqrt{w(i)}}{\mathrm{vol}(G)}\max_{j\in F^c}\sqrt{\boldsymbol{w}(j)} = -\beta_i^{F^c}.$$

Consequently, $\sum_{i\in F}(\langle \boldsymbol{x}, \widehat{\boldsymbol{\sigma}}_i^+\rangle + \beta_i^{F_c}) \geq \sum_{i\in F^c}(-\beta_i^{F^c} + \beta_i^{F^c}) = 0$, so indeed $\boldsymbol{x} \in \widehat{\mathcal{H}}_F$. The proof for the $\widehat{\mathcal{S}}_G^+$ and $\widehat{\mathcal{H}}_F^+$ is almost identical. ☒

We might expect that Lemma 3.19 yields a hyperplane representation of the normalized simplex, as did Lemma 3.8 for the combinatorial simplex. Unfortunately however, the issue is once again complicated by the vertex weights and the relation between $\widehat{\boldsymbol{\Sigma}}^+$ and $\widehat{\boldsymbol{\Sigma}}$. Let us illustrate the problem by focusing on $\widehat{\mathcal{S}}$.

As opposed to Section 3.4, $\widehat{\mathcal{S}}_{\{i\}^c}$ is not contained in the hyperplane $\widehat{\mathcal{H}}_i = \{\boldsymbol{x} : \langle \boldsymbol{x}, \widehat{\boldsymbol{\sigma}}_i^+\rangle + \beta_i = 0\}$, where we take $\beta_i = \beta_i^{\{i\}^c} = \sqrt{w(i)}\max_{j\neq i}\sqrt{w(j)}/\mathrm{vol}(G)$. To see this, take any $k \notin \mathrm{argmax}_{j\neq i}\sqrt{w(j)}$ (such a k exists iff the graph is not regular) and note that while $\boldsymbol{\sigma}_k \in \widehat{\mathcal{S}}_U$ it is not in $\widehat{\mathcal{H}}_i$:

$$\langle \boldsymbol{\sigma}_k, \boldsymbol{\sigma}_i^+\rangle = \boldsymbol{\chi}_k\widehat{\boldsymbol{\Sigma}}^t\widehat{\boldsymbol{\Sigma}}^+\boldsymbol{\chi}_i = -\frac{\sqrt{w(k)w(i)}}{\mathrm{vol}(G)} \neq \beta_i,$$

by assumption. The other way to see this is to note that $\widehat{\boldsymbol{\sigma}}_i^+$ is not perpendicular to $\mathcal{S}_{\{i\}^c}$ in general by Corollary 3.2. Thus, it is not clear how to generate an analogous description to Equation (3.6) for the normalized simplex. While this may seem relatively inconsequential, it severely complicates finding the dual of $\widehat{\mathcal{S}}_G$, which is the question we turn to next.

What is $\widehat{\mathcal{S}}_G^*$? Given that $\widehat{\mathcal{S}}_G^+$ is not the dual of $\widehat{\mathcal{S}}_G$ in general, it seems appropriate to ask "what on earth *is* the dual of the normalized simplex?". Somewhat surprisingly, this question is intimately related to the hyperplane representation—or lack thereof—of $\widehat{\mathcal{S}}_G$.

We can obtain an implicit representation for the dual vertices $\{\widehat{\boldsymbol{\sigma}}_i^*\}$ by noting that they must satisfy $\langle \widehat{\boldsymbol{\sigma}}_i^*, \widehat{\boldsymbol{\sigma}}_j - \widehat{\boldsymbol{\sigma}}_n \rangle = \delta_{ij}$ for all $i, j \neq n$. This translates to

$$\sum_{\ell=1}^{n} \widehat{\boldsymbol{\sigma}}_i^*(\ell)(\widehat{\varphi}_k(j) - \widehat{\varphi}_k(n))\widehat{\lambda}_k^{1/2} = \delta_{ij},$$

but extracting values of $\widehat{\boldsymbol{\sigma}}_i^*$ which meet this condition is not trivial. We might, however, try a different tactic. Note that in the case of the combinatorial simplices, the dual vertices are encoded in their hyperplane representation by Equation (3.6): $\mathcal{S}_G = \bigcap_i \{\boldsymbol{x} : \langle \boldsymbol{x}, \boldsymbol{\sigma}_i^+ \rangle \geq -1/n\}$. It is thus natural to wonder whether this relationship holds for every simplex, that is, if given a simplex described as the intersection of haldspaces, say $\mathcal{T} = \bigcap_i \{\boldsymbol{x} : \langle \boldsymbol{z}_i, \boldsymbol{x} \rangle \geq b_i\}$ are the vectors $\boldsymbol{z}_i$ are parallel to the dual vertices of $\mathcal{T}$. The following lemma gives gives sufficient conditions as to when this is the case.

Lemma 3.20. *Let $\mathcal{T} \subseteq \mathbb{R}^{n-1}$ be a centred simplex with $\mathcal{T} = \bigcap_{i=1}^n \{\boldsymbol{x} \in \mathbb{R}^{n-1} : \langle \boldsymbol{x}, \boldsymbol{z}_i \rangle \geq \alpha_i\}$. Then $\{-\boldsymbol{z}_i/(\alpha_i n)\}$ are the vertices of $\mathcal{T}^D$.*

Proof. As usual, let $\{\boldsymbol{\sigma}_i\}$ be the vertices of $\mathcal{T}$. Put $\boldsymbol{\gamma}_i = -\boldsymbol{z}_i/(\alpha_i n)$. We need to show that $\{\boldsymbol{\gamma}_i\}_{i=1}^{n-1}$ is the sister basis to $\{\boldsymbol{\sigma}_i - \boldsymbol{\sigma}_n\}_{i=1}^{n-1}$. Let H_i be the boundary of the halfspace $\{\boldsymbol{x} : \langle \boldsymbol{x}, \boldsymbol{z}_i \rangle \geq \alpha_i\}$, so $H_i = \{\boldsymbol{x} : \langle \boldsymbol{x}, \boldsymbol{z}_i \rangle = \alpha_i\}$. Enumerate the vertices $\{\boldsymbol{\sigma}_i\}$ such that $\mathcal{S}_{\{i\}^c} \subseteq H_i$. Fix $i \in [n-1]$. We claim that

$$\boldsymbol{\sigma}_i \in \bigcap_{j \neq i} H_i.$$

Indeed, $\mathcal{S}_{\{j\}^c}$ is the $n-1$ dimensional simplex with vertices $\{\boldsymbol{\sigma}_\ell\}_{\ell \neq j}$. Hence $\boldsymbol{\sigma}_i \in \mathcal{S}_{\{j\}^c}$ for all $j \neq i$ and thus also lies in $\cap_{j \neq i} H_j$. Therefore, $\langle \boldsymbol{\sigma}_i, \boldsymbol{z}_j \rangle = \alpha_j$ for all $j \neq i$, from which it follows that $\langle \boldsymbol{\gamma}_j, \boldsymbol{\sigma}_i - \boldsymbol{\sigma}_n \rangle = -\langle \boldsymbol{z}_j, \boldsymbol{\sigma}_i \rangle/(\alpha_j n) + \langle \boldsymbol{z}_j, \boldsymbol{\sigma}_n \rangle/(\alpha_j n) = 1/n - 1/n = 0$. It remains to show that $\langle \boldsymbol{\gamma}_i, \boldsymbol{\sigma}_i - \boldsymbol{\sigma}_n \rangle = 1$ for all $i \neq n$. Since $\mathcal{T}$ is centred by assumption, we have $\boldsymbol{\sigma}_i = -\sum_{j \neq i} \boldsymbol{\sigma}_j$. Consequently,

$$\langle \boldsymbol{\gamma}_i, \boldsymbol{\sigma}_i - \boldsymbol{\sigma}_n \rangle = -\sum_{j \neq i} \langle \boldsymbol{\gamma}_i, \boldsymbol{\sigma}_j \rangle - \langle \boldsymbol{\gamma}_i, \boldsymbol{\sigma}_n \rangle = \frac{1}{n}(n-1) + \frac{1}{n} = 1,$$

as was to be shown. ⊠

Lemma 3.20 allows us to extract the dual given a hyperplane description of a centred simplex. The next natural question is then how the hyperplane description of an arbitrary simplex relates to the hyperplane description of its centred counterpart. This is answered by the following lemma.

Lemma 3.21. *Let $\mathcal{T} = \cap_i \{\boldsymbol{x} : \langle \boldsymbol{x}, \boldsymbol{z}_i \rangle \geq \alpha_i\}$ be a simplex. Its centred version, $\mathcal{T}_0$, can be written as $\cap_i \{\boldsymbol{x} : \langle \boldsymbol{x}, \boldsymbol{z}_i \rangle \geq \alpha_i - \langle \boldsymbol{c}(\mathcal{T}), \boldsymbol{z}_i \rangle\}$.*

Proof. As usual, take $\mathcal{H}_i = \{\boldsymbol{x} : \langle \boldsymbol{x}, \boldsymbol{z}_i \rangle = \alpha_i\}$ to be the hyperplanes bounding the simplex. The hyperplanes bounding the centred simplex, are parallel to the hyperplanes $\mathcal{H}_i$ and can thus be written as

$$\mathcal{H}_{i0} = \{\boldsymbol{x} : \langle \boldsymbol{x}, \boldsymbol{z}_i \rangle = \beta_i\},$$

for some β_i. Moreover, just as $\boldsymbol{\sigma}_j \in \mathcal{H}_i$ for $j \neq i$, we have $\boldsymbol{\sigma}_j - \boldsymbol{c}(\mathcal{T}) \in \mathcal{H}_{i0}$, since $\{\boldsymbol{\sigma}_j - \boldsymbol{c}(\mathcal{T})\}$ are the vertices of $\mathcal{T}_0$. As such, $\langle \boldsymbol{\sigma}_j - \boldsymbol{c}(\mathcal{T}), \boldsymbol{z}_i\rangle = \beta_i$, and

$$\langle \boldsymbol{\sigma}_j - \boldsymbol{c}(\mathcal{T}), \boldsymbol{z}_i\rangle = \langle \boldsymbol{\sigma}_j, \boldsymbol{z}_i\rangle - \langle \boldsymbol{c}(\mathcal{T}), \boldsymbol{z}_i\rangle = \alpha_i - \langle \boldsymbol{c}(\mathcal{T}), \boldsymbol{z}_i\rangle,$$

whence $\beta_i = \alpha_i - \langle \boldsymbol{c}(\mathcal{T}), \boldsymbol{z}_i\rangle$. It then follows that

$$\mathcal{T}_0 = \bigcap_i \mathcal{H}_{i0}^{\geq},$$

where $\mathcal{H}_{i0}^{\geq} = \{\boldsymbol{x} : \langle \boldsymbol{x}, \boldsymbol{z}_i\rangle \geq \alpha_i - \langle \boldsymbol{c}(\mathcal{T}), \boldsymbol{z}_i\rangle\}$. ⊠

Taken together, Lemmas 3.20 and 3.21 provide a path to try and determine the dual simplex of $\widehat{\mathcal{S}}_G$. In particular, if we could determine a hyperplane representation of any simplex congruent to $\widehat{\mathcal{S}}_G$, then we can obtain a hyperplane representation of its centred version by Lemma 3.21 and to the dual of its centred version by Lemma 3.20. Since the dual is common to all congruent simplices by Observation 2.3, this would yield $\mathcal{S}_G^*$. The trick is simply to determine a hyperplane representation of $\mathcal{S}_G$—which we leave as an exercise for the reader. Just kidding.

Not worth fleshing out until we have more content for this section.

Noting that

$$\boldsymbol{c}(\widehat{\mathcal{S}}) = \frac{1}{n}\bigg(\sum_{\ell=1}^n \widehat{\boldsymbol{\sigma}}_\ell(1), \dots, \sum_{\ell=1}^n \widehat{\boldsymbol{\sigma}}_\ell(n)\bigg)^t,$$

we see that the vertices of $\widehat{\mathcal{S}}_0$ have coordinates

$$\widehat{\boldsymbol{\sigma}}_i(j) - \boldsymbol{c}(\widehat{\mathcal{S}})(j) = \widehat{\boldsymbol{\varphi}}_j(i)\widehat{\lambda}_j^{1/2} - \frac{1}{n}\sum_{\ell=1}^n \widehat{\boldsymbol{\varphi}}_j(\ell)\widehat{\lambda}_j^{1/2} = \widehat{\lambda}_j^{1/2}\bigg(\widehat{\boldsymbol{\varphi}}_j(i) - \frac{1}{n}\langle \widehat{\boldsymbol{\varphi}}_j, \mathbf{1}\rangle\bigg).$$

Likewise, the vertices of $\widehat{\mathcal{S}}_0^+$ have coordinates

$$\widehat{\boldsymbol{\sigma}}_i^+(j) = \widehat{\lambda}_j^{-1/2}\bigg(\widehat{\boldsymbol{\varphi}}_j(i) - \frac{1}{n}\langle \widehat{\boldsymbol{\varphi}}_j, \mathbf{1}\rangle\bigg).$$

Let $\boldsymbol{c}$ be the centroid of the centred normalized Laplacian. Noting that $(\boldsymbol{c}, \boldsymbol{c}, \dots, \boldsymbol{c}) = \boldsymbol{c}\mathbf{1}^t$, the Gram Matrix of $\widehat{\mathcal{S}}_0$ is

$$\begin{aligned}(\widehat{\boldsymbol{\Sigma}} - \boldsymbol{c}\mathbf{1}^t)^t(\widehat{\boldsymbol{\Sigma}} - \boldsymbol{c}\mathbf{1}^t) &= \widehat{\boldsymbol{\Sigma}}^t\widehat{\boldsymbol{\Sigma}} - \widehat{\boldsymbol{\Sigma}}^t\boldsymbol{c}\mathbf{1}^t - \mathbf{1}\boldsymbol{c}^t\widehat{\boldsymbol{\Sigma}} + \mathbf{1}\boldsymbol{c}^t\boldsymbol{c}\mathbf{1}^t \\ &= \widehat{\boldsymbol{L}}_G - \frac{1}{n}\widehat{\boldsymbol{\Sigma}}^t\widehat{\boldsymbol{\Sigma}}\mathbf{1}\mathbf{1}^t - \frac{1}{n}\mathbf{1}\mathbf{1}^t\widehat{\boldsymbol{\Sigma}}^t\widehat{\boldsymbol{\Sigma}} + \frac{1}{n^2}\widehat{\boldsymbol{\Sigma}}^t\widehat{\boldsymbol{\Sigma}}\mathbf{1}\mathbf{1}^t \\ &= \widehat{\boldsymbol{L}}_G - \frac{1}{n}\widehat{\boldsymbol{L}}_G\mathbf{J} - \frac{1}{n}\mathbf{J}\widehat{\boldsymbol{L}}_G + \frac{1}{n^2}\mathbf{J}\widehat{\boldsymbol{L}}_G\mathbf{J}.\end{aligned}$$

What are the properties of this matrix? It has an eigenvector of $\mathbf{1}$ with eigenvalue 0, but it does not seem to be a Laplacian.

Chapter 4

Further Properties of the Correspondence

The previous chapter introduced the graph-simplex correspondence and devoted several sections to the basic properties of the simplices associated to a given graph. In this chapter we continue the study of the correspondence and present several of its more significant and advanced properties.

§4.1. Block Matrix Equations

In this section we present matrix equations pertaining to both hyperacute simplices and the effective resistance of graphs. The equations appeal to the relationship between hyperacute simplices and graphs by using well known results from the literature on electrical networks and effective resistance. The goal of this section is to demonstrate to the reader the utility of the graph-simplex correspondence in generating statements about hyperacute simplices by hijacking our knowledge of graph theory, and vice versa.

We begin with a block matrix equation describing some aspects of the geometry between a hyperacute simplex and its dual. It is closely related to an equation given by Fiedler in Theorem 1.4.1 in [Fie11]. Instead of a direct proof, we use the results of Van Mieghem *et al.* [VMDC17] and prove it by leveraging aspects of the effective resistance of a graph.

Let a centred, hyperacute simplex $\mathcal{T}$ be given. Let $\bar{d}$ be the average squared distance between all the vertices of $\mathcal{T}$, that is

$$\bar{d} \overset{\text{def}}{=} \frac{1}{n^2} \sum_{i \leq j} \left\| \boldsymbol{\gamma}_i - \boldsymbol{\gamma}_j^+ \right\|_2^2. \tag{4.1}$$

Let $\xi(i)$ give the average squared distance of vertex i from other vertices minus the total average distance,

$$\xi(i) \overset{\text{def}}{=} \frac{1}{n} \sum_{j} \left\| \boldsymbol{\gamma}_i^+ - \boldsymbol{\gamma}_j^+ \right\|_2^2 - \bar{d}, \tag{4.2}$$

and put $\boldsymbol{\xi} = (\xi(1), \ldots, \xi(n))$. Then we have the following result.

