The Graph-Simplex Correspondence and its Algorithmic Foundations

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Abstract

We present and study the graph-simplex correspondence—a tool providing a series of relationships between weighted, undirected graphs on n vertices and simplices in $(n-1)$-dimensional Euclidean space. The core of the correspondence is a bijection between graphs and hyperacute simplices, first uncovered by Miroslav Fiedler. We consolidate Fiedler's work on the subject and expand on it in several ways.

The first relates purely to the mathematical properties of the correspondence. Among other things, we extend the correspondence to the normalized Laplacian matrix $\widehat{\boldsymbol{L}}_G$ (whereas previously only the combinatorial Laplacian, $\boldsymbol{L}_G$, had been used), develop new equations and inequalities relating aspects of the simplex to those of the graph, and give an isometry between a graph's "inverse combinatorial simplex" and an n-dimensional polytope arising from the Laplacian's pseudoinverse.

Secondly, we examine the algorithmic underpinnings and consequences of the correspondence. We begin by demonstrating that it can be used to draw conclusions about the computational complexity of various geometric problems. We then provide lower bounds on the complexity of transitioning between graphs and simplices, and end by studying low dimensional representations of the simplices. This provides theoretical justification for recent empirical work on Laplacian eigenmaps.

Of possible independent interest, we provide a formula for the non-zero eigenvalues of $\widehat{\boldsymbol{L}}_G$ in terms of the total weight of spanning trees in the graph G, relate the volume of an arbitrary simplex to the eigenvalues of the Gram matrix of its dual simplex (an object we introduce), and give an equation for the adjugate of $\widehat{\boldsymbol{L}}_G$ in terms of the weights of the vertices in G.

Keywords: Graph theory, simplex geometry, Laplacian matrix, effective resistance, convex polyhedra.

Lay Summary

The most significant features of mathematical research, to the astonishment of many, do not involve generating contrived calculus questions with which to torture sleep-deprived undergraduates. Instead of course, one focus of such research is on further developing its different branches—geometry, probability, number theory, etc. Another concern, however, is to seek connections between these different areas. Such connections are elusive, but often point to some deeper and beautiful (stay with me) mathematical structure.

This dissertation is concerned with research of the latter type. During his illustrious career, Miroslav Fiedler began exploring what we are calling the "graph-simplex correspondence". The reader is invited to draw several dots on a piece of paper and connect each one with several (or all) of the others by drawing lines between them. There; you have just succeeded in drawing a graph. Your graph can be described by listing the dots (formally called vertices), and whether or not there is a connection between them. Regardless of how far apart the dots are on the page are, we are simply interested in whether or not there is a connection between each pair of vertices. Thus, a graph lacks inherent geometry; it can be described with lists only. A simplex, on the other hand, is essentially a triangle but generalized to higher dimensions. Is it therefore inherently geometric, which makes a connection between graphs and simplices all the more surprising.

When studying an abstract topic, one can never be sure whether the work will remain only of interest to theoreticians or will find some practical application. That being said, we expect this research to be highly applicable—it will most likely help develop interstellar travel, 6G networks, and clarify broad macroeconomic trends. Just kidding. We do hope, however, that this work will serve to inspire researchers to include the graph-simplex correspondence in their mathematical toolkit when investigating graphs and/or simplices, and will thereby contribute to future research.

Acknowledgements

Having recently read A.J. Jacobs' *Thanks a Thousand* and being of persuadable character, I am inclined to search out and thank everyone who has helped with this thesis and made my time at Oxford so extraordinary.

This, of course, would be a terrible idea. Where would I stop? Alas, resigned to the fact that I must commit a kind of thanksism and draw an arbitrary line between those I thank and those I don't, I do however wish to extend my gratitude to several people.

Thanks is due to Renaud, who unflinchingly allowed an all-too-enthusiastic master's student to pursue his topic of choice, and follow any path he found interesting. This freedom was greatly appreciated. I also owe a great deal of thanks to Karel, who provided insight into the topic which I would have never garnered by myself, and who was always willing to answer my (incessant) questions—even while on holiday. He was also a constant source of motivation and proofread a draft of this work.