Lemma 4.1. *Let $\mathcal{T} \subseteq \mathbb{R}^{n-1}$ be a hyperacute simplex with squared distance matrix $\boldsymbol{D}$, and average squared distance vector $\boldsymbol{\xi}$. Denote by $\boldsymbol{\Gamma}$ the vertex matrix of the dual simplex to $\mathcal{T}$.*

Then,

$$-\frac{1}{2}\begin{pmatrix} 0 & \mathbf{1}_n^t \\ \mathbf{1}_n & \boldsymbol{D}\end{pmatrix} = \begin{pmatrix} \boldsymbol{\xi}^t\boldsymbol{\Gamma}^t\boldsymbol{\Gamma}\boldsymbol{\xi}+4\bar{d} & -(\boldsymbol{\Gamma}^t\boldsymbol{\Gamma}\boldsymbol{\xi}+2\mathbf{1}/n)^t \\ -(\boldsymbol{\Gamma}^t\boldsymbol{\Gamma}\boldsymbol{\xi}+2\mathbf{1}/n) & \boldsymbol{\Gamma}^t\boldsymbol{\Gamma}\end{pmatrix}^{-1}. \tag{4.3}$$

Moreover, the vertices of the dual simplex to $\mathcal{S}$ and the distance matrix of $\mathcal{S}$ are related by the equation

$$\boldsymbol{\Gamma}^t\boldsymbol{\Gamma}\boldsymbol{D}\boldsymbol{\Gamma}^t\boldsymbol{\Gamma} = -2\boldsymbol{\Gamma}^t\boldsymbol{\Gamma}, \tag{4.4}$$

and in the space $\mathrm{span}(\mathbf{1})^\perp$ *it holds that*

$$\boldsymbol{D}\boldsymbol{\Gamma}^t\boldsymbol{\Gamma}\boldsymbol{D} = -2\boldsymbol{D}.$$

Proof. As above, $\mathcal{S}$ is the inverse simplex of some graph G, and therefore, $\boldsymbol{D}=\boldsymbol{R}$, where $\boldsymbol{R}$ is the effective resistance matrix. Therefore, we can rewrite $\xi(i)$ as

$$\frac{1}{n}\sum_j r^{\mathrm{eff}}(i,j) - \frac{1}{n^2}\sum_{i<j} r^{\mathrm{eff}}(i,j),$$

and $\boldsymbol{\xi}$ as

$$\boldsymbol{\xi} = \frac{1}{n}\boldsymbol{R}\mathbf{1} - \frac{1}{n^2}\mathbf{1}\mathbf{1}^t\boldsymbol{R}\mathbf{1} = \frac{1}{n}\boldsymbol{R}\mathbf{1} - \frac{1}{n^2}\mathbf{J}\boldsymbol{R}\mathbf{1}.$$

Meanwhile, the dual simplex to $\mathcal{S}$ is the simplex of the graph G, and hence obeys $\boldsymbol{\Gamma}^t\boldsymbol{\Gamma}=\boldsymbol{L}_G$. Consequently, letting $\mathbf{u}=\frac{1}{n}\boldsymbol{R}\mathbf{1}-\frac{1}{n^2}\mathbf{J}\boldsymbol{R}\mathbf{1}$, we can rewrite Equation 4.3 as the purely graph theoretic statement

$$-\frac{1}{2}\begin{pmatrix} 0 & \mathbf{1}_n^t \\ \mathbf{1}_n & \boldsymbol{R}\end{pmatrix} = \begin{pmatrix} \mathbf{u}^t\boldsymbol{L}_G\mathbf{u}+\frac{4}{n^2}R & -(\boldsymbol{L}_G\mathbf{u}+\frac{2}{n}\mathbf{1})^t \\ -(\boldsymbol{L}_G\mathbf{u}+\frac{2}{n}\mathbf{1}) & \boldsymbol{L}_G\end{pmatrix}^{-1}.$$

where $R=\sum_{i<j} r^{\mathrm{eff}}(i,j)$ is the total effective resistance in the graph. The above equality was proved by Van Mieghem *et al.* [VMDC17], and in a more general form by Fiedler [Fie93, Fie11], but we prove it here for completeness. Multiplying out the left hand side, the top left-hand corner of the resulting block matrix is

$$-\frac{1}{2}(\mathbf{1}^t\boldsymbol{L}_G - \frac{2}{n}\mathbf{1}^t\mathbf{1}) = 1,$$

since $\mathbf{1}^t\boldsymbol{L}_G=\mathbf{1}^t\boldsymbol{L}_G^t=\mathbf{0}$. Likewise the top-right hand corner is $\mathbf{0}$. The bottom left-hand corner is

$$-\frac{1}{2}\bigg(\mathbf{1}\boldsymbol{\xi}^t\boldsymbol{L}_G\boldsymbol{\xi}+\frac{4}{n^2}R\mathbf{1}-\boldsymbol{R}\boldsymbol{L}_G\boldsymbol{\xi}-\frac{2}{n}\boldsymbol{R}\mathbf{1}\bigg), \tag{4.5}$$

where, using that $\boldsymbol{R}=\boldsymbol{\xi}\mathbf{1}^t+\mathbf{1}\boldsymbol{\xi}^t-2\boldsymbol{L}_G^+$ and $\mathbf{1}^t\boldsymbol{L}_G=\mathbf{0}$,

$$\boldsymbol{R}\boldsymbol{L}_G = \mathbf{1}\boldsymbol{\xi}^t\boldsymbol{L}_G - 2\bigg(\mathbf{I}-\frac{1}{n}\mathbf{J}\bigg). \tag{4.6}$$

Equation (4.5) thus becomes

$$\begin{aligned}\frac{1}{n}\boldsymbol{R}\mathbf{1}-\frac{2}{n^2}R\mathbf{1}-\left(\mathbf{I}-\frac{1}{n}\mathbf{J}\right)\boldsymbol{\xi} &= \frac{1}{n}\boldsymbol{R}\mathbf{1}-\frac{2}{n^2}R\mathbf{1}-\left(\mathbf{I}-\frac{1}{n}\mathbf{J}\right)\left(\frac{1}{n}\boldsymbol{R}\mathbf{1}-\frac{1}{n^2}\mathbf{J}\boldsymbol{R}\mathbf{1}\right)\\ &= -\frac{2}{n^2}R\mathbf{1}+\frac{1}{n^2}\boldsymbol{R}\mathbf{1}+\frac{1}{n^2}\mathbf{J}\boldsymbol{R}\mathbf{1}-\frac{1}{n^3}\mathbf{J}^2\boldsymbol{R}\mathbf{1}\\ &= -\frac{2}{n^2}R\mathbf{1}+\frac{1}{n^2}\mathbf{J}\boldsymbol{R}\mathbf{1}=\mathbf{0},\end{aligned}$$

using that $\mathbf{J}^2=n\mathbf{J}$, $R=\frac{1}{2}\mathbf{1}^t\boldsymbol{R}\mathbf{1}$, and $\mathbf{J}\boldsymbol{R}\mathbf{1}=\mathbf{1}(\mathbf{1}^t\boldsymbol{R}\mathbf{1})=\mathbf{1}R$. Finally, again using (4.6), the bottom right-hand side is

$$\frac{1}{2}\mathbf{1}\boldsymbol{\xi}^t\boldsymbol{L}_G+\frac{1}{n}\mathbf{1}\mathbf{1}^t-\frac{1}{2}\boldsymbol{R}\boldsymbol{L}_G=\frac{1}{n}\mathbf{J}+\left(\mathbf{I}-\frac{1}{n}\mathbf{J}\right)=\mathbf{I}.$$

This demonstrates that (4.5) holds. We now show that $\boldsymbol{L}_G\boldsymbol{R}\boldsymbol{L}_G=-2\boldsymbol{L}_G$ and that $\boldsymbol{R}\boldsymbol{L}_G\boldsymbol{R}\boldsymbol{x}=-2\boldsymbol{R}\boldsymbol{x}$ for all $\boldsymbol{x}\in\operatorname{span}(\mathbf{1})^\perp$, which will complete the proof. Applying Equation (4.6) we have

$$\boldsymbol{L}_G\boldsymbol{R}\boldsymbol{L}_G=\boldsymbol{L}_G\mathbf{1}\boldsymbol{\xi}^t\boldsymbol{L}_G=-2\boldsymbol{L}_G+\frac{2}{n}\boldsymbol{L}_G\mathbf{1}\mathbf{1}^t=-2\boldsymbol{L}_G.$$

In the same way as (4.6) was derived, we see that

$$\boldsymbol{L}_G\boldsymbol{R}=\boldsymbol{L}_G\boldsymbol{\xi}\mathbf{1}^t-2\left(\mathbf{I}-\frac{1}{n}\mathbf{J}\right),$$

and so

$$\boldsymbol{R}\boldsymbol{L}_G\boldsymbol{R}=\left(\boldsymbol{R}\boldsymbol{L}_G\boldsymbol{\xi}^t+\frac{2}{n}\mathbf{1}\right)\mathbf{1}^t-2\boldsymbol{R},$$

as desired. ⊠

Putting aside simplex geometry for the moment, it is worth meditating on the significance of Equation (4.3) as applied to electrical networks. As demonstrated in [VMDC17], the result translates into the matrix equation

$$-\frac{1}{2}\begin{pmatrix}0 & \mathbf{1}^t\\ \mathbf{1} & \boldsymbol{R}\end{pmatrix}=\begin{pmatrix}\mathbf{u}^t\boldsymbol{L}_G\mathbf{u}+4R_G/n^2 & -(\boldsymbol{L}_G\mathbf{u}+\frac{2}{n}\mathbf{1})^t\\ -(\boldsymbol{L}_G\mathbf{u}+\frac{2}{n}\mathbf{1}) & \boldsymbol{L}_G\end{pmatrix}^{-1}, \tag{4.7}$$

where $\mathbf{u}=\operatorname{diag}(\boldsymbol{L}_G^+(i,i))$, which is interesting in its own right. Taken together, Equations (4.11) and (4.7) allow us to translate between knowledge of the effective resistance of a graph, and the underlying geometry of its simplex. For example, we can relate the volume of the simplex to the effective resistances in the graph. To see this, we need to introduce a particular object from the field of distance geometry. Let $\boldsymbol{D}(\mathcal{X})$ be the distance matrix of a set $\mathcal{X}$ of d points. The matrix

$$\begin{pmatrix}0 & \mathbf{1}^t\\ \mathbf{1} & \boldsymbol{D}(\mathcal{X})\end{pmatrix}\in\mathbb{R}^{(d+1)\times(d+1)}, \tag{4.8}$$

is called the *Menger matrix of* X, the determinant of which is called the *Cayley-Menger determinant*, named after Arthur Cayley and Karl Menger [Cay41, Men28]. The Cayley-

Menger determinant is related to the volume of the underlying set of points as follows.

Lemma 4.2 ([Men31]). *Let $\boldsymbol{D}(\mathcal{X})$ be the distance matrix of a set $\mathcal{X}$ of d points. The $d-1$ dimensional volume*[1] *of the convex hull of $\mathcal{X}$ is proportional to the root of the determinant of the Menger matrix:*

$$\mathrm{vol}(\mathrm{conv}(\mathcal{X}))^2 = \frac{(-1)^d}{((d-1)!)^2 2^{d-1}} \det \begin{pmatrix} 0 & \boldsymbol{1}^t \\ \boldsymbol{1} & \boldsymbol{D}(\mathcal{X}) \end{pmatrix}.$$

The relation between the Menger matrix and the volume combined with the matrix equations above, allows us to give a concise formula for the volume of any hyperacute simplex. This was first pointed out in [VMDC17].

Lemma 4.3. *Let $\mathcal{T} \subseteq \mathbb{R}^{n-1}$ be a hyperacute simplex, and let G be its associated graph. Then $\mathcal{T}$'s $n-1$ dimensional volume is*

$$\mathrm{vol}(\mathcal{T}) = \frac{1}{(n-1)! \cdot \Gamma_G^{1/2}}, \tag{4.9}$$

where Γ_G is the total weight of all spanning trees of G.

We remind the reader that Γ_G was discussed in Section 2.3.2; see Equation 2.18 in particular. Before proceeding to the proof, we remind the reader of the equation of the determinant of a matrix in terms of its co-factor expansion. Let $\boldsymbol{Q} \in \mathbb{R}^{m\times m}$. For any $i, j \in [m]$, let $\boldsymbol{Q}_{-i,-j}$ denote the matrix obtained by removing row i and column j from $\boldsymbol{Q}$. The cofactor expansion along row $i \in [n]$ is the relationship

$$\det(\boldsymbol{Q}) = \sum_{k=1}^{m} (-1)^{i+k} \boldsymbol{Q}(i,k) \det\big(\boldsymbol{Q}_{-i,-k}\big),$$

while the cofactor expansion along column $j \in [n]$ reads

$$\det(\boldsymbol{Q}) = \sum_{k=1}^{m} (-1)^{j+k} \boldsymbol{Q}(k,j) \det\big(\boldsymbol{Q}_{-k,-j}\big).$$

We may now give the proof.

Proof. Let $\boldsymbol{D}$ be the distance matrix of $\mathcal{T}$, and recall that $\boldsymbol{D} = \boldsymbol{R}$ where $\boldsymbol{R}$ is the effective resistance matrix of the graph G. Set

$$\boldsymbol{r} = -\left(\boldsymbol{L}_G \mathrm{diag}(\boldsymbol{L}_G^+(i,i)) + \frac{2}{n}\boldsymbol{1}\right), \quad \alpha = \mathrm{diag}(\boldsymbol{L}_G^+(i,i))^t \boldsymbol{L}_G \mathrm{diag}(\boldsymbol{L}_G^+(i,i)) + 4R_G/n^2.$$

Combining Lemma 4.2 and Equation 4.7, write

$$\mathrm{vol}(\mathcal{T})^2 = \frac{(-1)^n}{((n-1)!)^2 2^{n-1}} \det\left(-2\begin{pmatrix} \alpha & \boldsymbol{r} \\ \boldsymbol{r} & \boldsymbol{L}_G \end{pmatrix}^{-1}\right)$$

[1]That is, the volume as calculated in $\mathbb{R}^{d-1}$.

$$= \frac{-4}{((n-1)!)^2} \det \begin{pmatrix} \alpha & \boldsymbol{r} \\ \boldsymbol{r} & \boldsymbol{L}_G \end{pmatrix}^{-1},$$

where we've employed the basic determinant properties $\det(\beta \boldsymbol{Q}) = \beta^m \det(\boldsymbol{Q})$ for $\boldsymbol{Q} \in \mathbb{R}^{m\times m}$ and $\det\big(\boldsymbol{Q}^{-1}\big) = \det(\boldsymbol{Q})^{-1}$ for $\boldsymbol{Q}$ invertible. We are thus left with task of evaluating the above determinant. We claim it is equal to $-4\Gamma_G$, which will complete the proof. Put

$$\boldsymbol{Q} = \begin{pmatrix} \alpha & \boldsymbol{r} \\ \boldsymbol{r} & \boldsymbol{L}_G \end{pmatrix} \in \mathbb{R}^{n+1\times n+1}.$$

First we carry out a cofactor expansion along the first row, which yields

$$\det(\boldsymbol{Q}) = \alpha \det(\boldsymbol{L}_G) + \sum_{j=2}^{n+1} (-1)^{1+j} r(j-1) \det\big(\boldsymbol{Q}_{-1,-j}\big) = \sum_{j=1}^{n} (-1)^j r(j) \det\big(\boldsymbol{Q}_{-1,-j+1}\big).$$

For each j, carrying out a cofactor expansion of the first column of $\boldsymbol{Q}_{-1,-j+1}$ yields

$$\det\big(\boldsymbol{Q}_{-1,-j+1}\big) = \sum_{k=1}^{n} (-1)^{k+1} r(k) \det(\boldsymbol{L}_{-k,-j}),$$

hence,

$$\det(\boldsymbol{Q}) = -\sum_{j=1}^{n}\sum_{k=1}^{n} r(j)r(k)(-1)^j(-1)^k \det\big(\boldsymbol{Q}_{-k,-j}\big) = -\sum_{j=1}^{n}\sum_{k=1}^{n} r(j)r(k)\Gamma_G,$$

by Theorem 2.2. It remains only to note that $-\sum_{j,k=1}^n r(j)r(k) = -(\sum_j r(j))^2 = -\langle \boldsymbol{1}, \boldsymbol{r}\rangle^2 = -4$ by definition of $\boldsymbol{r}$. ⊠

We can use these results to produce a surprising equation concerning the diagonal entries of the pseudoinverse Laplacian. In particular, $\boldsymbol{L}_G^+(i,i)$ is proportional to the ratio of the weight of spanning trees in G to this weight when the vertex i is removed.

Lemma 4.4. *Let G be a connected graph and fix $i \in V(G)$. Put $G_{\{i\}^c} = G[V \setminus \{i\}]$. Then*

$$\boldsymbol{L}_G^+(i,i) = \frac{(n-1)\Gamma_G^{1/2}}{n^2 \Gamma_{G_{\{i\}^c}}^{1/2}}. \tag{4.10}$$

Proof. Let $\mathcal{S}^+$ be the hyperacute simplex of G with vertices $\boldsymbol{\sigma}_1^+, \dots, \boldsymbol{\sigma}_n^+$. For an arbitrary simplex $\mathcal{T}$ with vertices $\{\gamma_i\}$, Fiedler [Fie11, Chapter 2] gave the formula can we derive this ourselves?

$$\langle \boldsymbol{\gamma}_i^*, \boldsymbol{\gamma}_j^* \rangle = \frac{\mathrm{vol}(\boldsymbol{\gamma}_1, \dots, \boldsymbol{\gamma}_{i-1}, \boldsymbol{\gamma}_{i+1}, \dots, \boldsymbol{\gamma}_n)}{(n-1)^2 \mathrm{vol}(\mathcal{T})},$$

where $\{\boldsymbol{\gamma}_i^*\}$ are the dual vertices. Translating this to a statement about $\mathcal{S}$ and $\mathcal{S}^+$ and applying Lemma 4.3 gives

$$\boldsymbol{L}_G(i,i) = \|\boldsymbol{\sigma}_i\|_2^2 = \frac{\mathrm{vol}(\mathcal{S}^+_{\{i\}^c})}{(n-1)^2\mathrm{vol}(\mathcal{S}^+)} = \frac{1}{(n-2)!\cdot\Gamma^{1/2}_{G_{\{i\}^c}}} \Bigg/ \frac{(n-1)^2}{(n-1)!\cdot\Gamma^{1/2}_G},$$

which simplifies to the desired expression.

⊠

Our next set of results demonstrate the the inverse relation can be used not only to infer geometry properties of simplices, but also graph-theoretic properties. A variant of the following was proved by Fiedler [Fie11].

LEMMA 4.5. *For a weighted and connected tree $T=(V,E,w)$ on n vertices let the matrix $\boldsymbol{S}_T$ describe the inverse distances between vertices, i.e., for $(i,j)\in E$, $\boldsymbol{S}_T(i,j)=1/w(i,j)$ and for $(i,j)\notin E$, $\boldsymbol{S}_T(i,j)=\sum_{\ell=1}^{k-1}1/w(v_\ell,v_{\ell+1})$ where $i=v_1,v_2,\ldots,v_k=j$ is the unique path between i and j. Then,*

$$-\frac{1}{2}\begin{pmatrix}0 & \mathbf{1}^t\\ \mathbf{1} & \boldsymbol{S}_T\end{pmatrix}\begin{pmatrix}\sum_{i\sim j}1/w(i,j) & (\boldsymbol{d}-2\mathbf{1})^t\\ \boldsymbol{d}-2\mathbf{1} & \boldsymbol{L}_T\end{pmatrix} = \mathbf{I}. \tag{4.11}$$

Proof. We begin by computing the left hand side of the matrix equation. Note that for connected trees on n nodes, there are precisely $n-1$ edges. Therefore, $\mathbf{1}^t\boldsymbol{d}-2n=\sum_i\deg(i)-2n=2|E|-2n=-2$, by the handshaking lemma. Since $\mathbf{1}^t\boldsymbol{L}_T=\mathbf{0}$, it follows that the top row of the resulting matrix is as desired. Next, let us consider the term

$$\sum_{i\sim j}\frac{\mathbf{1}}{w(i,j)}+\boldsymbol{S}_T(\boldsymbol{d}-2\mathbf{1}),$$

which we need to demonstrate is equal to $\mathbf{0}$. Consider the k-th row of the above vector,

$$\sum_{i\sim j}\frac{1}{w(i,j)}+\sum_{\ell\in[n]}\boldsymbol{S}_T(k,\ell)(\deg(\ell)-2). \tag{4.12}$$

Denote the sum on the right by S. Fix some $(i,j)\in E$ and let us consider how many occurrences of $1/w(i,j)$ there are in S. Since T is a tree, we may partition V into two disjoint sets of vertices, V_i and V_j (so that $V_i\cup V_j=V$ and $V_i\cap V_j=\emptyset$) where $i\in V_i$, $j\in V_j$, and $T[V_i]$, $T[V_j]$ are both connected trees. That is, the original graph T is a union of $T[V_i]$, $T[V_j]$ and the edge (i,j) which connects them. Now, the edge (i,j) will be on the path between two vertices if and only if one lies in V_i and the other in V_j. (Again, this is due to the fact that T is a tree—there is thus no other path between the components V_i and V_j other than via (i,j).) Assume without loss of generality that $k\in V_i$. Then, by the above argument, $1/w(i,j)$ appears only in those terms $\boldsymbol{S}_T(k,\ell)$ with $\ell\in V_j$. Consequently, collecting and summing over all the terms $1/w(i,j)$, we may rewrite S as

$$\sum_{i\sim j}\frac{1}{w(i,j)}\sum_{\ell\in V_j}(\deg_T(\ell)-2).$$

Since $T[V_j]$ is a tree, $\sum_{\ell\in V_j}\deg_{T[V_j]}(\ell)=2(|V_j|-1)$ (using the same arguments as above). Moreover, $\deg_{T[V_j]}(\ell)=\deg_T(\ell)$ for every $\ell\in V_j\setminus\{j\}$, since no other vertex besides j shares an edge with any vertex in V_i. On the other hand, since $(i,j)\in E$, $\deg_{T[V_j]}(j)=\deg_T(j)-1$. Hence,

$$\sum_{\ell\in V_j}(\deg_T(\ell)-2)=2(|V_i|-1)+1-2|V_i|=-1.$$

We have thus shown that $S=-\sum_{i\sim j}1/w(i,j)$, and so (4.12) is indeed 0. Finally, we consider the term $\mathbf{1}^t\boldsymbol{d}-2\mathbf{1}\mathbf{1}^t+\boldsymbol{S}_T\boldsymbol{L}_T$, which we need to show is $-2I$. Let us expand the (k,ℓ)-th component of this matrix:

$$\begin{aligned}\deg(\ell)-2+\sum_{i\in[n]}\boldsymbol{S}_T(k,i)\boldsymbol{L}_T(\ell,k)&=\deg(\ell)-2+\boldsymbol{S}_T(k,\ell)\boldsymbol{L}_T(\ell,\ell)+\sum_{i\neq\ell}\boldsymbol{S}_T(k,i)\boldsymbol{L}_T(\ell,k)\\&=\deg(\ell)-2+\boldsymbol{S}_T(k,\ell)w(\ell)-\sum_{i\in\delta(\ell)}\boldsymbol{S}_T(k,i)\\&=\deg(\ell)-2+\sum_{i\in\delta(\ell)}w(i,\ell)(\boldsymbol{S}_T(k,\ell)-\boldsymbol{S}_T(k,i)).\end{aligned}$$

For $k=\ell$, we have $\boldsymbol{S}_T(k,\ell)=0$ and $\boldsymbol{S}_T(k,i)=\boldsymbol{S}_T(\ell,i)=1/w(i,\ell)$. It follows that the above sum is -2, as desired. Now consider $k\neq\ell$. Fix $i\in\delta(\ell)$ and let $P=(k=v_1,\dots,v_r=\ell)$ be the unique path between k and ℓ. First, suppose that $i\in P$ so that $i=v_{r-1}$. Then $\boldsymbol{S}_T(k,\ell)-\boldsymbol{S}_T(k,i)=\sum_{s=1}^{r-1}1/w(v_s,v_{s+1})-\sum_{s=1}^{r-2}1/w(v_s,v_{s+1})=1/w(v_{r-1},v_r)=1/w(i,\ell)$. Otherwise, if $i\in P$ then the unique path between i and k in T is $P\cup\{\ell\}=(v_1,\dots,v_r,i)$. In this case $\boldsymbol{S}_T(k,ell)-\boldsymbol{S}_T(k,i)=\sum_{s=1}^{r-1}1/w(v_s,v_{s+1})-(\sum_{s=1}^{r-1}1/w(v_s,v_{s+1})+1/w(i,\ell))=-1/w(i,\ell)$. Finally, we note that there can be at most one neighbour of ℓ which is on the shortest path between k and ℓ. Therefore, $\sum_{i\in\delta(\ell)}w(i,\ell)(\boldsymbol{S}_T(k,\ell)-\boldsymbol{S}_T(k,i))=1-(|\delta(\ell)|-1)=2-\deg(\ell)$, demonstrating that the (k,ℓ)-th component is zero, completing the proof. ⊠

Corollary 4.1. *Let T be a weighted and connected tree. Then*

$$\boldsymbol{\xi}^t\boldsymbol{L}_T\boldsymbol{\xi}+\frac{4R_T}{n^2}=\sum_{i,j}\frac{1}{w(i,j)},\quad \text{and}\quad \boldsymbol{L}_G\boldsymbol{\xi}=\left(2-\frac{2}{n}\right)\mathbf{1}-\boldsymbol{d},$$

where $\boldsymbol{\xi}=diag(\boldsymbol{L}_T^+(i,i))=\frac{1}{n}\boldsymbol{R}\mathbf{1}-\frac{1}{n^2}\mathbf{J}\boldsymbol{R}\mathbf{1}$ and $\boldsymbol{d}=(\deg(1),\dots,\deg(n))$.

Proof. Let $\boldsymbol{S}_T$ be as it was in Lemma 4.5. It's well known that in trees, the effective resistance between nodes i,j is equal to $\sum_{s=1}^{r-1}1/w(v_s,v_{s+1})$ where $i=v_1,\dots,v_r=j$ is the shortest path between i and j in T (see e.g., [Ell11]). That is, $\boldsymbol{R}_T=\boldsymbol{S}_T$. Since matrix inverses are unique, combining Equations (4.11) and (4.7) yields

$$\begin{pmatrix} \sum_{i\sim j} 1/w(i,j) & (\boldsymbol{d}-2\mathbf{1})^t \\ \boldsymbol{d}-2\mathbf{1} & \boldsymbol{L}_T \end{pmatrix} = \begin{pmatrix} \boldsymbol{\xi}^t\boldsymbol{L}_T\boldsymbol{\xi} + 4R_T/n^2 & -(\boldsymbol{L}_T\boldsymbol{\xi}+\frac{2}{n}\mathbf{1})^t \\ -(\boldsymbol{L}_T\boldsymbol{\xi}+\frac{2}{n}\mathbf{1}) & \boldsymbol{L}_T \end{pmatrix},$$

from which the claim follows. ☒

§4.2. Inequalities

In this section we demonstrate how the graph-simplex may be used to obtain both geometric and graph-theoretic inequalities. We begin with an inequality relating the quadratic form $\mathcal{L}$ to the "weight" of the cuts associated with the pseudoinverse. It was first proved by Devriendt and Van Mieghem [DVM18]. Interestingly, a parallel result for the normalized Laplacian form does not seem to exist.

Lemma 4.6. *For any f with $\langle f, \mathbf{1}\rangle = 0$,*

$$\mathcal{L}(f) \geq \frac{\|f\|_1^2}{4w(\partial^+F^+)},$$

for $F^+ \stackrel{def}{=} \{i : f(i) \geq 0\}$.

Proof. Let F^+ be as above and let $F^- \stackrel{\text{def}}{=} [n] \setminus F^+ = \{i : f(i) < 0\}$. Observe that

$$\|f\|_1 = \sum_i |f(i)| = \langle \boldsymbol{\chi}_{F^+} - \boldsymbol{\chi}_{F^-}, f\rangle = (\boldsymbol{\chi}_{F^+} - \boldsymbol{\chi}_{F^-})^t f = (\boldsymbol{\chi}_{F^+} - \boldsymbol{\chi}_{F^-})^t(\mathbf{I} - \mathbf{J}/n)f,$$

where the last inequality follows since f is orthogonal to $\mathbf{1}$ by assumption. Using the pseudoinverse relation (3.4), we can continue as

$$\begin{aligned} \|f\|_1 &= (\chi_{F^+} - \boldsymbol{\chi}_{F^-})^t(\boldsymbol{\Sigma}^+)^t\boldsymbol{\Sigma} f \\ &= (\boldsymbol{\chi}_{F^+} - \mathbf{1} + \boldsymbol{\chi}_{F^+})^t(\boldsymbol{\Sigma}^+)^t\boldsymbol{\Sigma} f \\ &= 2\boldsymbol{\chi}_{F^+}^t(\boldsymbol{\Sigma}^+)^t\boldsymbol{\Sigma} f - (\boldsymbol{\Sigma}^+\mathbf{1})^t\boldsymbol{\Sigma} f \\ &= 2\langle \boldsymbol{\Sigma}^+\boldsymbol{\chi}_{F^+}, \boldsymbol{\chi}_{F^+}^t(\boldsymbol{\Sigma}^+)^t\boldsymbol{\Sigma} f\rangle && \text{since } \boldsymbol{\Sigma}^+\mathbf{1} = \mathbf{0} \\ &\leq 2\|\boldsymbol{\Sigma}\chi_{F^+}\|_2 \cdot \left\|\boldsymbol{\Sigma}^+ f\right\|_2 && \text{by Cauchy-Schwartz}^2 \\ &= 2\left(\boldsymbol{\chi}_{F^+}\boldsymbol{L}^+\boldsymbol{\chi}_{F^+} \cdot f^t\boldsymbol{L}f\right)^{1/2}. \end{aligned}$$

Squaring both sides and recalling that $\chi_{F^+}\boldsymbol{L}^+\chi_{F^+} = w(\delta^+F^+)$ gives the desired result. ☒

Given the combinatorial simplex $\mathcal{S}_G$ of the graph G, it has a natural corresponding normalized simplex, namely $\widehat{\mathcal{S}}_G$. Using Cheeger's inequality [CG97]

$$\kappa_G \geq \widehat{\lambda}_{n-1} \geq \frac{\kappa_G^2}{2},$$

where $\widehat{\lambda}_1 \geq \widehat{\lambda}_{n-1} > \widehat{\lambda}_n = 0$ are the eigenvalues of the normalized Laplacian of G, and κ_G is the *conductance of* G,

$$\kappa_G \stackrel{\text{def}}{=} \min_{U:vol(U)\leq \mathrm{vol}(G)/2} \frac{\mathrm{vol}(\partial U)}{|U|},$$

we can relate the centroids of $\mathcal{S}_G$ to $\widehat{\mathcal{S}}_G$ as follows.

Observation 4.1.

$$\min_{U:\mathrm{vol}(U)\leq \mathrm{vol}(G)/2} \|\boldsymbol{c}(\mathcal{S}_U)\|_2^4 |U|^2 \leq \min_{i=1}^{n} (\widehat{\boldsymbol{\Sigma}}\widehat{\boldsymbol{\Sigma}}^t)(i,i) \leq \min_{U:\mathrm{vol}(U)\leq \mathrm{vol}(G)/2} \|\boldsymbol{c}(\mathcal{S}_U)\|_2^2 |U|.$$

Proof. Use that $\|\boldsymbol{c}(\mathcal{S}_U)\|_2^2 = |U|^{-2}\boldsymbol{\chi}_U \boldsymbol{L}_G \boldsymbol{\chi}_U$ (Section 3.4) and that $\widehat{\boldsymbol{\Sigma}}\widehat{\boldsymbol{\Sigma}}^t = \widehat{\boldsymbol{\Lambda}}$ (Equation (3.1)) and apply Cheeger's inequality. ⊠

Still working on this content. Since $\boldsymbol{R}_G = n\sum_i \lambda_i^{-1} = n\,\mathrm{tr}\big(\boldsymbol{\Sigma}\boldsymbol{\Sigma}^t\big)$, facts/inequalities pertaining to the effective resistance can be translated to the simplex.

§4.3. Quadrics

Here we explore several quadrics associated with the simplices of G. We remind the reader that a *quadric* in $\mathbb{R}^d$ is a hypersurface of dimension $d-1$ of the form

$$\{\boldsymbol{x} \in \mathbb{R}^d : \boldsymbol{x}^t\boldsymbol{Q}\boldsymbol{x} + \boldsymbol{r}^t\boldsymbol{x} + s = 0\},$$

for some $\boldsymbol{Q} \in \mathbb{R}^{d\times d}, \boldsymbol{r} \in \mathbb{R}^d$ and $s \in \mathbb{R}$. In $\mathbb{R}^3$, typical examples of quadrics are spheroids and ellipsoids ($\boldsymbol{r} = \boldsymbol{0}$ in these cases), paraboloids, hyperboloids, and cylinders. In what follows we focus on ellipsoids, in particular on *circumscribed* ellipsoids. Such a quadric of interest in simplex geometry is the following.

Definition 4.1 ([Kra83]). The *Steiner Circumscribed Ellipsoid*, or simply the *Steiner Ellipsoid* of a simplex $\mathcal{S}$ with vertices $\{\boldsymbol{\sigma}_i\}$ is a quadric which contains the vertices and whose tangent plane at $\boldsymbol{\sigma}_i$ is parallel to the affine plane spanned by $\{\boldsymbol{\sigma}_j\}_{j\neq i}$.

It's existence and uniqueness is guaranteed by the following theorem.

Theorem 4.1 ([Fie05]). *The Steiner ellipsoid of a simplex $\mathcal{S}$ is unique and moreover, is the ellipsoid with minimum volume which contains $\mathcal{S}$.*

Owing to its uniqueness, we denote the Steiner ellipsoid of the simplex $\mathcal{S}$ by $\mathcal{E}(\mathcal{S})$. The following lemma gives an explicit representation of the circumscribed ellipsoid of the combinatorial simplex of G—which we will henceforth call the *(Steiner) circumscribed ellipsoid of* G—and of its inverse, which we call the *inverse (Steiner) circumscribed Ellipsoid of* G.

Lemma 4.7 ([Fie05]). *The Steiner circumscribed ellipsoid of G and its inverse are described by*

$$\mathcal{E}(\mathcal{S}_G) = \left\{\boldsymbol{x} : \boldsymbol{x}^t\boldsymbol{\Sigma}^+(\boldsymbol{\Sigma}^+)^t\boldsymbol{x} - \frac{n-1}{n} = 0\right\}, \tag{4.13}$$

and

$$\mathcal{E}(\mathcal{S}_G^+) = \left\{ \boldsymbol{x} : \boldsymbol{x}^t \boldsymbol{\Sigma}\boldsymbol{\Sigma}^t \boldsymbol{x} - \frac{n-1}{n} = 0 \right\}. \tag{4.14}$$

Proof. We prove Equation (4.13) only; Equation (4.14) follows similarly. Set $\boldsymbol{M} = \boldsymbol{\Sigma}^+(\boldsymbol{\Sigma}^+)^t$ and $E = \{\boldsymbol{x} : \boldsymbol{x}^t \boldsymbol{M} \boldsymbol{x} = (n-1)/n\}$. The claim is that $\mathcal{E}(\mathcal{S}) = E$. First we demonstrate that the vertices of $\mathcal{S}$ are contained in E. Noticing that $\mathbf{J}^2 = n\mathbf{J}$, we compute

$$\boldsymbol{\sigma}_i^t \boldsymbol{M} \boldsymbol{\sigma}_i = \chi_i^t \boldsymbol{\Sigma}^t \boldsymbol{\Sigma}^+ (\boldsymbol{\Sigma}^+)^t \boldsymbol{\Sigma} \chi_i = \chi_i^t \left(\mathbf{I} - \frac{1}{n}\mathbf{J}\right)^2 \chi_i = \chi_i^t \left(\mathbf{I} - \frac{1}{n}\mathbf{J}\right) \chi_i = 1 - \frac{1}{n},$$

so indeed the vertices $\boldsymbol{\sigma}_i$ are contained in E. Now, define the hyperplane

$$\mathcal{H} \stackrel{\text{def}}{=} \left\{ \boldsymbol{x} : \boldsymbol{x}^t \boldsymbol{M} \boldsymbol{\sigma}_i = -\frac{1}{n} \right\}.$$

We claim that $\mathcal{H}$ is the plane containing the points $\{\boldsymbol{\sigma}_j\}_{j \neq i}$. Indeed, consider $\boldsymbol{\sigma}_j$ for some fixed $j \neq i$. Then, as above

$$\boldsymbol{\sigma}_j^t \boldsymbol{M} \boldsymbol{\sigma}_i = \chi_j^t \left(\mathbf{I} - \frac{1}{n}\mathbf{J}\right) \chi_i = -\frac{1}{n}.$$

It remains to show that $\mathcal{H}$ is parallel to the tangent plane of E at the point $\boldsymbol{\sigma}_i$. But this tangent plane is defined by the equation [Fie05] Should figure out how this is actually done

$$\boldsymbol{x}^t \boldsymbol{M} \boldsymbol{\sigma}_i = \frac{n-1}{n},$$

which is clearly parallel to $\mathcal{H}$. This completes the proof. ⊠

Perhaps a more insightful representation of $\mathcal{E}(\mathcal{S})$ comes from appealing to Equation (3.2), i.e., $\boldsymbol{\Sigma}\boldsymbol{\Sigma}^t = \boldsymbol{\Lambda}^{-1/2}$. Hence, by (4.13),

$$\mathcal{E}(\mathcal{S}) = \left\{ \boldsymbol{x} : \boldsymbol{x}^t \boldsymbol{\Lambda}^{-1} \boldsymbol{x} = \frac{n-1}{n} \right\}. \tag{4.15}$$

This allows us to give explicit formulas for the semi-axes of $\mathcal{E}(\mathcal{S})$. The *semi-axes* of an ellipsoid written in the standard form $\boldsymbol{x}^t \boldsymbol{D}^2 \boldsymbol{x} = 1$ with $\boldsymbol{D} \in \mathbb{R}^{d \times d}$ a diagonal matrix are the d vectors $\boldsymbol{e}_i \cdot \boldsymbol{D}(i,i)^{-1}$. They are the unique vectors $\mathbf{u}_i$ such that any point $\boldsymbol{x}$ on the ellipsoid can be written as $\boldsymbol{x} = \sum_i \mathbf{u}_i \alpha_i$ with $\sum_i \alpha_i^2 = 1$ [DVM18].