This year would not have been one tenth as exciting (albeit perhaps ten times as productive) without the St. Cross student community and the Wolfson College Boat Club. Though small in quadrangle count (it's how you use them that counts), St. Cross proved itself full of friendly and talented students. More importantly, it provided lunch—by far the most epic on campus. The yogurt by itself redeems the odd smell in the library that nobody wants to talk about. WCBC ensured that I caught many crabs, lengthened my strokes, and perfected my hip swing. Sometimes I even rowed. While I can no longer drink gin without thinking of Denmark, I could not have asked for a better group of people with whom to be trapped in a boat early in the morning, being yelled at about pineapples and early squares. In the words of a large Swiss gentlemen, this year "was better than ..."

My parents provide a constant source of support and encouragement for which I am incredibly grateful. I would be nowhere without you both.

Much love to all.

Contents

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Nomenclature[2]

Simplex Geometry

$\mathcal{T}$	General simplex	Section 2.5
$\boldsymbol{\Sigma}(\mathcal{T})$	Vertex matrix of simplex $\mathcal{T}$	
$\{\boldsymbol{\gamma}_i\}$	Vertices of $\mathcal{T}$	
$\cong$	Translational congruency between simplices	
$\boldsymbol{x}_U$	Barycentric coordinate for face $\mathcal{T}_U$	
$\boldsymbol{a}(\mathcal{T}_U)$	Altitude vector from $\mathcal{T}_U$ to $\mathcal{T}_{U^c}$	
$\boldsymbol{c}(\mathcal{T}_U)$	Centroid of simplex $\mathcal{T}_U$	Equation (2.21)
$\mathcal{T}\restriction_U, \mathcal{T}_U, \mathcal{T}[U]$	Face of simplex $\mathcal{T}$ restricted to U	Equation (2.19)
$\mathcal{T}_0$	Canonical/Centred Simplex of $\mathcal{T}$	Definition 2.5
$[\mathcal{T}]$	Congruence class of simplices	Equation (2.20)
$\mathcal{T}^*$	Dual simplex to $\mathcal{T}$	Section 2.5.1
$\boldsymbol{\Sigma}^* = \boldsymbol{\Sigma}(\mathcal{T}^*)$	Dual vertex matrix	
$\{\boldsymbol{\gamma}_i^*\}$	Vertices of $\mathcal{T}^*$	
$\mathcal{S}_G$ ($\widehat{\mathcal{S}}_G$)	(Normalized) Simplex of G	Section 3.2
$\mathcal{S}_G^+$ ($\widehat{\mathcal{S}}_G^+$)	Inverse simplex of $\mathcal{S}_G$ ($\widehat{\mathcal{S}}_G$)	
$\boldsymbol{\Sigma}_G$ ($\widehat{\boldsymbol{\Sigma}}_G$)	Vertex matrix of the simplex $\mathcal{S}_G$ ($\widehat{\mathcal{S}}_G$)	
$\boldsymbol{\Sigma}_G^+$ ($\widehat{\boldsymbol{\Sigma}}_G^+$)	Vertex matrix of the simplex $\mathcal{S}_G^+$ ($\widehat{\mathcal{S}}_G^+$)	
$\{\boldsymbol{\sigma}_i\}$ ($\{\widehat{\boldsymbol{\sigma}}_i\}$)	Vertex vectors of (normalized) simplex	
θ_{ij} (θ_{ij}^+)	Angle between $\mathcal{S}_{\{i\}^c}$ ($\mathcal{S}_{\{i\}^c}^+$) and $\mathcal{S}_{\{j\}^c}$ ($\mathcal{S}_{\{j\}^c}^+$)	
ϕ_{ij} (ϕ_{ij}^+)	Angle between $\boldsymbol{\sigma}_i$ ($\boldsymbol{\sigma}_i^+$) and $\boldsymbol{\sigma}_j$ ($\boldsymbol{\sigma}_j^+$)	
$\mathcal{H}_i$ ($\mathcal{H}_i^+$)	Hyperplane containing $\mathcal{S}_{\{i\}^c}$ ($\mathcal{S}_{\{i\}^c}^+$)	Equation (3.7)
$\mathcal{E}(\mathcal{T})$	Steiner circumscribed ellipsoid of $\mathcal{T}$	Definition 4.1
$\bar{d}$	Avg. squared distance in a simplex	Equation (4.2)
$\boldsymbol{\xi}$	Avg. squared distance of vertices minus $\bar{d}$	Equation (4.3)