Lemma 4.8. *The semi-axes of the Steiner Cirscumscribed Ellipsoid $\mathcal{E}(\mathcal{S}_G)$ of the graph G are*

$$\frac{\boldsymbol{e}_i}{\sqrt{\lambda_i}} \cdot \left(\frac{n}{n-1}\right)^{1/2},$$

for $i = 1, \ldots, n-1$.

Proof. The diagonal matrix $\boldsymbol{D} = \boldsymbol{\Lambda}^{-1/2}(\frac{n}{n-1})^{1/2}$ has entries $D(i,i) = \boldsymbol{e}_i(\frac{n}{(n-1)\lambda_i})^{1/2}$, and equation (4.15) demonstrates that $\mathcal{E}(\mathcal{S}_G) = \{\boldsymbol{x} : \boldsymbol{x}^t\boldsymbol{D}^2\boldsymbol{x} = 1\}$. Apply the definition of semi-axes. ⊠

Next we investigate the circumscribed sphere of the combinatorial simplex. Similarly to the circumscribed ellipsoid, the *cirscumscribed sphere of a convex body* $\mathcal{P}$ is the sphere whose boundary contains all the vertices of $\mathcal{P}$. The circumscribed sphere does not exist in general. However, just as it is possible to always draw a circle containing the endpoints of a triangle, so the circumscribed sphere of a hyperacute simplex always exists as is demonstrated by the following lemma.

Lemma 4.9 ([Fie93]). *Let $\mathcal{S}^+ \subseteq \mathbb{R}^{n-1}$ be a hyperacute simplex. The circumscribed sphere of $\mathcal{S}^+$ exists and is given by the set of points $\{\boldsymbol{x} : \boldsymbol{x} = \boldsymbol{\Sigma\alpha},\ \langle\boldsymbol{\alpha}, \mathbf{1}\rangle = 1,\ \langle\boldsymbol{\alpha}, \boldsymbol{D\alpha}\rangle = 0\}$, which is a sphere centred at the point $\frac{1}{2}\boldsymbol{\Sigma}(\boldsymbol{L}_G\boldsymbol{\xi} + \mathbf{1}/n)$ with radius $\frac{1}{2}\sqrt{\boldsymbol{\xi}^t\boldsymbol{L}_G\boldsymbol{\xi} + 4R_G/n^2}$ where G is $\mathcal{S}^+$'s associated graph, and $\boldsymbol{\xi} = diag(\boldsymbol{L}_G^+(i,i))$.*

Proof. Set $\boldsymbol{\zeta} = \frac{1}{2}(\boldsymbol{L}_G\boldsymbol{\xi} + \mathbf{1}/n)$ and $r = \boldsymbol{\xi}^t\boldsymbol{L}_G\boldsymbol{\xi} + 4R_G/n^2$. Let us expand $\boldsymbol{x}$ in barycentric coordinates in accordance with Lemma 2.6. Put $\boldsymbol{x} = \sum_i \alpha_i\boldsymbol{\sigma}_i$ where $\sum_i \alpha_i = \sum_i \beta_i = 1$. Let $\boldsymbol{\alpha} = (\alpha_1, \ldots, \alpha_n)$. The claim is that the circumscribed sphere of $\mathcal{S}^+$ is given by the equation

$$\|\boldsymbol{x} - \boldsymbol{\Sigma\zeta}\|_2^2 = \frac{1}{4}r, \tag{4.16}$$

and that this equation is equivalent to $\boldsymbol{\alpha}^t\boldsymbol{D\alpha} = 0$. Note first that due to Equation 4.7, $\langle\mathbf{1}, -2\boldsymbol{\zeta}\rangle = \langle\mathbf{1}, -\boldsymbol{L}_G\boldsymbol{\xi} - \frac{2}{n}\mathbf{1}\rangle = -2$, so $\boldsymbol{\zeta} = (\zeta_1, \ldots, \zeta_{n-1})$ obeys $\sum_i \zeta_i = 1$. The left hand side of (4.16) then becomes

$$\begin{aligned}\langle\boldsymbol{x} - \boldsymbol{\Sigma\zeta}, \boldsymbol{x} - \boldsymbol{\Sigma\zeta}\rangle &= \sum_{i,j\in[n]} (\alpha_i - \zeta_i)(\alpha_j - \zeta_j)\langle\boldsymbol{\sigma}_i, \boldsymbol{\sigma}_j\rangle \\ &= \sum_{i,j\in[n]} (\alpha_i - \zeta_i)(\alpha_j - \zeta_j)\langle\boldsymbol{\sigma}_i - \boldsymbol{\sigma}_n, \boldsymbol{\sigma}_j - \boldsymbol{\sigma}_n\rangle,\end{aligned}$$

where the last line uses that $\boldsymbol{\sigma}_n\sum_i(\alpha_i - \zeta_i) = \mathbf{0}$. Observing that

$$\langle\boldsymbol{\sigma}_i - \boldsymbol{\sigma}_n, \boldsymbol{\sigma}_j - \boldsymbol{\sigma}_n\rangle = \frac{1}{2}(\|\boldsymbol{\sigma}_i - \boldsymbol{\sigma}_n\|_2^2 + \|\boldsymbol{\sigma}_j - \boldsymbol{\sigma}_n\|_2^2 - \|\boldsymbol{\sigma}_i - \boldsymbol{\sigma}_j\|_2^2),$$

we may proceed as

$$\begin{aligned}\langle\boldsymbol{x} - \boldsymbol{\Sigma\zeta}, \boldsymbol{x} - \boldsymbol{\Sigma\zeta}\rangle &= \frac{1}{2}\Big(\sum_j(\alpha_j - \zeta_j)\sum_i(\alpha_i - \zeta_i)\|\boldsymbol{\sigma}_i - \boldsymbol{\sigma}_n\|_2^2 \\ &\qquad + \sum_i(\alpha_i - \zeta_i)\sum_j(\alpha_j - \zeta_j)\|\boldsymbol{\sigma}_j - \boldsymbol{\sigma}_n\|_2^2 \\ &\qquad - \sum_{i,j}(\alpha_i - \zeta_i)(\alpha_j - \zeta_j)\|\boldsymbol{\sigma}_i - \boldsymbol{\sigma}_j\|_2^2\Big) \\ &= -\frac{1}{2}\sum_{i,j}(\alpha_i - \zeta_i)(\alpha_j - \zeta_j)\|\boldsymbol{\sigma}_i - \boldsymbol{\sigma}_j\|_2^2. \end{aligned} \tag{4.17}$$

Recalling the block matrix equation (4.7) for hyperacute simplices, for all i we have $\mathbf{1}(\boldsymbol{\xi}^t \boldsymbol{L}_G \boldsymbol{\xi} + 4R_G/n^2) - \boldsymbol{D}(\boldsymbol{L}_G \boldsymbol{\xi} + 2\mathbf{1}/n) = \mathbf{0}$, i.e., $r\mathbf{1} - 2\boldsymbol{D} = \mathbf{0}$. Hence

$$\langle \boldsymbol{D}(i,\cdot), \boldsymbol{\zeta} \rangle = \frac{r}{2}.$$

Using this, we rewrite the summation on the right hand side of (4.17) as

$$\begin{aligned}
\sum_{i,j} (\alpha_i - \zeta_i)(\alpha_j - \zeta_j)\boldsymbol{D}(i,j) &= \sum_i (\alpha_i - \zeta_i)\Big(\sum_j \alpha_j \boldsymbol{D}(i,j) - \sum_j \alpha_j \boldsymbol{D}(i,j) \Big) \\
&= \sum_j \alpha_j \sum_i (\alpha_i - \zeta_i)\boldsymbol{D}(i,j) - \frac{1}{2} r \sum_i (\alpha_i - \zeta_i) \\
&= \sum_j \alpha_j \Big(\sum_i \alpha_i \boldsymbol{D}(i,j) - \frac{1}{2} r \Big) \\
&= \sum_{i,j} \alpha_i \boldsymbol{D}(i,j)\alpha_j - \frac{1}{2} r = \boldsymbol{\alpha}^t \boldsymbol{D} \boldsymbol{\alpha} - \frac{1}{2} r.
\end{aligned}$$

The equation of the sphere in (4.16) now becomes $\frac{1}{4}r - \frac{1}{2}\boldsymbol{\alpha}^t \boldsymbol{D}\boldsymbol{\alpha} = \frac{1}{4}r$, i.e., $\boldsymbol{\alpha}^t \boldsymbol{D} \boldsymbol{\alpha} = \mathbf{0}$ as was claimed. Now, to see that this sphere contains the vertices of $\mathcal{S}^+$, $\{\boldsymbol{\sigma}_i^+\}$, we need only note that the barycentric coordinate of $\boldsymbol{\sigma}_\ell^+$ is $\boldsymbol{\chi}_\ell$ and that $\boldsymbol{\chi}_\ell^t \boldsymbol{D} \boldsymbol{\chi}_\ell = \sum_{i,j} \boldsymbol{\chi}_\ell(i) \boldsymbol{D}(i,j) \boldsymbol{\chi}_\ell(j) = \boldsymbol{D}(\ell,\ell) = 0$. ⊠

Until this point, we have been examining only the quadrics associated with the combinatorial simplices. We now consider the normalized simplices. Since all the vertices of the normalized simplex lie on the unit sphere, it's clear that the circumscribed sphere of $\widehat{\mathcal{S}}_G$ is precisely $\{\boldsymbol{x} : \boldsymbol{x}^t \boldsymbol{x} = 1\}$. It's not as straightforward to see what they circumscribed ellipsoid, $\mathcal{E}(\widehat{\mathcal{S}})$, is on the other hand. One might suspect that it obeys the equation $\boldsymbol{x}^t \widehat{\boldsymbol{\Sigma}} + (\widehat{\boldsymbol{\Sigma}}^+)^t = 1 - 1/n$, as this is the natural analogue of (4.13). However, because $\widehat{\boldsymbol{\Sigma}}^+$ and $\widehat{\boldsymbol{\Sigma}}$ obey a non-constant pseudoinverse relation, this equation fails the first test: $\widehat{\boldsymbol{\sigma}}_i^t \widehat{\boldsymbol{\Sigma}}^+ (\widehat{\boldsymbol{\Sigma}}^+)^t \widehat{\boldsymbol{\sigma}}_i = \boldsymbol{\chi}_i^t (\mathbf{I} - \sqrt{\boldsymbol{w}}\sqrt{\boldsymbol{w}}^t/\mathrm{vol}(G))\boldsymbol{\chi}_i = 1 - \sqrt{w(i)w(j)}/\mathrm{vol}(G)$ is non-constant. However, at this point we recall that beyond being simply the inverse simplex of $\mathcal{S}$, $\mathcal{S}^+$ is also its dual. We might thus hazard a guess that the correct matrix is $\widehat{\boldsymbol{\Sigma}}^* (\widehat{\boldsymbol{\Sigma}}^*)^t$, where $\widehat{\boldsymbol{\Sigma}}^*$ is the vertex matrix of $\widehat{\mathcal{S}}^*$. This is in fact correct, but to see this we first need to demonstrate that any set of simplex vertices and their duals obey the same relationship as do the vertices of the combinatorial simplex and its inverse.

Lemma 4.10. *Let $\mathcal{T} \subseteq \mathbb{R}^{n-1}$ be any simplex, and $\mathcal{T}^*$ its dual, where $\boldsymbol{\Sigma} = \boldsymbol{\Sigma}(\mathcal{T}) = (\boldsymbol{\sigma}_i)$ and $\boldsymbol{\Sigma}^* = \boldsymbol{\Sigma}(\mathcal{T}^*) = (\widehat{\boldsymbol{\sigma}}_i^*)$. For all $i,j \in [n]$, $\langle \widehat{\boldsymbol{\sigma}}_i, \widehat{\boldsymbol{\sigma}}_j^* \rangle = \delta_{i,j} - 1/n$.*

Proof. By definition of the dual simplex, for all $i, j \neq n$, $\langle \widehat{\boldsymbol{\sigma}}_i, \widehat{\boldsymbol{\sigma}}_j^* - \widehat{\boldsymbol{\sigma}}_n^* \rangle = \delta_{ij}$. Recalling that $\widehat{\boldsymbol{\sigma}}_n^* = -\sum_{\ell<n} \widehat{\boldsymbol{\sigma}}_\ell^*$, write

$$\langle \widehat{\boldsymbol{\sigma}}_i, \widehat{\boldsymbol{\sigma}}_n^* \rangle = -\sum_{\ell<n} \langle \widehat{\boldsymbol{\sigma}}_i, \widehat{\boldsymbol{\sigma}}_\ell^* \rangle$$

$$= -\sum_{\ell<n} \delta_{i,\ell} + \langle \widehat{\boldsymbol{\sigma}}_i, \widehat{\boldsymbol{\sigma}}_n^* \rangle$$
$$= -1 - (n-1)\langle \widehat{\boldsymbol{\sigma}}_i, \widehat{\boldsymbol{\sigma}}_n^* \rangle.$$

Rearranging the above yields $\langle \widehat{\boldsymbol{\sigma}}_i, \widehat{\boldsymbol{\sigma}}^* \rangle = -1/n$. Therefore, $\langle \widehat{\boldsymbol{\sigma}}_i, \widehat{\boldsymbol{\sigma}}_j^* \rangle = \delta_{ij} - 1/n$. It remains to show that $\langle \widehat{\boldsymbol{\sigma}}_n, \widehat{\boldsymbol{\sigma}}_n^* \rangle = 1 - 1/n$. Proceeding as above, we have

$$\langle \widehat{\boldsymbol{\sigma}}_n, \widehat{\boldsymbol{\sigma}}_n^* \rangle = -\sum_{\ell<n} \langle \widehat{\boldsymbol{\sigma}}, \widehat{\boldsymbol{\sigma}}_\ell^* \rangle = -\sum_{\ell<n} \frac{-1}{n} = \frac{n-1}{n}. \qquad \boxtimes$$

From this we can extract the equations of $\mathcal{E}(\widehat{\mathcal{S}})$ and $\mathcal{E}(\widehat{\mathcal{S}}^+)$.

Corollary 4.2. *The normalized Steiner ellipsoid of G is*

$$\mathcal{E}(\widehat{\mathcal{S}}) = \left\{ \boldsymbol{x} : \boldsymbol{x}^t \widehat{\boldsymbol{\Sigma}}^* (\widehat{\boldsymbol{\Sigma}}^*)^t \boldsymbol{x} = \frac{n-1}{n} \right\},$$

and the inverse is

$$\mathcal{E}(\widehat{\mathcal{S}}) = \left\{ \boldsymbol{x} : \boldsymbol{x}^t (\widehat{\boldsymbol{\Sigma}}+)^* ((\widehat{\boldsymbol{\Sigma}}^+)^*)^t \boldsymbol{x} = \frac{n-1}{n} \right\}.$$

where $\widehat{\boldsymbol{\Sigma}}^*$ contains the vertices of $\widehat{\mathcal{S}}_G^*$ and $(\widehat{\boldsymbol{\Sigma}}^+)^*$ those of $(\widehat{\mathcal{S}}_G^+)^*$.

Proof. The computational is almost identical to that in the proof of Lemma 4.7. $\boxtimes$

§4.4. Resistive Polytope

In this section we explore the relationship between the inverse combinatorial simplex of G and another geometric object related to the effective resistance of the graph. Consider the vertices $\boldsymbol{\mu}_i = \boldsymbol{L}_G^{+/2} \boldsymbol{\chi}_i \in \mathbb{R}^n$, for $i \in [n]$. This yields n points in $\mathbb{R}^n$, also with pairwise squared distances equal to the effective resistance of the graph:

$$\left\| \boldsymbol{\mu}_i - \boldsymbol{\mu}_j \right\|_2^2 = \left\| \boldsymbol{L}_G^{+/2} (\boldsymbol{\chi}_i - \boldsymbol{\chi}_j) \right\|_2^2 = (\boldsymbol{\chi}_i - \boldsymbol{\chi}_j)^t \boldsymbol{L}_G^+ (\boldsymbol{\chi}_i - \boldsymbol{\chi}_j) = r^{\text{eff}}(i,j).$$

This embedding has been referred to as a *resistive embedding* [Gha15, DLP11], and is an example of an ℓ_2^2 metric [ARV09] owing to the fact that, as we saw in Section 2.4, that effective resistance is a metric. That being said however, while the mapping seems to be known, there is very little literature on its properties.

We set

$$\mathcal{R}_G \overset{\text{def}}{=} \operatorname{conv}(\{\mu_i\}), \tag{4.18}$$

and call $\mathcal{R}_G$ the *resistive polytope of* G. Note that $\boldsymbol{L}_G^{+/2}$ is $\mathcal{R}_G$'s vertex matrix. As usual, we may omit the subscript G for convenience. We emphasize that while the vertices $\{\boldsymbol{\mu}_i\}$ obey the same pairwise distances as those of the inverse simplex $\mathcal{S}_G^+$, $\mathcal{R}_G$ is not the same object as $\mathcal{S}_G^+$. First, of course, there is the fact that it sits in $\mathbb{R}^n$. However, we also note that the entries of μ_i (the first $n-1$, at least) do not match those of $\boldsymbol{\sigma}_i^+$. Indeed,

$$\mu_i(\ell) = \boldsymbol{L}_G^{+/2}(\ell, i) = \sum_{j\in[n]} \lambda_j^{-1/2}\boldsymbol{\varphi}_j\boldsymbol{\varphi}_j^t(\ell, i) = \sum_{j\in[n]} \lambda_j^{-1/2}\boldsymbol{\varphi}_j(\ell)\boldsymbol{\varphi}_j(i).$$

Recalling the formula for the vertices of the inverse simplex $\mathcal{S}^+$ demonstrates that

$$\mu_i(\ell) = \sum_{j\in[n]} \boldsymbol{\sigma}_\ell^+(j)\boldsymbol{\varphi}_j(i) = \sum_{j\in[n]} \boldsymbol{\sigma}_i^+(j)\boldsymbol{\varphi}_j(\ell).$$

Hence, in general, $\mu_i(\ell) \neq \boldsymbol{\sigma}_i(\ell)$. However, the dot products between the vertices of $\mathcal{R}_G$ does respect the same relationships as those between the vertices of $\mathcal{S}_G^+$:

$$\begin{aligned}\langle \boldsymbol{\mu}_i, \boldsymbol{\mu}_j\rangle &= \sum_{\ell\in[n]} \boldsymbol{L}_G^{+/2}(\ell, i)\boldsymbol{L}_G^{+/2}(\ell, j)\\ &= \langle \boldsymbol{L}_G^{+/2}(\cdot, i), \boldsymbol{L}_G^{+/2}(\cdot, j)\rangle\\ &= \langle \boldsymbol{L}_G^{+/2}(\cdot, i), \boldsymbol{L}_G^{+/2}(j, \cdot)\rangle = \boldsymbol{L}_G^{+}(i, j),\end{aligned}$$

since $\boldsymbol{L}_G^{+/2}$ is symmetric and $\boldsymbol{L}_G^{+/2}\boldsymbol{L}_G^{+/2} = \boldsymbol{L}_G^+$. We can also see this from recalling that

$$r^{\text{eff}}(i, j) = \boldsymbol{L}_G^+(i, i) + \boldsymbol{L}_G^+(j, j) - \frac{1}{2}\boldsymbol{L}_G^+(i, j),$$

combined with the facts that $\left\|\boldsymbol{\mu}_i - \boldsymbol{\mu}_j\right\|_2^2 = r^{\text{eff}}(i, j)$ and $\|\boldsymbol{\mu}_i\|_2^2 = \boldsymbol{L}_G^+(i, i)$. Moreover, the centroid of $\mathcal{R}_G$ also coincides with the origin of $\mathbb{R}^n$:

$$\boldsymbol{c}(\mathcal{R}_G) = \frac{1}{n}\boldsymbol{L}_G^{+/2}\mathbf{1} = \frac{1}{n}\sum_{i\in[n-1]} \lambda_i^{-1/2}\boldsymbol{\varphi}_i\boldsymbol{\varphi}_i^t\mathbf{1} = \mathbf{0}.$$

One therefore begins to suspect that $\mathcal{R}_G$ is the same object of $\mathcal{S}_G^+$, simply projected onto some hyperplane of $\mathbb{R}^n$. The following lemma demonstrates that this is indeed the case, and that the hyperplane is that which is has $\operatorname{span}(\mathbf{1})$ as its orthogonal complement.

LEMMA 4.11. *The all ones vector is orthogonal to $\mathcal{R}_G$.*

Proof. We need to show that for all $\boldsymbol{p}, \boldsymbol{q} \in \mathcal{R}_G$, $\langle \mathbf{1}, \boldsymbol{p} - \boldsymbol{q}\rangle = 0$. As usual, let $\boldsymbol{x}$ and $\boldsymbol{y}$ be the barycentric coordinates of $\boldsymbol{p}$ and $\boldsymbol{q}$ so that $\boldsymbol{p} = \boldsymbol{L}_G^{+/2}\boldsymbol{x}$ and $\boldsymbol{q} = \boldsymbol{L}_G^{+/2}\boldsymbol{y}$. We have

$$\langle \mathbf{1}, \boldsymbol{p}\rangle = \sum_{\ell\in[n]} (\boldsymbol{L}_G^{+/2}\boldsymbol{x})(\ell) = \sum_{\ell\in[n]}\sum_{j\in[n]} \boldsymbol{L}_G^{+/2}(\ell, j)x(j) = \sum_{j\in[n]} x(j)\sum_{\ell\in[n]} \boldsymbol{L}_G^{+/2}(\ell, j),$$

where for any j,

$$\sum_{\ell\in[n]} \boldsymbol{L}_G^{+/2}(\ell, j) = \mathbf{1}^t\boldsymbol{L}_G^{+/2}\boldsymbol{\chi}_j = \sum_{\ell\in[n-1]} \lambda_\ell^{-1/2}\mathbf{1}^t\boldsymbol{\varphi}_\ell\boldsymbol{\varphi}_\ell^t\boldsymbol{\chi}_j = 0,$$

since $\boldsymbol{\varphi}_i \in \text{span}(\mathbf{1})^\perp$ for all $i < n$. Hence $\langle \mathbf{1}, \boldsymbol{p} \rangle = 0$ meaning that $\langle \mathbf{1}, \boldsymbol{p} - \boldsymbol{q} \rangle = 0$ as well. ⊠

The relationship between $\mathcal{R}$ and $\mathcal{S}$ gives us an alternate way to prove equalities such as (3.13): There exists an isometry[3] between $\mathcal{R}$ and $\mathcal{S}$, so

$$\left\|\boldsymbol{c}(\mathcal{S}_U^+)\right\|_2^2 = \|\boldsymbol{c}(\mathcal{R}_U)\|_2^2 = \frac{1}{|U|^2}\left\|\boldsymbol{L}_G^{+/2}\boldsymbol{\chi}_U\right\|_2^2 = \frac{1}{|U|^2}w(\delta^+ U).$$

Additionally, just as $\mathcal{S}_G^+$ has the inverse $\mathcal{S}_G$, $\mathcal{R}_G$ has an inverse which respects the same relationships. As one might guess, this inverse has vertex matrix $\boldsymbol{L}_G^{1/2}$. To see this, for any $i, j \neq k$, we have

$$\langle \boldsymbol{L}_G^{1/2}\boldsymbol{\chi}_i, \boldsymbol{L}_G^{+/2}\boldsymbol{\chi}_j - \boldsymbol{L}_G^{+/2}\boldsymbol{\chi}_k \rangle = \boldsymbol{\chi}^t \boldsymbol{L}_G^{1/2}\boldsymbol{L}_G^{+/2}(\boldsymbol{\chi}_j - \boldsymbol{\chi}_k)\rangle,$$

where

$$\boldsymbol{L}_G^{1/2}\boldsymbol{L}_G^{+/2} = \sum_{r,s=1}^{n-1} \lambda_r^{1/2}\lambda_s^{1/2}\boldsymbol{\varphi}_r\boldsymbol{\varphi}_r^t\boldsymbol{\varphi}_s\boldsymbol{\varphi}_s^t = \sum_{r=1}^{n-1}\boldsymbol{\varphi}_r\boldsymbol{\varphi}_r^t,$$

and

$$\sum_{r=1}^{n-1}\boldsymbol{\chi}_i\boldsymbol{\varphi}_r\boldsymbol{\varphi}_r^t\boldsymbol{\chi}_j = \sum_{r=1}^{n-1}\boldsymbol{\varphi}_r(i)\boldsymbol{\varphi}_r(j) = \delta_{ij} - \frac{1}{n},$$

using Equation (3.3). Hence,

$$\boldsymbol{\chi}_i^t\boldsymbol{L}_G^{1/2}\boldsymbol{L}_G^{+/2}(\boldsymbol{\chi}_j - \boldsymbol{\chi}_k) = \delta_{ij} - \frac{1}{n} - (\delta_{ik} - \frac{1}{n}) = \delta_{ij}.$$

Still investigating this relationship and its properties.

§4.5. Random Walks

[3] A distance preserving map.

Chapter 5

Algorithmics

This final technical chapter will discuss some of the algorithmic foundations and consequences of the graph-simplex correspondence. Vis-à-vis foundations, we will chiefly be concerned with transitioning between a graph and its various simplices. We will explore lower bounds for how quickly this can be done if we wish to obtain the precise result[1], and whether we can "approximate" any of the constructions (e.g., given the graph G can we quickly obtain a simplex which serves as an approximation[2] to $\mathcal{S}_G$.) With respect to algorithmic consequences on the other hand, we will attempt to leverage knowledge we have in the hitherto relatively unrelated areas of computational graph theory and high-dimensional computational geometry to draw new conclusions about the complexity of several problems in these areas. For instance, if a graph theoretic problem has an analogue in the simplex, any fact regarding the problems difficulty—whether it's NP-complete, say—translates to an immediate result about its geometric counterpart. In particular, since the simplex of a graph can be generate in polynomial time given the graph (due to the fact that an eigendecomposition can be computed in polynomial time) and vice versa, problems which are solvable in polynomial in either the simplex or graph domain translate to polynomial (yet perhaps not optimal!) problems in the other domain and likewise, problems which are NP-hard in one domain have analogues which are NP-hard in the other.

For the benefit of the (undoubtedly confused) reader unfamiliar with computational complexity and reductions, we begin the chapter with a short section containing this background material. We will also discuss computational representations of a simplex therein.

§5.1. Preliminaries

Asymptotics. We begin with asymptotic notation which will be used to analyze the running time of various algorithms. We use the standard definitions—see any reference text on algorithm design for more background (e.g., [KT06]). Let $f, g : U \subseteq \mathbb{R} \to \mathbb{R}$ be functions. Write $f = O(g)$ (or $f(n) = O(g(n))$) if $\limsup_{x\to\infty} |f(x)/g(x)| < \infty$, and $f = \Omega(g)$ if $g = O(f)$. Write $f = o(g)$ as $x \to c$ if $\lim_{x\to\infty} |f(x)/g(x)| = 0$ and $f = \omega(g)$ if $g = o(f)$. If $f = O(g)$ and $f = \Omega(g)$ we write $f = \Theta(g)$. We will also use the tilde to hide polylog factors. Say $f = \widetilde{O}(g)$ if $f(n) = O(g(n)\log^c n)$ and $f = \widetilde{\Omega}(g)$ if $f(n) = \Omega(g(n)\log^{-c} n)$, for

[1] Ignoring issues of floating point number accuracy

[2] The notion of approximating a simplex is rather ambiguous and will be expounded upon at a later time.

some $c \geq 0$.

Simplex representations. In order to discuss the algorithmics pertaining to simplices and convex polyhedra in general, we must discuss how such objects are represented by a machine. Clearly, we cannot simply enumerate all the points enclosed by a body in high-dimensional space. Instead we must concisely represent the boundaries of the polytope. The two most common such descriptions are

- V-*description*, in which we are given the vertex vectors of the polytope;
- H-*description*, in which we are given the parameters of the half-spaces whose intersection defines the polytope. That is, if $\mathcal{T} = \bigcap_i \{\boldsymbol{x} : \langle \boldsymbol{z}_i, \boldsymbol{x} \rangle \geq b_i\}$, then an H-description of $\mathcal{T}$ would be the vectors $\{\boldsymbol{z}_i\}$ and the scalars $\{b_i\}$.

It's not at all clear whether these descriptions are equivalent in the sense that one can easily generate one from the other. Indeed, the complexity of vertex enumeration (generating a V-description from an H-description) and facet enumeration (generating an H-description from a V-description) remains an open problem for general polytopes [KP03], although there exist polynomial time algorithms when the polytopes are simplices (e.g., [BFM98]). We will return to this fact later on.

Reductions. Some background on computational models and reductions will also be useful. For more details see [KT06] or [Knu11]. We will use the typical computational model for analyzing algorithms. Without diving too far into the minutiae, we assume that single arithmetic operations require $O(1)$-time, i.e., constant. We will analyze the runtime of an algorithm as a function of how many bits it takes to represent the input. A common tool for providing upper bounds on the runtime of an algorithm is to "reduce" it to a problem for which a bound is already known. Assume problem P requires time $\Omega(f_P(n))$ to solve—meaning that *any* algorithm requires time $\Omega(f_P(n))$—where n represents the size of the input and $f_P(n)$ is some function of n, e.g., $f_P(n) = n^2 \log n$. Let Q be a distinct problem and suppose that for every instance of P we can transform the input of P to a valid input for Q, and transform the output of Q to a valid output of P, both in time $O(f_P(n))$. We have then established that $f_Q(n) = \Omega(f_P(n))$, where f_Q the runtime required to solve Q, since we can solve P in time $f_Q(n) + O(f_P(n))$ by transforming any input to P to the input of Q, solving Q, and transforming the output back. Such a technique will be used extensively throughout the next few sections.

The complexity classes NP, NP-hard, and NP-Complete. For brevity, we restrict ourselves to a very brief presentation of these concepts. The interested reader can find more background in any reference on computational complexity theory.

The class NP is the set of all decision problems[3] which have solutions which are *verifiable* in polynomial time. It is possible, for example, to check in polynomial time whether a given

[3] That is, problems to which we seek a yes/no answer.

set is in fact an independent set of a certain size. Thus the decision variant of Independent-Set lies in NP. NP stands for "non-deterministic polynomial time", as it is formally the set of all decision problems solvable by a non-deterministic Turing Machine [Pap03].

The class NP-hard comprises all the problems to which any problem in NP can be reduced in polynomial time (see above). That is, $P \in \mathsf{NP}$-hard iff for all $Q \in \mathsf{NP}$, Q can be reduced to P in polynomial time. Thus, to show that $P \in \mathsf{NP}$-hard, it suffices to reduce another problem $R \in \mathsf{NP}$-hard to P (in polynomial time) since, in this case, if all problems in NP are reducible to R they are in turn reducible to P. We tend to think of NP as the set of "hard" problems.

Finally, the class NP-complete is the intersection of the classes NP and NP-hard. Informally then, it is the class of all "hard" decision problems.

§5.2. Computational Complexity

In this section we investigate the relationships between problems in one domain—either the graph-theoretic or geometric domain—and their analogues in the other. The following result exemplifies the power of the graph-simplex correspondence in yielding results which seem otherwise to be difficult to obtain (certainly more difficult than the following proof, at any rate). The following result was first stated by Devriendt and Van Mieghem [DVM18], although it was stated only for inverse simplices of graphs. We observe that it can be generalized as follows.

Lemma 5.1. *Computing the altitude of minimum length in a hyperacute polytope is NP-hard. Consequently, computing the minimum length altitude in general polyhedra is NP-hard.*

Proof. The relationship $\left\|\boldsymbol{a}(\mathcal{S}_U^+)\right\|_2^2 = w(\delta U)^{-1}$ (Lemma 3.13) for the inverse simplex of a graph G demonstrates that the problem of computing a minimum length altitude in any hyperacute simplex is NP-hard, because computing the maximum weight cut in any weighted graph is NP-hard [Kar72]. Since the class of convex polytopes contains the class of hyperacute simplices, the result follows. ⊠

Remark 5.1. In the above statement and its proof, the description of the polytope and simplex was not specified. This is due to the fact that—as discussed above—for simplices there is a polynomial time algorithm to translate betweent the various descriptions. With regard to NP-completeness therefore, the description makes no difference.

Remark 5.2. As exemplified by the statement of Lemma 5.1 the fact that a problem is NP-hard for hyperacute simplices immediately implies that it is so for general polyhedra (since simplices are a subclass of polyhedra). We will still, however, often state a result in terms of general polyhedra because it seems most likely to be useful in this form.

The remainder of this section is dedicated to obtaining more results of this type.

We begin by investigating independent sets. Given a graph $G = (V, E, w)$, recall that an *independent set* is a subset $I \subseteq V$ such that if $i, j \in I$ then $(i, j) \notin E$. The weight of an independent set is nicely described by the Laplacian quadratic form. If I is an independent set note that

$$\mathrm{vol}(I) = w(\delta I),$$

and so

$$\mathcal{L}(\boldsymbol{\chi}_I) = \sum_{i\sim j} w(i,j)(\boldsymbol{\chi}_I(i) - \boldsymbol{\chi}_I(j))^2 = \sum_{i\in I}\sum_{j:j\sim i} w(i,j) = \sum_{i\in I} w(i) = w(\delta I),$$

where the second and fourth inequalities follows from the fact that I is an independent set. Now, suppose we assign each vertex i a weight $f(i) \geq 0$. The Max-Weight Independent-Set problem consists of maximizing $f(I) \overset{\mathrm{def}}{=} \sum_{i\in I} f(i)$ over all independent sets I. Clearly Max-Weight Independent-Set is NP-hard in general, seeing as it reduces to the usual independent set maximization problem by taking $f(i) = 1$ for all i. If f is a linear function of the weights so that $f(i) = \alpha w(i)$ for all i and some $\alpha > 0$, we call the corresponding problem α-Vertex-Weighted Independent-Set. We will focus on the case $\alpha = 1$ for clarity, and call the corresponding problem just Vertex-Weighted Independent-Set. The difficulty of this problem is not immediately clear, since it is more structured than simply Max-Weight Independent-Set. The next lemma removes any doubt as to the problems tractability.