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	
$w_G(i)$	Weight of vertex $i \in V(G)$	
$\boldsymbol{A}_G$	Adjacency matrix of graph G	
$\boldsymbol{W}_G$	Weight matrix of graph G	

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

$G[U]$, G_U	Graph restricted to vertices in U	
$w_G(i,j)$	Weight of edge (i,j) in G	
$\partial_G(i)$	Set of neighbours of i in G	Equation (2.6)
$\partial_G U$	Cut set of U in G	Section 3.5
$\mathrm{vol}_G(U)$	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 (2.16)
$r_G^{\mathrm{eff}}(i,j)$	Effective resistance between i and j	Definition 2.2
$\boldsymbol{R}_G$	Effective resistance matrix of G	
R_G^{tot}	Total effective resistance of G	
$\mathcal{R}_G$	Effective Polytope of G	Equation (4.21)

Linear Algebra & Spectral Graph Theory

$\lVert\cdot\rVert_p$	p-norm in $\mathbb{R}^d$	Section 2.2
$\perp$	Perpendicular to; orthogonal complement	
$\dim \boldsymbol{Q}$	Dimension of space spanned by $\boldsymbol{Q}$	
range Q	Range of $\boldsymbol{Q}$	
$\ker \boldsymbol{Q}$	Kernel of $\boldsymbol{Q}$	
$\boldsymbol{Q}^+$	Pseudoinverse of matrix $\boldsymbol{Q}$	Section 2.2.1
$\boldsymbol{L}_G$	Combinatorial Laplacian Matrix of G	Equation (2.8)
$\widehat{\boldsymbol{L}}_G$	Normalized Laplacian Matrix of G	Equation (2.11)
$\mathcal{L}_G$	Quadratic form associated with $\boldsymbol{L}_G$	Equation (2.10)
$\widehat{\mathcal{L}}_G$	Quadratic form associated with $\widehat{\boldsymbol{L}}_G$	Equation (2.13)
$\{\lambda_i\}$ ($\{\widehat{\lambda}_i\}$)	Eigenvalues of $\boldsymbol{L}_G$ ($\widehat{\boldsymbol{L}}_G$)	Section 2.3.1
$\boldsymbol{\Lambda}_G$ ($\widehat{\boldsymbol{\Lambda}}_G$)	Diagonal Eigenvalue matrix of $\boldsymbol{L}_G$ ($\widehat{\boldsymbol{L}}_G$)	
$\{\boldsymbol{\varphi}_i\}$ ($\{\widehat{\boldsymbol{\varphi}}_i\}$)	Eigenvectors of $\boldsymbol{L}_G$ ($\widehat{\boldsymbol{L}}_G$)	
$\boldsymbol{\Phi}_G$ ($\widehat{\boldsymbol{\Phi}}_G$)	Eigenvector matrix of $\boldsymbol{L}_G$ ($\widehat{\boldsymbol{L}}_G$)	
$\boldsymbol{\Delta}$	Vector of diagonals of $\boldsymbol{L}_G^+$	Section 2.4

Miscellaneous

$\mathbb{R}$	Real numbers	Section 2.1
$\mathbb{Q}$	Rational 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 (2.1)

Chapter 1

Introduction

Confusion is the natural state of the mathematician.

— Lior Silberman

What if I slept a little more and forgot about all this nonsense.

— Franz Kafka, *The Metamorphosis*

This thesis is concerned with uniting two fundamental mathematical objects: the graph and the simplex. A graph is fundamentally a *combinatorial* object—it can be described purely by means of finite sets and must not refer to any underlying geometric space. Simplices, on the other hand, are inherently geometric. Essentially a high dimensional triangle, any complete description of a simplex must include certain geometric information; the distance between its vertices, for example. Thus, a simplex cannot be divorced from an underlying metric space.