Lemma 5.2. Vertex-Weighted Independent-Set *is* NP*-Complete.*

Proof. Given a purported independent I, it is easily checkable in polynomial time whether $\mathrm{vol}(I)$ is of a certain size—hence Vertex-Weighted Independent-Set is in NP. To that it is NP-hard, we reduce from Independent-Set. Let $G = (V(G), E(G))$ and $k \in \mathbb{N}$ be an instance of Independent-Set. The intuition behind the following reduction is to create a separate graph H which, for each independent set $I \subseteq V(G)$, has an independent set J in H such that $\mathrm{vol}_H(J) = |I|$ in H and conversely, for each maximal independent set J in H there exists an independent set I in G with $|I| = \mathrm{vol}_H(J)$. From this relationship it follows that G, k constitutes a yes instance to Independent-Set iff H, k is a yes instance to Max-Weight Independent-Set. After wordsmithing the intuition, let us proceed to the formal argument.

Construct a graph $H = (V(H), E(H))$ as follows. For each vertex $u \in V(G)$, create $\deg_G(u) + 1$ vertices $u_0, u_1, \ldots, u_{\deg_G(u)}$ in $V(H)$. For $1 \leq k \leq \deg_G(u)$ set

$$w_H(u_k) = \frac{1}{\deg_G(u)}.$$

Construct the edge set $E(H)$ such that the neighbours of each vertex are described by

$$\delta_H(u_k) = \{u_0\} \cup \bigcup_{v\in\delta_G(u)} \{v_\ell : 0 \leq \ell \leq \deg_G(v)\}.$$

In words, u_k is connected to all the vertices representing v if $(u, v) \in E(G)$, and to u_0. Now, let $I \subseteq V(G)$ be an independent set in G and consider the set

$$J = \{v_k : v \in I, 1 \leq k \leq \deg_G(v)\}.$$

We claim that J is an independent set in H. Indeed, if $v_k, u_\ell \in J$ and $(v_k, u_\ell) \in E(H)$ for some $k \in [\deg_G(v)]$, $\ell \in [\deg_G(u)]$ then $v \in d_G(u)$ by definition of $\delta_H(u)$. Since I is an independent set however, both u and v are not in I, a contradiction. This demonstrates that J is bonafide independent set. Moreover,

$$\mathrm{vol}_H(J) = \sum_{v\in I} \sum_{k=1}^{\deg_G(u)} w_H(v_k) = \sum_{v\in I} \sum_{k=1}^{\deg_G(u)} \frac{1}{\deg_G(u)} = |I|.$$

Conversely, let J be an independent set in H. We claim that there exists an independent J' in H with $\mathrm{vol}_H(J') \geq \mathrm{vol}_H(J)$ containing only vertices of the form v_ℓ for $\ell \geq 1$, i.e., not v_0. Initially, set $J' = J$ but suppose $v_0 \in J$. Replace v_0 by $v_1, \ldots, v_{\deg_G(v)}$ in J'. None of the these vertices share edges, and aside from one another, v_ℓ and v_0 for $\ell > 0$ have the same edge set. It follows that J' remains an independent set. Moreover, since $w_H(v_0) < w_H(v_\ell)$ by construction, we have $\mathrm{vol}_H(J) < \mathrm{vol}_H(J')$. Let us remark further that if J contains vertices $\{v_\ell\}_{\ell\in F}$ for some $F \subsetneq [\deg_G(v)]$, then we may add the missing vertices v_k, $k \in [\deg_G(v)] \setminus F$ while maintaining the property that J is an independent set (this follows since $\delta_H(v_k) = \delta_H(v_\ell)$ for all $\ell, k \geq 1$). We have thus argued that every maximal independent set in H can be written in the form $J = \cup_{v\in I}\{v_k : 1 \leq k \leq \deg_G(v)\}$ for some set $I \subseteq V(G)$. We now claim that I is an independent set in G. The argument is similar to above: If not, then $u, v \in I$ with $u \sim v$, but this implies that $v_k \sim v_\ell$ in H meaning that J is not an independent set. Additionally, as above, $\mathrm{vol}_H(J) = |I|$. Therefore, there exists an independent set J in H with $\mathrm{vol}_H(J) \geq k$ iff there exists an independent set I in G with $|I| \geq k$, concluding the argument. ⊠

This result allows us to conclude that certain optimizations problems in hyperacute simplices—thus convex polytopes in general—are NP-hard.

Lemma 5.3. *Let $\mathcal{P}$ be a convex polytope with vertex set V. The optimization problem*

$$\begin{aligned} \min_{I\subseteq V, I\neq\emptyset} \quad & \frac{\|\boldsymbol{c}(\mathcal{P}_I)\|_2^2}{|I|} \\ s.t. \quad & \langle \boldsymbol{\sigma}_i, \boldsymbol{\sigma}_j\rangle = 0,\ i,j \in I, \end{aligned}$$

is NP-hard. In particular, it is NP-hard whenever $\mathcal{P}$ is the combinatorial simplex of a graph.

Proof. Let $\mathcal{P}$ be the combinatorial simplex of a graph G. Using that $\langle \boldsymbol{\sigma}_i, \boldsymbol{\sigma}_j\rangle = w(i,j)$, the condition that $\langle \boldsymbol{\sigma}_i, \boldsymbol{\sigma}_j\rangle = 0$ for all $i, j \in I$ translates to $(i,j) \in E(G)$ for all $i, j \in I$. Moreover, Equation (3.13) in Section 3.4 gives us

$$\frac{|I|}{\|c(\mathcal{S}_I)\|_2^2} = w_G(\delta I) = \mathrm{vol}(I),$$

for I an independent set. The above optimization problem can consequently be formulated as

$$\max_{I\subseteq V(G)} \mathrm{vol}_G(I), \quad \text{s.t.} \quad I \text{ is an independent set.}$$

which is precisely the Vertex-Weighted Independent-Set problem. ⊠

We can play a similar game by using the relationships furnished by the normalized Laplacian as opposed to the combinatorial Laplacian. Doing this removes the normalizing factor of $|I|$ from the optimization problem in the previous result.

Lemma 5.4. *Let $\mathcal{P}$ be a convex polytope with vertex set V. The optimization problem*

$$\begin{aligned} \min_{I\subseteq V, I\neq\emptyset} \quad & \|\boldsymbol{c}(\mathcal{P}_I)\|_2^2 \\ s.t. \quad & \langle \boldsymbol{\sigma}_i, \boldsymbol{\sigma}_j\rangle = 0,\ i,j\in I, \end{aligned}$$

is NP*-hard. In particular, it is hard for those polytopes and simplices with all vertices on the unit sphere.*

Proof. The proof is similar to the previous lemma. For $\mathcal{P}$ the normalized simplex of a graph G, the condition $\langle \boldsymbol{\sigma}_i, \boldsymbol{\sigma}_j\rangle = 0$ once again implies that I must be an independent set. Notice that for such an I, if $i\in I$ then $\delta(i)\cap I^c = \delta(i)$ (none of i's neighbours are in I). Therefore, Equation (3.16) yields

$$\widehat{\mathcal{L}}(\boldsymbol{\chi}_I) = \sum_{i\in I}\frac{1}{w(i)}\sum_{j\in I^c\cap\delta(i)} w(i,j) = \sum_{i\in I}\frac{w(i)}{w(i)} = |I|.$$

Equation (3.17) then implies that

$$\|c(\mathcal{P}_I)\|_2^2 = \frac{1}{|I|^2}\widehat{\mathcal{L}}_G(\boldsymbol{\chi}_I) = \frac{1}{|I|},$$

so the optimization problem can be formulated as

$$\max_{I\subseteq V(G)} |I|, \quad \text{s.t.} \quad I \text{ is an independent set},$$

which is the Independent-Set problem. ⊠

Next we extract a result based on the most (in)famous problem in computational graph theory: Graph isomorphism. An *isomorphism* between two graphs G_1 and G_2 is a bijection $f: V(G_1)\to V(G_2)$ such that $(u,v)\in E(G_1)$ iff $(f(u),f(v))\in E(G_2)$. We write $G_1\cong G_2$ if G_1 is isomorphic to G_2. The Graph-Isomorphism problem asks, given G_1, G_2 whether they are isomorphic. It's clear that Graph-Isomorphism $\in$ NP, but whether it is NP-complete remains an open question [MP14]. László Babai recently claims to have solved the problem in quasipolynomial time [Bab16]; the work is still being verified. Accordingly, we call a problem *Graph Isomorphism Hard* if it can be reduced to to Graph-Isomorphism. The more general problem of *subgraph* isomorphism, which asks whether G_1 has a subgraph isomorphic to G_2, is NP-complete [Coo71, Kar72]. We are interested in the relationship between graph isomorphism and polytope congruence.

THEOREM 5.1. *Deciding whether two hyperacute simplices are congruent is Graph Isomorphism Hard. Moreover, given two hyperacute simplices $\mathcal{S}_1 \in \mathbb{R}^d$ and $\mathcal{S}_2 \in \mathbb{R}^k$, deciding whether there exists k-dimensional face of $\mathcal{S}_1$ congruent to $\mathcal{S}_2$ is* NP*-hard.*

Proof. Let two graphs G_1 and G_2 be given. Compute their corresponding inverse simplices $\mathcal{S}_1^+$ and $\mathcal{S}_2^+$. We claim that $\mathcal{S}_1^+ \cong \mathcal{S}_2^+$ iff $G_1 \cong G_2$. If $\mathcal{S}_1^+ \cong \mathcal{S}_2^+$ then because they are both centred at the origin there exists a rotation matrix $\boldsymbol{Q}$ such that $\boldsymbol{Q}\boldsymbol{\Sigma}_1^+ = \boldsymbol{\Sigma}_2^+$. Since a rotation matrix does not change the relationship between the inner product of vectors[4], we see that $(\boldsymbol{\Sigma}_1^+)^t\boldsymbol{\Sigma}_1^+$ and $(\boldsymbol{\Sigma}_2^+)^t\boldsymbol{\Sigma}_2^+$ define the same Laplacian. Hence G_1 is isomorphic to G_2. Conversely, if $G_1 \cong G_2$, then there exists a relabelling of the vertices such that their Laplacian matrices are identical, as are the simplices. The second part of the statement follows by a similar reduction, and the fact that SUBGRAPH-ISOMORPHISM $\in$ NP-complete. ⊠

Kaibel and Schwarz [KS08] investigated the problem of polytope isomorphism. They define two polytopes is isomorphic if they have the same *face-lattice*—the lattice in which the nodes correspond to subsets of the vertices, and the lattice ordering is by face inclusion. Since congruent simplices share the same face lattice up to labelling, Theorem 5.1 implies their result.

§5.3. There and Back Again: A Tale of Graphs and Simplices

In this section we investigate the computational aspects of transitioning between the various objects which we've studied thus far. As one should expect given that the mapping between graphs and simplices relies on the eigenvalues and eigenvectors of graph Laplacians, the complexity of these transitions is intimately related with the complexity of computing eigendecompositions. Moreover, as we will see, if we are prepared to compute eigendecompositions (which is essentially cubic), then we can essentially compute all the objects from one another. We thus begin with a foray into the computational complexity of eigendecompositions, as we will be mostly interested in circumstances in which a transition can be computed in less time than this. Unfortunately, it will become clear that the complexity of computing a Laplacian eigendecomposition is actually a lower bound to many of the transitions.

Let $M(n)$ denote the complexity of the eigendecomposition problem. It is known that $M(n) = \widetilde{\Omega}(n^3 + n\log^2\log\epsilon)$ to obtain a relative error[5] of $2^{-\epsilon}$, while there exists algorithms which run in time $O(n^3 + n\log^2\log\epsilon)$ [PC99]. Let LAPLACIAN EIGENDECOMPOSION refer to the problem of computing the eigendecomposition of the Laplacian of a graph, i.e., computing its eigenvalues and eigenvectors. The complexity of LAPLACIAN EIGENDECOMPOSION does not seem to be known, really need to figure this out—how can it not be known? and we thus denote the lower bound by $\Omega(n^\tau)$ for some τ. We will assume, based on the difficulty of general eigendecomposition that $\tau > 2$.

Now, observe that given G, we can compute the combinatorial and nornalized Laplacians (and their inverses) by first constructing the combinatorial or normalized Laplacian

[4] A rotation matrix $\boldsymbol{Q}$ obeys $\boldsymbol{Q}^t\boldsymbol{Q} = \mathbf{I}$, hence $\langle \boldsymbol{Q}\mathbf{u}, \boldsymbol{Q}\mathbf{v}\rangle = \mathbf{u}^t\boldsymbol{Q}^t\boldsymbol{Q}\mathbf{v} = \langle \mathbf{u}, \mathbf{v}\rangle$.

[5] We note that the relative error is a necessary parameter of any algorithm because eigenvalues may be irrational.

			V				H			
From/To		G	$\mathcal{S}_G$	$\mathcal{S}_G^+$	$\widehat{\mathcal{S}}_G$	$\widehat{\mathcal{S}}_G^+$	$\mathcal{S}_G$	$\mathcal{S}_G^+$	$\widehat{\mathcal{S}}_G$	$\widehat{\mathcal{S}}_G^+$
	G	—	$\Omega(n^\tau)$	$\Omega(n^\tau)$	$\Omega(n^\tau)$	$\Omega(n^\tau)$	$\Omega(n^\tau)$	$\Omega(n^\tau)$		
V	$\mathcal{S}_G$	$O(n^3)$	—	$\Omega(n^\tau)$	$O(n^2)$		$\Omega(n^\tau)$	$O(1)$		
V	$\mathcal{S}_G^+$		$\Omega(n^\tau)$	—			$O(1)$	$\Omega(n^\tau)$		
V	$\widehat{\mathcal{S}}_G$		? / $O(n^2)$		—	$\Omega(n^\tau)$				
V	$\widehat{\mathcal{S}}_G^+$				$\Omega(n^\tau)$	—				
H	$\mathcal{S}_G$		$\Omega(n^\tau)$	$O(n^2)$			—	$\Omega(n^\tau)$		
H	$\mathcal{S}_G^+$		$O(n^2)$	$\Omega(n^\tau)$			$\Omega(n^\tau)$	—		
H	$\widehat{\mathcal{S}}_G$								—	
H	$\widehat{\mathcal{S}}_G^+$									—

Figure 5.1: Summary of results for precise mappings. A slash refers to a difference in runtimes when the graph is available versus when it isn't. The quantity before the slash indicates the runtime *without* the graph, after the slash the runtime *with* the graph. A question mark indicates that the runtime isn't known.

in $O(n^2)$, performing an eigendecomposition in time $O(n^\tau)$, and constructing the vertices of the simplices from the eigenvalues and eigenvectors in time $O(n^2)$. Using our assumption that $\tau > 2$, this takes total time $O(n^\tau)$. Moreover, starting with a simplex with vertex set $\mathbf{\Sigma}$, one can compute $\mathbf{\Sigma}^t\mathbf{\Sigma}$ in the time required for matrix multiplication, which is currently $O(n^{2.3727})$ [Wil12] and whose lower bound is $\Theta(n^\kappa)$ for some $2 \leq \kappa \leq 2.3727$ [Sto10]. If the simplex is the simplex of a graph then this yields the Laplacian (or its pseudoinverse) of the graph in time $O(n^{2.3727})$, and from here to any of its simplices in time $O(n^\tau)$. Hence, we can transition between the various simplices in time $O(n^{\max\{2.3727,\tau\}})$. In what follows therefore, we attempt to beat the barrier of $O(n^\tau)$.

Another question in which we might be interested is one of *certification*. That is, verifying whether a given simplex is one of the combinatorial or normalized simplices of a graph. We will investigate this possibility at the end of this section.

We begin by investigating the relationship between $\mathcal{S}$ and $\widehat{\mathcal{S}}$, when either $\mathcal{S}$ or $\widehat{\mathcal{S}}$ are given and we are told a priori that they are the simplices of a graph. The results obtained in this section are summarized in Figure 5.1.

Between $\mathcal{S}$ and $\widehat{\mathcal{S}}$. Let us consider the computational complexity of transitioning between $\mathcal{S}$ and $\widehat{\mathcal{S}}$ and vice versa. Let ϕ_{ij} (resp., $\widehat{\phi}_{ij}$) be the angle between $\boldsymbol{\sigma}_i$ and $\boldsymbol{\sigma}_j$ (resp., $\widehat{\boldsymbol{\sigma}}_i$ and $\widehat{\boldsymbol{\sigma}}_j$). Using the typical formula for the dot product in Euclidean space we have

$$\cos\phi_{ij} = \frac{\langle \boldsymbol{\sigma}_i, \boldsymbol{\sigma}_j \rangle}{\|\boldsymbol{\sigma}_i\|_2 \|\boldsymbol{\sigma}_j\|_2} = \frac{\boldsymbol{L}_G(i,j)}{\sqrt{w(i)w(j)}} = \widehat{\boldsymbol{L}}_G(i,j), \quad \text{and} \quad \cos\widehat{\phi}_{ij} = \frac{\langle \widehat{\boldsymbol{\sigma}}_i, \widehat{\boldsymbol{\sigma}}_j \rangle}{\|\widehat{\boldsymbol{\sigma}}_i\|_2 \|\widehat{\boldsymbol{\sigma}}_j\|_2} = \widehat{\boldsymbol{L}}_G(i,j),$$

using that $\|\widehat{\boldsymbol{\sigma}}_i\|_2 = 1$ for all i. That is, the angles between vertices in $\mathcal{S}$ in $\widehat{\mathcal{S}}$ are the same. Suppose we are given the simplex $\mathcal{S}$ and told it is the combinatorial simplex of a graph. For each $\boldsymbol{\sigma}_i = \boldsymbol{\Sigma}(\mathcal{S})$, define a new vertex

$$\boldsymbol{\gamma}_i = \frac{\boldsymbol{\sigma}_i}{\|\boldsymbol{\sigma}_i\|_2}.$$

Is it evident that the angle between $\boldsymbol{\gamma}_i$ and $\boldsymbol{\gamma}_j$ is identical to that between $\boldsymbol{\sigma}_i$ and $\boldsymbol{\sigma}_j$:

$$\frac{\langle \gamma_i, \gamma_j \rangle}{\|\gamma_i\|_2 \|\gamma_j\|_2} = \left\langle \frac{\boldsymbol{\sigma}_i}{\|\boldsymbol{\sigma}_i\|_2}, \frac{\boldsymbol{\sigma}_j}{\|\boldsymbol{\sigma}_j\|_2} \right\rangle = \cos(\phi_{ij}).$$

Therefore, it follows that the simplex with vertices is congruent to $\widehat{\mathcal{S}}$. This yields the following result.

Lemma 5.5. *Given a combinatorial simplex $\mathcal{S}$, a simplex congruent to $\widehat{\mathcal{S}}$ can be computed in time $O(n^2)$.*

Proof. Given $\mathcal{S}$, define the vertices $\boldsymbol{\gamma}_i$ as above. Computing $\|\boldsymbol{\sigma}_i\|_2$ takes time $O(n)$ and must be done for each vertex. ⊠

Given the relative ease with which we can transition from $\mathcal{S}$ to $\widehat{\mathcal{S}}$, it is somewhat surprising that it is much more difficult to transition from $\widehat{\mathcal{S}}$ to $\mathcal{S}$, especially if the underlying graph G is not given. The obvious tactic is, given the vertices $\{\widehat{\boldsymbol{\sigma}}_i\}$, to define vertices $\widehat{\boldsymbol{\sigma}}_i\sqrt{w(i)}$, which, since $\sqrt{w(i)} = \|\boldsymbol{\sigma}_i\|_2$, have the same magnitude as $\boldsymbol{\sigma}_i$. As above, the scaling does not affect the angle between the vertices, and thus the simplex with these vertices is congruent to $\mathcal{S}$. However, it's not clear how to obtain the value $\sqrt{w(i)}$ from $\widehat{\mathcal{S}}$. Using that $\langle \widehat{\boldsymbol{\sigma}}_i, \widehat{\boldsymbol{\sigma}}_j \rangle = (w(i)w(j))^{-1/2}$ we can write

$$w(i)^{1/2} = -\sum_{j \neq i} w(j)^{-1/2} \Big/ \sum_{j \neq i} \langle \widehat{\boldsymbol{\sigma}}_i, \widehat{\boldsymbol{\sigma}}_j \rangle,$$

which yields a non-linear system of equations.

Of course, if we are given the graph then we have access to $\sqrt{w(i)}$ and can compute $\widehat{\boldsymbol{\sigma}}_i w(i)^{1/2}$ in time $O(n)$. The following result is then immediate.

Lemma 5.6. *Given a graph $G = (V, E, w)$ and its normalized simplex $\widehat{\mathcal{S}}_G$, a simplex congruent to the combinatorial simplex $\mathcal{S}_G$ can be computed in $O(n^2)$ time.*

Think about possible lower bounds on computing $\mathcal{S}$ from $\widehat{\mathcal{S}}$ when no graph is given. Doing so would imply knowledge of $\sqrt{\boldsymbol{w}}$ (taking ratio of lengths of vertices). What does this imply? Does knowledge of $\boldsymbol{w}$ give us some knowledge of the graph structure from which we can extract a lower bound?

$\mathcal{S}$ and $\mathcal{S}^+$. Let us suppose that we can generate $\mathcal{S}^+$ from $\mathcal{S}$ (or vice versa) in time $O(g(n))$. Note that for $i < n$,

$$\lambda_i = \frac{\lambda_i^{1/2}\boldsymbol{\varphi}_j(i)}{\lambda_i^{-1/2}\boldsymbol{\varphi}_j(i)} = \frac{\boldsymbol{\sigma}_i(j)}{\boldsymbol{\sigma}_i^+(j)}, \quad \text{and} \quad \boldsymbol{\varphi}_i(j) = \frac{\boldsymbol{\sigma}_j(i)}{\lambda_i^{1/2}},$$

hence knowledge of $\{\boldsymbol{\sigma}_i\}$ and $\{\boldsymbol{\sigma}_i^+\}$ yields knowledge of the eigendecomposition of the underlying graph G in $O(n^2)$ time ($O(n)$ to determine all the eigenvalues and $O(n^2)$ to determine the eigenvectors). The same argument holds *mutatis mutandis* for the normalized Laplacian.

Lemma 5.7. *If a* V*-description of* $\mathcal{S}^+$ *(resp.,* $\widehat{\mathcal{S}}^+$*) can be generated from a* V*-description of* $\mathcal{S}$ *(resp.,* $\widehat{\mathcal{S}}$*) or vice versa in time* $O(g(n))$*, then* Laplacian Eigendecomposion *can be solved in time* $O(g(n) + n^2)$ *for arbitrary weighted graphs. Consequently* $g(n) = \Omega(n^\tau)$*.*

An alternate way of seeing that constructing the inverse simplex from its dual is computationally challenging is to recall from Section 3.4 that $\mathcal{S}_{\{i\}^c}$ is contained in the hyperplane $\{\boldsymbol{x} \in \mathbb{R}^{n-1} : \langle \boldsymbol{x}, \boldsymbol{\sigma}_i^+\rangle = -1/n\}$ (Lemma 3.8) and that that $\boldsymbol{\sigma}_i^+$ is perpendicular to $\mathcal{S}_{\{i\}^c}$ (Lemma 3.4). Hence, computing the inverse simplex would imply that we had computed normal vectors to n hyperplanes, the typical procedure for which typically involves computing an $n \times n$ determinant and requires $O(n^3)$ time.

We now consider transitioning between different descriptions of $\mathcal{S}$ and $\mathcal{S}^+$. Let us recall that the H-description of $\mathcal{S}$ and $\mathcal{S}^+$ yield immediate insight into the vertices of its inverse as $\mathcal{S} = \cap_i\{\boldsymbol{x} : \langle \boldsymbol{x}, \boldsymbol{\sigma}_i^+\rangle \geq -1/n\}$ and $\mathcal{S}^+ = \cap_i\{\boldsymbol{x} : \langle \boldsymbol{x}, \boldsymbol{\sigma}_i\rangle \geq -1/n\}$ (Equations (3.7) and (3.8)). Consequently, given given a H-description of one of these simplices, the vertices of its inverse are recoverable in quadratic time. This yields the following result.

Lemma 5.8. *Suppose that in time* $t(n)$ *we can compute an* H*-description of* $\mathcal{S}$ *(resp.,* $\mathcal{S}^+$*) given its* V*-description. Then a* V*-description of* $\mathcal{S}^+$ *(resp.,* $\mathcal{S}$*) is recoverable in time* $t(n) + O(n^2)$*, implying by Lemma 5.7 that* $t(n) = \Omega(n^\tau)$*.*

We also note that a consequence of the relationship between the vertices of $\mathcal{S}$ and the H-description of $\mathcal{S}^+$ that given V-description of $\mathcal{S}$ or $\mathcal{S}^+$, we have immediate access to the H-description of its inverse.

A similar result for going from between the H-description of the combinatorial simplices. The argument runs as usual: Given an H-description of $\mathcal{S}$, suppose we can generate an H-description of $\mathcal{S}^+$ in time $t(n)$. We can obtain the vertices $\{\boldsymbol{\sigma}_i^+\}$ from the H-description of $\mathcal{S}$, and the vertices $\{\boldsymbol{\sigma}_i\}$ from the H-description of $\mathcal{S}^+$. Using these, we can then obtain the eigendecomposition of G in time $O(n^2)$. That is, we can solve Laplacian Eigendecomposion in time $t(n) + O(n^2)$ yielding that $t(n) = \Omega(n^\tau)$.

Lemma 5.9. *Generating an* H*-description of* $\mathcal{S}_G$ *given an* H*-description of* $\mathcal{S}_G^+$*, and vice versa, requires time* $\Omega(n^\tau)$*.*

Between G and $\mathcal{S}$ or $\widehat{\mathcal{S}}$. Similar kinds of results hold in these cases. Assume that we obtain the simplex $\mathcal{S}_G$ from G. Notice that

$$\sum_{i=1}^{n-1} \boldsymbol{\sigma}_i(j)^2 = \lambda_j \sum_{i=1}^{n-1} \boldsymbol{\varphi}_j(i) = \lambda_j \left(1 - \frac{1}{n}\right),$$

so

$$\lambda_j = \frac{\sum_{i=1}^{n-1} \boldsymbol{\sigma}_i(j)}{1 - 1/n},$$

which can be computed in $O(n)$ time. Then, as above, knowledge of the eigenvalues furnishes knowledge of the eigenvectors in $O(n^2)$ time. Running almost identical arguments for $\mathcal{S}^+$, $\widehat{\mathcal{S}}$, or $\widehat{\mathcal{S}}^+$ yields an almost equivalent result as in the previous section.

Lemma 5.10. *If either the combinatorial or normalized simplex or their inverses can be generated from a graph G in $O(g(n))$ time, then* Laplacian Eigendecomposion *can be solved in time $O(g(n) + n^2)$ for arbitrary weighted graphs. Consequently $g(n) = \Omega(n^\tau)$.*

The information encoded in the dot products between vertices allow us to make queries regarding the edge weights, but each query takes $O(n)$ time since we must compute a dot product between two vectors of length $n-1$. Hence, re-constructing the graph or its Laplacian takes $O(n^3)$ if we wish do it precisely.

Let us now consider transitioning between G and the H-description of a simplex. The following lemma summarizes the consequences of this relationship.

Lemma 5.11. *Given a graph G suppose an H-description of $\mathcal{S}$ (resp., $\mathcal{S}^+$) can be generated in time $g(n)$. Then a V-description of $\mathcal{S}^+$ (resp., $\mathcal{S}$ can be obtained in time $O(g(n) + n^2)$ starting from G. Consequently, by Lemma 5.10, $g(n) = \Omega(n^\tau)$.*

Between different descriptions of the simplices. Here we investigate the interplay between the various different descriptions of the simplices.

The following is an immediate consequence of Lemma 3.20.

Corollary 5.1. *If $\mathcal{T}$ is a centred simplex in H-description, we can obtain a V-description of $\mathcal{T}^D$ in quadratic time. In particular, given an H-description of the combinatorial simplex $\mathcal{S}_G$ (resp., inverse combinatorial simplex $\mathcal{S}_G^+$) of a graph G, a V-description of $\mathcal{S}_G^+$ (resp., $\mathcal{S}_G$) is obtainable in quadratic time.*

Due to the fact that $\widehat{\mathcal{S}}_G^+$ is not the dual of $\widehat{\mathcal{S}}_G$ Lemma 3.20 is less useful here.

Lemma 5.12. *Generating an V-description of the simplex $\mathcal{S}$ given its H-description requires time $\Omega(n^\tau)$ for any $\mathcal{S} \in \{\mathcal{S}_G, \mathcal{S}_G^+\}$.*

Proof. Consider $\mathcal{S}_G$; the argument is similar for $\mathcal{S}_G^+$. Suppose obtaining the H-description takes time $t(n)$. Due to the properties of the hyperplane representations, this yields access to both sets of vertices in time $t(n) + O(n^2)$. Using the arithmetic in the previous section, this implies that we can obtain the eigenvalues and eigenvectors of G in time $O(n^2)$, i.e., we can solve Laplacian Eigendecomposion in time $t(n) + O(n^2)$ implying that $t(n) = \Omega(n^\tau)$. ⊠

Verification. We now turn to discussing the complexity of verifying whether a given simplex is the simplex of graph. In time $O(n^{2.3727})$ we can compute $\mathbf{\Sigma}^t\mathbf{\Sigma}$. We can check whether this is equal to $\boldsymbol{L}_G$ for some G by verifying whether (i) $\mathbf{\Sigma}^t\mathbf{\Sigma}\mathbf{1} = \mathbf{0}$, (ii) $(\mathbf{\Sigma}^t\mathbf{\Sigma})(i,i) > 0$ for all i and (iii) $(\mathbf{\Sigma}^t\mathbf{\Sigma})(i,j) \leq 0$ for all $i \neq j$. These three steps require time $O(n^3)$. We can check whether $\mathbf{\Sigma}^t\mathbf{\Sigma}$ is equal to $\widehat{\boldsymbol{L}}_G$ for some G by first ensuring, similarly to above, that (iii) holds and that $(\mathbf{\Sigma}^t\mathbf{\Sigma})(i,i) = 1$ for all i. Then we compute the kernel of $\mathbf{\Sigma}^t\mathbf{\Sigma}$ in cubic time by means of Gaussian elimination [KS99] to obtain a vector $\mathbf{v}$ equal to $\sqrt{\boldsymbol{w}_G}$ (if indeed $\mathbf{\Sigma}^t\mathbf{\Sigma} = \widehat{\boldsymbol{L}}_G$) up to scaling. To determine whether $\mathbf{v}$ does represent valid weightings of the vertices, we check whether $(\mathbf{\Sigma}^t\mathbf{\Sigma})(i,j)\mathbf{v}(j)$ is constant for all i. In this case $\mathbf{\Sigma}^t\mathbf{\Sigma}$ is equal to the normalized Laplacian of some graph. This can also be done in cubic time. We therefore see that we can verify whether a given simplex is the combinatorial or normalized simplex of a graph in cubic time. It's not clear whether it can be done faster, however. Unsure, think about this.

Moreover, we note that in cubic time we can check whether all the angles θ_{ij} between the faces $\mathcal{T}_{\{i\}^c}$ and $\mathcal{T}_{\{j\}^c}$ are non-obtuse, in which case $\mathcal{T}$ is the inverse simplex of some graph.

§5.4. Approximations

Here we are concerned with approximations of various sorts. We begin with an eye towards the problem of dimensionality. Specifically, Theorem 3.1 yields simplices of dimension $n-1$ for a graph on n vertices. In many application areas, graphs may have thousands to millions of vertices. Working in a Euclidean space of this size can be unwieldy. Our first result, therefore, demonstrates that we can "approximate" the simplex in a lower dimensional space.

5.4.1. Embedding $\mathcal{S}^+$ in lower dimensions

The idea is to map each vertex to a point in $\mathbb{R}^d$, for $d \ll n$, while maintaining the general form of the simplex. By this we mean that we'd like the distance between the new points to remain approximately as they were. If possible, we'd also like to new, lower dimensional object (note that it won't be a simplex because there will be n points in R^d) to retain some of the properties which relate it to the underlying graph. In particular, we'd like the gram matrix of the new points to approximate the gram matrix of the original set of points. As it turns out, a mapping meeting both of these criteria exists and is computable in polynomial time. It will rely on the Johnson-Lindenstrauss (JL) Lemma [JL84, DG03].

Theorem 5.2 (Johnson-Lindenstrauss). *Let $\mathcal{X} \subseteq \mathbb{R}^k$ be a set of n points, for some $k \in \mathbb{N}$. For any $\epsilon > 0$ and $d \geq 8\log(n)\epsilon^{-2}$ there exists a map $g_\epsilon : \mathbb{R}^k \to \mathbb{R}^d$ such that*

$$(1-\epsilon)\|\mathbf{u}-\mathbf{v}\|_2^2 \leq \|g_\epsilon(\mathbf{u}) - g_\epsilon(\mathbf{v})\|_2^2 \leq (1+\epsilon)\|\mathbf{u}-\mathbf{v}\|_2^2,$$

for all $\mathbf{u},\mathbf{v} \in \mathcal{X}$.

Now, let us suppose we have the vertices $\{\boldsymbol{\sigma}_i^+\}$ of the inverse simplex. Let $\mathcal{X} = \{\boldsymbol{\sigma}_i^+\} \cup \{\mathbf{0}\}$. Apply the JL Lemma to $\mathcal{X}$ to obtain $n+1$ points in $\mathbb{R}^d$, for $d = O(\log(n)/\epsilon^2)$. Let f be the mapping, e.g., $\boldsymbol{\sigma}_i^+$ is sent to $f(\boldsymbol{\sigma}_i^+)$. By JL, have

$$(1-\epsilon)\|\boldsymbol{x}-\boldsymbol{y}\|_2^2 \leq \|f(\boldsymbol{x})-f(\boldsymbol{y})\|_2^2 \leq (1+\epsilon)\|\boldsymbol{x}-\boldsymbol{y}\|_2^2,$$

for all $\boldsymbol{x},\boldsymbol{y} \in \{\boldsymbol{\sigma}_1^+,\dots,\boldsymbol{\sigma}_n^+,\mathbf{0}\}$. Apply a linear transformation to the points so that $f(\mathbf{0})$ coincides with the origin $\mathbf{0} \in \mathbb{R}^d$. Note that this does not affect the distances between the points themselves, and does not damage the approximation. Update f to reflect this transformation. For all i,j, let $\epsilon_{i,j}$ denote the true error of the mapping, i.e.,

$$\left\|f(\boldsymbol{\sigma}_i^+)-f(\boldsymbol{\sigma}_j^+)\right\|_2^2 = (1+\epsilon_{i,j})\left\|\boldsymbol{\sigma}_i^+-\boldsymbol{\sigma}_j^+\right\|_2^2,$$

where $|\epsilon_{i,j}| \leq \epsilon$. Define $\epsilon_{i,\mathbf{0}}$ similarly. Then,

$$\|f(\boldsymbol{\sigma}_i^+)\|_2^2 = \|f(\boldsymbol{\sigma}_i^+)-f(\mathbf{0})\|_2^2 = (1+\epsilon_{i,\boldsymbol{o}})\|\boldsymbol{\sigma}_i^+\|_2^2 = (1+\epsilon_{i,\boldsymbol{o}})\boldsymbol{L}_G^+(i,i),$$

hence,

$$\begin{aligned}\left\|f(\boldsymbol{\sigma}_i^+)-f(\boldsymbol{\sigma}_j^+)\right\|_2^2 &= \langle f(\boldsymbol{\sigma}_i^+)-f(\boldsymbol{\sigma}_j^+), f(\boldsymbol{\sigma}_i^+)-f(\boldsymbol{\sigma}_j+)\rangle \\ &= \|f(\boldsymbol{\sigma}_i^+)\|_2^2 + \left\|f(\boldsymbol{\sigma}_j^+)\right\|_2^2 - 2\langle f(\boldsymbol{\sigma}_i^+), f(\boldsymbol{\sigma}_j^+)\rangle,\end{aligned}$$