The dubious reader may interject that graphs can *of course* be viewed geometrically. For instance, he or she continues, it is well-known that the shortest path between two vertices constitutes a metric on the graph. We in turn interrupt the interrupter and remark that while graphs *can* be given geometric interpretations, it is *not necessary* that they are. Indeed, a graph can be described by two finite lists: a list of its vertices and a second of the connections between these vertices (perhaps with weights given to the edges). No underlying geometric space need be defined.

Due to the combinatorial nature of the graph and the geometric nature of the simplex, a connection between the two objects might seem unlikely a priori. It is precisely this fact which makes such a connection worth studying. The original link between graphs and simplices was uncovered by Miroslav Fiedler in his 1993 paper entitled "A geometric approach to the Laplacian matrix of a graph" [Fie93]. Here he introduced the machinery needed to define what will be a central object in our study of the relationship between graphs and simplices: a bijection between connected, weighted graphs and hyperacute simplices. However, we will be concerned with more than this single bijective mapping. Indeed, what we will term the *graph-simplex correspondence* includes four (not necessarily bijective) mappings between graphs and simplices. They arise as natural extensions of Fiedler's original work.

Unfortunately (we believe) for the mathematical community, Fiedler's investigations in this area have gone relatively unnoticed. Convinced as we are of the beauty and utility of such work, this dissertation aims to present Fiedler's results in a concise, clarifying, and self-contained fashion, expand on the mathematical foundations of the correspondence, and explore new applications thereof. Our primary motivation is to convince the reader that the graph-simplex correspondence is a useful tool for studying graphs and simplices, and can shed light on various aspects of both which are overlooked by other methods. Given the ubiquity of graphs in the mathematical sciences, both in theory and in application, the possibility of a new tool with which to analyze them is highly appealing.

§1.1. Prior Work

As we stated above, Miroslav Fiedler was the "primary mover" in uncovering the graph-simplex correspondence [Fie93, Fie05, Fie11]. A lifelong geometer [Vav95], Fiedler made many contributions to both simplex geometry [Fie54, Fie55, Fie56], matrix theory [Fie98, Fie95], and graph theory [Fie73, Fie75, Fie76, Fie89]. However, his work connecting graph theory and simplex geometry remained largely unnoticed until very recently, when Devriendt and Van Mieghem used the simplex geometry of the graph as intuition behind investigating a graph's "best conducting node" [VMDC17] and, in a later work, provided a summary of Fiedler's results [DVM18]. All of this work is concerned with a connected and possibly weighted graph G and what we will henceforth refer to as its *combinatorial simplices*, denoted $\mathcal{S}_G$ and $\mathcal{S}_G^+$. (This is in contrast its *normalized simplices*, which we will define and explore later.)

Fiedler uncovered the graph-simplex correspondence by means of a more general relationship between matrices and simplices. In particular, he associated with each symmetric matrix $\boldsymbol{Q}$ whose range space is orthogonal to the all ones vector (i.e., $\boldsymbol{Q}\boldsymbol{1} = \boldsymbol{0}$) a unique (up to congruence) hyperacute simplex. Since the Laplacian matrix $\boldsymbol{L}_G$ of a connected, weighted graph G obeys this constraint, this associates with each such graph a hyperacute simplex $\mathcal{S}_G^+$. For reasons which will become clear later, we call $\mathcal{S}_G^+$ the *inverse* (combinatorial) simplex of G. Fiedler associated $\boldsymbol{L}_G$ and $\mathcal{S}_G^+$ by means of a block matrix equation which involved several somewhat complex components, including the Gram matrix of the outer normals of the simplex and the radius of its circumscribed ellipsoid. While this matrix representation is useful for various reasons—elaborated upon in Section 4.2—the correspondence can be simplified by means of working solely with the graph's Laplacian matrix. This is the approach recently taken by Devriendt and Van Mieghem [DVM18]. They simplify and summarize Fiedler's main results and focus mainly on one side of the correspondence—namely, given G, they examine the properties of its associated simplices $\mathcal{S}_G$ and $\mathcal{S}_G^+$. Devriendt and Van Mieghem also make explicit the connection between a graph's (combinatorial) simplex, $\mathcal{S}_G$, and its inverse simplex, $\mathcal{S}_G^+$. While Fiedler was aware of the existence of $\mathcal{S}_G$—he later examines the properties of its circumscribed ellipsoid [Fie05]—the majority of his work on the graph-simplex correspondence focuses on the inverse simplex, $\mathcal{S}_G^+$.

Due to Fiedler's more general interest in the relationship between matrices and simplices, the majority of his results pertaining to the graph-simplex correspondence are implicit consequences thereof. His block matrix approach lends itself more readily to the study of volumes, angles and circumscribed quadrics, which thus constitute the core of Fiedler's results. Devriendt and Van Mieghem make many of these implicit results explicit, giving equations

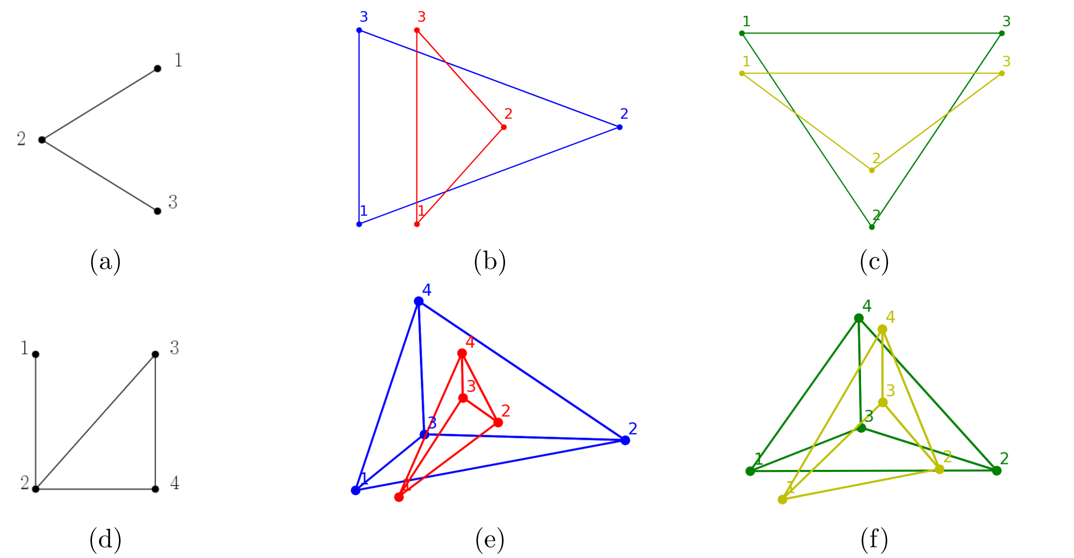

Figure 1.1: Two examples of graphs ((a) and (d)) and their combinatorial and normalized simplices. The combinatorial simplices are figures (b) and (e); the red (lighter) simplex is the inverse combinatorial simplex. The normalized simplices are figures (c) and (f); the yellow (lighter) simplex is the inverse normalized simplex. Observe that the upper graph on three vertices gives rise to simplices in $\mathbb{R}^2$, while that on four vertices to simplices in $\mathbb{R}^3$. The reader may notice that the inverse simplex seems to be smaller in volume—we will address this relationship in Chapter 3.

which directly relate properties of the graph to those of the simplex.

Very recently, the graph-simplex correspondence has been applied in computer science to the area of low dimensional graph embeddings. Such embeddings seek to realize the vertices of a given graph as points in Euclidean space (ideally a space whose dimension is much lower than the number of nodes of the graph) in such a way that particular graph properties are preserved [CZC18]. Torres, Chan, and Eliassi-Rad examine projections of $\mathcal{S}_G$ into a lower dimensional space as possible graph embeddings. [TCER19]. They give empirical results suggesting that this approach is highly effective for link prediction and graph reconstruction.

While this summarizes all the work done explicitly on the graph-simplex correspondence, the more general topic of geometric graph theory has garnered attention from many sources. There is a wide literature on graph embeddings and geometric graph visualizations (e.g., [Tam13, BCD$^+$07, KK89, FR91, DFPP90]), an area which typically seeks to represent a graph (sometimes multiple graphs [EKLN05, ELM16, BKR12]) in the plane or $\mathbb{R}^3$ under certain conditions. For example, we might seek an embedding in which the edges do not cross (a "planar" embedding [Kan93, NR04]), or one in which the vertices are represented as geometric objects [DH97].