implying that

$$\begin{aligned}\langle f(\boldsymbol{\sigma}_i^+), f(\boldsymbol{\sigma}_j^+)\rangle &= -\frac{1}{2}\left((1+\epsilon_{i,j})\left\|\boldsymbol{\sigma}_i^+-\boldsymbol{\sigma}_j^+\right\|_2^2 - (1+\epsilon_{i,\boldsymbol{o}})\boldsymbol{L}_G^+(i,i) - (1+\epsilon_{j,\boldsymbol{o}})\boldsymbol{L}_G^+(j,j)\right) \\ &= -\frac{1}{2}((1+\epsilon_{i,j})r(i,j) - (1+\epsilon_{i,\boldsymbol{o}})\boldsymbol{L}_G^+(i,i) - (1+\epsilon_{j,\boldsymbol{o}})\boldsymbol{L}_G^+(j,j)) \\ &= -\frac{1}{2}((1+\epsilon_{i,j})(\boldsymbol{L}_G^+(i,i) - \boldsymbol{L}_G^+(j,j) - 2\boldsymbol{L}_G^+(i,j)) \\ &\qquad - (1+\epsilon_{i,\boldsymbol{o}})\boldsymbol{L}_G^+(i,i) - (1+\epsilon_{j,\boldsymbol{o}})\boldsymbol{L}_G^+(j,j)) \\ &= (1+\epsilon_{i,j})\boldsymbol{L}_G^+(i,j) + \varepsilon(i,j),\end{aligned}$$

where

$$\varepsilon(i,j) \stackrel{\text{def}}{=} \frac{1}{2}(\epsilon_{i,\boldsymbol{o}}-\epsilon_{i,j})\boldsymbol{L}_G^+(i,i) + (\epsilon_{j,\boldsymbol{o}}-\epsilon_{i,j})\boldsymbol{L}_G^+(i,j),$$

is an error term dictated by $\epsilon_{i,j}, \epsilon_{i,\boldsymbol{o}}$ and $\epsilon_{j,\boldsymbol{o}}$. Setting

$$M = \max_i \boldsymbol{L}_G^+(i,i),$$

we can bound the error term via repeated applications of the triangle inequality:

$$\begin{aligned}|\varepsilon(i,j)| &\leq \frac{1}{2}\left(|(\epsilon_{i,\boldsymbol{o}}-\epsilon_{i,j})\boldsymbol{L}_G^+(i,i)| + |(\epsilon_{j,\boldsymbol{o}}-\epsilon_{i,j})\boldsymbol{L}_G^+(i,j|\right) \\ &\leq \frac{1}{2}\left([|\epsilon_{i,j}|+|\epsilon_{i,\boldsymbol{o}}|]\boldsymbol{L}_G^+(i,i) + [|\epsilon_{i,j}|+|\epsilon_{j,\boldsymbol{o}}|]\boldsymbol{L}_G^+(j,j)\right) \\ &\leq \frac{1}{2}(2\epsilon\boldsymbol{L}_G^+(i,i) + 2\epsilon\boldsymbol{L}_G^+(j,j)) \leq 2\epsilon M,\end{aligned}$$

since $|\epsilon_{i,j}|, |\epsilon_{i,\boldsymbol{o}}|, |\epsilon_{j,\boldsymbol{o}}| \leq |\epsilon|$. Setting $f(\boldsymbol{\Sigma}^+) = (f(\boldsymbol{\sigma}_1^+), \ldots, f(\boldsymbol{\sigma}_n^+)) \in \mathbb{R}^{d\times n}$, this approximation implies that

$$\boldsymbol{L}_G^+ - O(\epsilon M)\mathbf{I} \leq f(\boldsymbol{\Sigma}^+)^t f(\boldsymbol{\Sigma}^+) \leq \boldsymbol{L}_G^+ + O(\epsilon M)\mathbf{I}.$$

In other words, we can approximately recover the Gram matrix $\boldsymbol{L}_G^+ = \boldsymbol{\Sigma}^+\boldsymbol{\Sigma}^+$ using the lower dimensional matrix $f(\boldsymbol{\Sigma}^+)$.

The JL mapping maintains other approximate information of the graph. For example, it is well-known that the effective resistance between two vertices is related to the probability that this edge is in a random spanning tree as

$$r^{\text{eff}}(i,j) = \frac{1}{w(i,j)} \Pr_{T\sim\mu}[(i,j) \in T],$$

where μ is the uniform distribution over all spanning trees [BP93]. Hence,

$$\left\| f(\boldsymbol{\sigma}_i^+) - f(\boldsymbol{\sigma}_j^+) \right\|_2^2 \in \frac{1}{w(i,j)}[(1-\epsilon), (1+\epsilon)] \Pr_{T\sim\mu}[(i,j) \in T].$$

5.4.2. Approximating the distances of $\mathcal{S}^+$

Here we remark that we can leverage an elegant result of Spielman and Srivastava [SS11] in order to approximate the distance matrix $\boldsymbol{D}(\{\boldsymbol{\sigma}_i^+\})$.

Theorem 5.3 ([SS11]). *For any $\epsilon > 0$ and graph $G = (V, E, w)$, there exists an algorithm which computes a matrix $\widetilde{\boldsymbol{R}} \in \mathbb{R}^{O(\log(n)\epsilon^{-2})\times n}$ such that*

$$(1-\epsilon)r(i,j) \leq \left\| \widetilde{\boldsymbol{R}}(\boldsymbol{\chi}_i - \boldsymbol{\chi}_j) \right\|_2^2 \leq (1+\epsilon)r(i,j).$$

The algorithm runs in time $\widetilde{O}(|E|\log(r)/\epsilon^2)$, where

$$r = \frac{\max_{i,j} w(i,j)}{\min_{i,j} w(i,j)}.$$

Given a graph $G = (V, E, w)$, we use the algorithm of Theorem 5.3 to compute all the approximate distances $\left\| \boldsymbol{\sigma}_i^+ - \boldsymbol{\sigma}_j^+ \right\|_2^2 = r^{\text{eff}}(i,j)$ in time

$$\widetilde{O}(|E|\log(r)/\epsilon^2) + O(|E|\log(n)/\epsilon^2) = \widetilde{O}(|E|/\epsilon^2),$$

assuming $r = O(1)$. Note that we can compute a single effective resistance in time $O(\log n/\epsilon^2)$, since it involves simply computing the ℓ_2 norm the vector $\widetilde{\boldsymbol{R}}(\boldsymbol{\chi}_i - \boldsymbol{\chi}_j)$ which is simply the difference of two columns of $\widetilde{\boldsymbol{R}}$.

Will say more, but unclear exactly where this is heading.

5.4.3. Low Rank Approximations of $\boldsymbol{L}_G$

In Section 5.4.1, we asked how to reduce the dimension of the simplex while (approximately) maintaining several of its properties. However, we might instead reduce the dimensionality of the Laplacian. This section explores this prospect.

Let us suppose the we have obtained a low rank—k, say—approximation of $\boldsymbol{L}_G$, written $\widetilde{\boldsymbol{L}}$. We might then ask several questions:

1. Is $\widetilde{\boldsymbol{L}}$ still a gram matrix? That is, can $\widetilde{\boldsymbol{L}}$ be written $\widetilde{\boldsymbol{\Sigma}}^t\widetilde{\boldsymbol{\Sigma}}$ where $\widetilde{\boldsymbol{\Sigma}}$ is the vertex matrix of some set of points, $P = \{\boldsymbol{p}_1, \dots, \boldsymbol{p}_\ell\}$? If so, what is the relationship between $\boldsymbol{\Sigma}$ and $\widetilde{\boldsymbol{\Sigma}}$, where $\boldsymbol{\Sigma} = \boldsymbol{\Sigma}(\mathcal{S}_G)$ is the usual vertex matrix of the combinatorial simplex of G? If $\widetilde{\boldsymbol{L}}$ has rank k then P spans a subspace of dimension k and $\mathrm{conv}(P)$ forms a polytope in that space. What is the relationship between the geometry of $\mathrm{conv}(P)$ and $\mathcal{S}_G$?

2. Is $\widetilde{\boldsymbol{L}}$ useful in helping estimate properties of the simplex $\mathcal{S}_G$? For example, if one could bound the difference in the quadratic products of $\boldsymbol{L}_G$ and $\widetilde{\boldsymbol{L}}$, this would imply (via the results in Section 3.4) that we could estimate many of the properties of $\mathcal{S}_G$.

Of course, we have chosen to work with $\boldsymbol{L}_G$ and $\mathcal{S}_G$ for convenience; we could have asked the same questions of $\widehat{\boldsymbol{L}}_G$ and $\widehat{\mathcal{S}}_G$.

Still working on this — unsure if there's anything here. Let us examine a specific low rank approximation proposed by Drineas and Mahoney [DM05], which finds low rank approximations to Gram matrices. We will give a brief overview of their method in general, and then elaborate on how it applies to our case in particular. Let $\boldsymbol{M} \in \mathbb{R}^{n\times m}$ be a gram matrix. Using the probability distribution $F(i) = \boldsymbol{M}(i,i)^2/\operatorname{tr}(\boldsymbol{M}^2)$ sample $a \le m$ columns of $\boldsymbol{M}$ independently at random and with replacement, where a is some given parameter. Let $I \subseteq [n]$, $|I| \le a$, be the indices of sampled columns. Let $\boldsymbol{C} \in \mathbb{R}^{n\times a}$ be the matrix formed by these columns (that is, $\boldsymbol{C} = \boldsymbol{M}(\cdot, I)$). Let $\boldsymbol{Q}$ be the matrix $\boldsymbol{M}(I,I) \in \mathbb{R}^{a\times a}$, i.e., the submatrix of M with entries corresponding to indices in I, and $\boldsymbol{Q}_k^+$ the optimal rank k-approximation to $\boldsymbol{Q}^+$, the pseudoinverse of $\boldsymbol{Q}$ (section 2.2.1). The low rank approximation to $\boldsymbol{M}$ is then

$$\widetilde{\boldsymbol{M}} \stackrel{\text{def}}{=} \boldsymbol{C}\boldsymbol{M}(I,I)_k^+\boldsymbol{C}^t.$$

THEOREM 5.4 ([DM05]). *Let $\boldsymbol{M}$ be a gram matrix and let $\widetilde{\boldsymbol{M}}$ be as above. Let $\epsilon > 0$, $k \le c \in \mathbb{N}$. If $c = \Omega(k/\epsilon^4)$, then*

$$\left\|\boldsymbol{M} - \widetilde{\boldsymbol{M}}\right\|_\kappa \le \|\boldsymbol{M} - \boldsymbol{M}_k\|_\kappa + \epsilon \operatorname{tr}(\boldsymbol{M}^2),$$

for $\kappa = 2, F$.

Let us analyze how this result translates to the case when $\boldsymbol{M} = \boldsymbol{L}_G$. Let I and $\boldsymbol{C}$ be as above. First we observe that $\boldsymbol{L}_G(I,I)$ is simply the Laplacian on the subgraph $G[I]$. Put $\widetilde{G} = G[I]$. Performing an eigendecomposition, write

$$\boldsymbol{L}_{\widetilde{G}} = \sum_{r=1}^{|I|} \mu_r \boldsymbol{\nu}_r \boldsymbol{\nu}_r^t,$$

for where $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_{|I|} = 0$ and $\{\boldsymbol{\nu}_r\}$ are the eigenvalues and eigenvectors of $\boldsymbol{L}_{\widetilde{G}}$, respectively. The results of Section 2.2.1 then dictate that

$$\boldsymbol{L}_{\widetilde{G}}^{+} = \sum_{r=1}^{|I|} \frac{1}{\mu_r} \boldsymbol{\nu}_r \boldsymbol{\nu}_r^t,$$

and so the best rank k approximation to $\boldsymbol{L}_{\widetilde{G}}$ is given by

$$\boldsymbol{L}_k \stackrel{\text{def}}{=} (\boldsymbol{L}_{\widetilde{G}}^{+})_k = \sum_{r=1}^{k} \frac{1}{\mu_r} \boldsymbol{\nu}_r \boldsymbol{\nu}_r^t.$$

The approximation for $\boldsymbol{L}_G$ is thus given by $\widetilde{\boldsymbol{L}} = \boldsymbol{C}\boldsymbol{L}_k\boldsymbol{C}^t = \boldsymbol{C}\boldsymbol{L}_k^{1/2}\boldsymbol{L}_k^{t/2}\boldsymbol{C}^t = (\boldsymbol{L}_k^{t/2}\boldsymbol{C}^t)^t\boldsymbol{L}_k^{t/2}\boldsymbol{C}^t$. That is, we can view $\widetilde{\boldsymbol{L}}$ as the gram matrix of the vectors given by the columns of $\widetilde{\boldsymbol{\Sigma}} = (\boldsymbol{L}_k^{t/2}\boldsymbol{C}^t)$.

Let us examine $\widetilde{\boldsymbol{\Sigma}}^t = \mathbb{C}\boldsymbol{L}_k^{t/2}$. First consider $\operatorname{rank}(\boldsymbol{C})$, which we claim is $|I|$. Suppose $\boldsymbol{C}\boldsymbol{f} = \boldsymbol{0}$, where $\boldsymbol{f} : I \to \mathbb{R}$. Extend $\boldsymbol{f}$ to $\widehat{\boldsymbol{f}} : [n] \to \mathbb{R}$ by setting $\widehat{\boldsymbol{f}}(u) = 0$ for all $u \in [n] \setminus I$. Then

$$(\boldsymbol{L}_G\widehat{\boldsymbol{f}})(k) = \sum_{i\in[n]} \boldsymbol{L}_G(k,i)\widehat{\boldsymbol{f}}(i) = \sum_{i\in I} \boldsymbol{L}_G(k,i)\boldsymbol{f}(i) + \sum_{i\in[n]\setminus I} \boldsymbol{L}_G(k,i)\widehat{\boldsymbol{f}}(i) = \sum_{i\in I} \boldsymbol{C}(k,i)\boldsymbol{f}(i) = 0,$$

implying that $\boldsymbol{L}_G\widehat{\boldsymbol{f}} = \boldsymbol{0}$, so $\widehat{\boldsymbol{f}} \in \operatorname{span}(\boldsymbol{1})$). However, as long as $|I| \neq [n]$, this is impossible since $\widehat{\boldsymbol{f}}([n] \setminus I) = \boldsymbol{0}$. Therefore, so long as $c < n$, we have $\operatorname{rank}(\boldsymbol{C}) = c$. We now claim that $\operatorname{rank}(\boldsymbol{C}\boldsymbol{L}_k^{t/2}) = \operatorname{rank}(\boldsymbol{L}_k^{t/2})$, which is easier to prove in the abstract.

Lemma 5.13. *Let $\boldsymbol{S} : \mathbb{R}^n \to \mathbb{R}^\ell$, $T \in \mathbb{R}^m \to \mathbb{R}^n$ be linear maps with $\operatorname{rank}(\boldsymbol{S}) = \ell$. Then $\operatorname{rank}(\boldsymbol{S}\boldsymbol{T}) = \operatorname{rank}(\boldsymbol{T})$.*

Proof. If $\boldsymbol{T}\boldsymbol{f} = \boldsymbol{0}$ then clearly $\boldsymbol{S}\boldsymbol{T}\boldsymbol{f} = \boldsymbol{0}$ so $\dim\ker(\boldsymbol{T}) \leq \dim\ker(\boldsymbol{S}\boldsymbol{T})$. On the other hand, if $\boldsymbol{S}\boldsymbol{T}\boldsymbol{f} = \boldsymbol{0}$ then because $\boldsymbol{S}$ is full rank, $\boldsymbol{T}\boldsymbol{f} = \boldsymbol{0}$ implying that $\dim\ker\boldsymbol{T} \geq \ker\boldsymbol{S}\boldsymbol{T}$. By the rank nullity Theorem (e.g., [Axl97]) $\operatorname{rank}(\boldsymbol{S}\boldsymbol{T}) + \dim\ker\boldsymbol{S}\boldsymbol{T} = n = \operatorname{rank}(\boldsymbol{T}) + \dim\ker\boldsymbol{T}$ from which the result follows immediately. ⊠

Taking $\boldsymbol{C} = \boldsymbol{S}$ and $\boldsymbol{T} = \boldsymbol{L}_k^{t/2}$ in the above lemma gives that $\operatorname{rank}(\boldsymbol{C}\boldsymbol{L}_k^{t/2}) = k$. Consequently, the vertex matrix $\widetilde{\boldsymbol{\Sigma}} \in \mathbb{R}^{|I|\times n}$ contains n vectors in $\mathbb{R}^{|I|}$. Moreover,

$$\operatorname{rank}(\widetilde{\boldsymbol{L}}) = \operatorname{rank}(\widetilde{\boldsymbol{\Sigma}}^t\widetilde{\boldsymbol{\Sigma}}) = \operatorname{rank}(\widetilde{\boldsymbol{\Sigma}}) = k,$$

meaning the n vectors span a k-dimensional space.

One might hope that the approximation matrix $\widetilde{\boldsymbol{L}}$ was a Laplacian, but this does not seem to be the case in general. While it is true that $\widetilde{\boldsymbol{L}}(i,i) \geq 0$ (by virtue of being a gram matrix) and that $\widetilde{\boldsymbol{L}}\boldsymbol{1} = \boldsymbol{0}$ (this follows since $\boldsymbol{C}^t\boldsymbol{1} = \boldsymbol{0}$ because the rows of $\boldsymbol{C}^t$ are columns and hence rows of $\boldsymbol{L}_G$). However,

$$\widetilde{\boldsymbol{L}}(i,j) = \sum_{r,s=1}^{c} \boldsymbol{C}(i,r)\boldsymbol{C}(j,s)\boldsymbol{L}_k(r,s),$$

which does not look to be necessarily non-positive.

Chapter 6

Conclusion

§6.1. Open Problems and Future Directions

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