Computer scientists have also leveraged graph theory to analyze data. Datum with k features can naturally be viewed as points in k dimensional space—the "feature space". Laplacian Eigenmap methods [BN02] assume that the observed data lies on a lower dimensional manifold within the feature space and seeks to develop useful representations of the data. A distinct approach involves trying to generate a lower dimensional representation of the data given its graph structure (typically represented as an "affinity matrix"). This general approach is usually referred to as *spectral embedding* [BH03, BDR+04], and admits different instantiations, including *Principal Component Analysis (PCA)* [Jol11], *Multi-dimensional Scaling (MDS)* [KW78, CC00], and *Local Linear Embedding (LLE)* [RS00]. Related work seeks to apply techniques from topology to find structure in graphs, both from a purely theoretical viewpoint (e.g., topological graph theory [GT01]), and more recently with applications to complex networks in mind [SCL18, WMRB15].

There has also been work on graphs arising from general polyhedra, e.g., Steinitz's theorem [Ste22]. However, this work is not spectral in nature and therefore quite unrelated to the graph-simplex correspondence.

§1.2. Contribution

We provide a self-contained treatise of the graph-simplex correspondence, including both 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, enumerated below. For a preliminary taste of the correspondence, see the examples in Figure 1.1.

- **Introduction of the dual simplex.** Although at first seemingly unrelated to the correspondence itself, we introduce an object called the "dual simplex" of a given simplex. This object was remarked upon by Fiedler in his 2011 book [Fie11], but he did not investigate it. Our treatment of the dual simplex is also mathematically distinct from Fiedler's. We present several general properties of the dual simplex (e.g., Lemmas 2.13, 2.14, 3.23, 2.12) and use it to frame the graph-simplex correspondence, especially as it relates to the normalized Laplacian (see below).

- **Extension of correspondence to 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 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. Somewhat surprisingly, the normalized simplex is a significantly different object than the combinatorial simplex. Its analysis also proves more complicated because, as we will show, the inverse normalized simplex is *not* the dual of the normalized simplex in general, whereas the combinatorial simplex and its inverse are duals to one another. We refer the reader to Figure 1.2 for an illustration of the relationship between a graph and its various simplices.

- **New graph equations and inequalities.** Combining Fiedler's block matrix approach with that of Devriendt and Van Mieghem, we are able to uncover several new relationships. We show, for example, that the entries of the Laplacian and the vertices of $\mathcal{S}_G$ are related to the volumes of the facets of $\mathcal{S}_G^+$ (Lemma 4.6), give a general formula

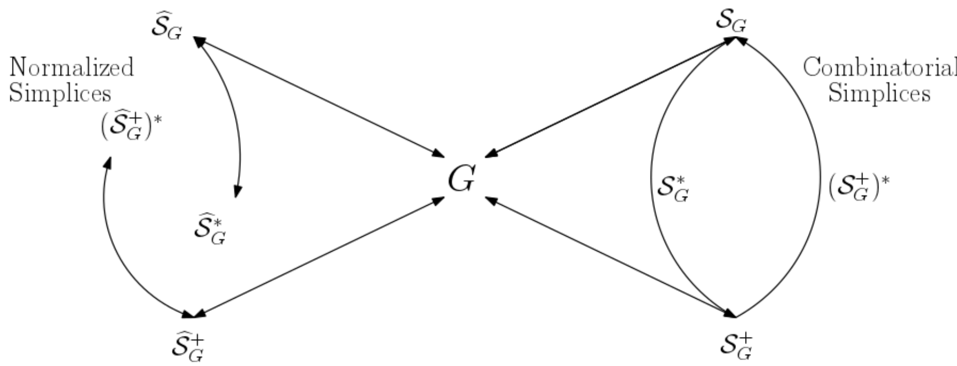

Figure 1.2: An illustration of the various objects and relationships in the graph-simplex correspondence. The combinatorial simplices sit to the right of G, while the normalized simplices sit to the left. Duality is marked by the superscript $*$. We see that $\mathcal{S}_G$ and $\mathcal{S}_G^+$ are duals to one another but the normalized simplices are not.

for the volume of a simplex in terms of the eigenvalues of the Gram matrix of its dual (Theorem 4.2), and a formula for Steiner ellipsoid of a simplex in terms of the vertex matrix of its dual (Lemma 4.19). We also relate the eigenvalues of $\widehat{\boldsymbol{L}}_G$ to the total weight of spanning trees in G, and consequently to the eigenvalues of $\boldsymbol{L}_G$ (Lemma 4.11). These results are given in Section 4.2, 4.3, and 4.4. Figure 1.3 demonstrates how one can utilize the correspondence to translate between the combinatorial properties of the graph and the geometric properties of its simplices.

- **Link between $\mathcal{R}_G$ and $\mathcal{S}_G^+$.** We uncover a link between the inverse combinatorial simplex of a graph and a geometric object related to the effective resistance of the graph, which we call the "resistive polytope" and denote $\mathcal{R}_G$. It seems that the existence of this object has been previously acknowledged (e.g., [Gha15]), but never rigorously studied. This material appears in Section 4.5.

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

  1. **Consequences for computational complexity.** We explore several consequences for computational complexity. Owing to the pervasiveness of graphs in theory and application, the complexity class 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 complexity of the analogous geometric problems may already be known in general convex polytopes, understanding the complexity in simplices can yield an improved understanding of their hardness threshold. We give several examples of such results in Section 5.2.

  2. **Lower bounds on computing the correspondence.** We then explore the natural question of whether various aspects of the correspondence can be computed

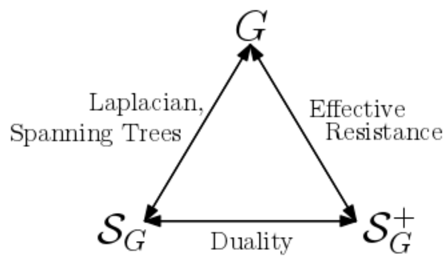

Figure 1.3: A visualization of how the correspondence can be used to apply graph-theoretic knowledge to the geometry of the simplices and vice versa. For example, leveraging that the geometry of $\mathcal{S}_G^+$ is intimately related to the effective resistances of G and relating the equations of $\mathcal{S}_G^+$ to those of $\mathcal{S}_G$ via duality allows us to, say, express equations of spanning trees in terms of effective resistances.

efficiently. For example, given G how quickly can we compute $\mathcal{S}_G$ or $\mathcal{S}_G^+$? 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 such a decomposition, but it is not immediate. It is a priori feasible that the various relationships between the eigenvalues and eigenvectors which define the vertices of the simplices are computable more quickly than the eigenvalues and eigenvectors themselves.

3. **Approximations.** 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. We also demonstrate that rank k approximations to the Laplacian give rise to convex polyhedra in $\mathbb{R}^k$, and that these polyhedra approximate the simplex $\mathcal{S}_G$ in various ways (with the accuracy depending on the size of the $(k+1)$-st largest eigenvalue of $\boldsymbol{L}_G$). We view these results as providing theoretical justification for recent work of Torres *et al.* mentioned in the previous section [TCER19].

We end this section by noting that while the dissertation is largely theoretical in nature, code implementing various aspects of the graph-simplex correspondence was written by the author and is publicly available. The figures throughout the manuscript were either generated by this software (via PYTHON and MATPLOTLIB), or by the drawing editor IPE [Che14].

§1.3. Organization

The rest of the thesis will be organized as follows. Chapter 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. Chapters 3 and 4 then explore the mathematical aspects of the graph-simplex correspondence, and Chapter 5 presents the algorithmic foundations. In order to conserve space, we have moved those proofs which were presented by either Fiedler or Devriendt and Van Mieghem to the appendix, in addition to those which are elementary and not directly related to the material at hand (e.g., those pertaining to background material).

Chapter 2

Background and Fundamentals

I have got my result, but I do not know yet how to get it.

— Carl Friedrich Gauss

This chapter is devoted to introducing the pre-requisite knowledge necessary to grapple with subsequent material. 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 strive—courageously, in the author's unbiased opinion—to use standard notation wherever possible in the hopes that readers familiar with linear algebra and spectral graph theory may skip this background material without losing the plot. Omitted proofs can be found in Appendix A.1.

§2.1. General Notation

We use the standard notation for sets of numbers: $\mathbb{R}$ (reals), $\mathbb{N}$ (naturals), $\mathbb{Z}$ (integers). For any $n \in \mathbb{N}$, set $[n] \stackrel{\text{def}}{=} \{1, 2, \ldots, n\}$. The complement of a set U (with respect to what will be clear from context) is denoted U^c. We let $\mathbb{R}^{n\times m}$ denote the set of $n \times m$ matrices (n rows and m columns) with entries in $\mathbb{R}$. Matrices will typically be denoted by uppercase letters in boldface, e.g., $\boldsymbol{Q} \in \mathbb{R}^{n\times m}$. Matrices may also be referred to as linear transformations and written, for example, as $\boldsymbol{Q} : \mathbb{R}^m \to \mathbb{R}^n$. We let $\boldsymbol{Q}(i, \cdot)$ (resp., $\boldsymbol{Q}(\cdot, i)$) denote the i-th row (resp., column) of the matrix $\boldsymbol{Q}$. Similarly, for sets B_1, B_2, we let $\boldsymbol{Q}(B_1, B_2)$ be the submatrix of $\boldsymbol{Q}$ indexed by the rows B_1 and columns B_2. We take $\boldsymbol{Q}_{-i,-j}$ to mean $\boldsymbol{Q}(\{i\}^c, \{j\}^c)$.

We work with $\mathbb{R}^n$ as a vector space. Vectors will typically be denoted by lowercase boldcase letters. It will often be intuitively useful to identify 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.

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: $\langle \boldsymbol{x}, \alpha\boldsymbol{y}_1 + \boldsymbol{y}_2 \rangle = \alpha\langle \boldsymbol{x}, \boldsymbol{y}_1 \rangle + \langle \boldsymbol{x}, \boldsymbol{y}_2 \rangle$ for $\alpha \in \mathbb{R}$. 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 $\boldsymbol{\chi}_U(i) = \chi(i \in U)$. We also set $\boldsymbol{\chi}_i = \boldsymbol{\chi}_{\{i\}}$.

By $\operatorname{diag}(y_1, y_2, \dots, y_n)$ we mean the $n \times n$ matrix $\boldsymbol{Q}$ entries $\boldsymbol{Q}(i,i) = y_i$ and $\boldsymbol{Q}(i,j) = 0$ for $i \neq j$. Given vectors $\boldsymbol{x}_1, \dots, \boldsymbol{x}_n$, we will often denote by $(\boldsymbol{x}_1, \dots, \boldsymbol{x}_n)$ or simply $(\boldsymbol{x}_i)$ the matrix whose i-th column is $\boldsymbol{x}_i$. The *Gram matrix* of a set of vectors $\boldsymbol{x}_1, \dots, \boldsymbol{x}_n$ is the matrix with (i,j)-th entry $\langle \boldsymbol{x}_i, \boldsymbol{x}_j \rangle$. The i-th coordinate of a vector $\boldsymbol{x}$ will be denoted either by $\boldsymbol{x}(i)$ or simply $x(i)$. We also set $\boldsymbol{x}^{1/2} = \sqrt{\boldsymbol{x}} = (\sqrt{x(1)}, \dots, \sqrt{x(n)})$.

For $1 \leq p < \infty$, the *p-norm* of $\boldsymbol{x} \in \mathbb{R}^d$ is $\|\boldsymbol{x}\|_p = \left(\sum_{i=1}^d x_i^p \right)^{1/p}$, 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 $\boldsymbol{Q}^t(i,j) = \boldsymbol{Q}(j,i)$. 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 $X = \{\boldsymbol{x}_1, \dots, \boldsymbol{x}_k\} \subseteq \mathbb{R}^n$ is

$$\operatorname{conv}(\mathcal{X}) \overset{\text{def}}{=} \left\{ \sum_{\ell} \alpha_i \boldsymbol{x}_i : \sum_{\ell} \alpha_i = 1,\ \alpha_i \geq 0 \right\}, \tag{2.1}$$

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—determinants, dimension, span, etc. We use the standard notation for these—det, dim, span, 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 ([Fie11]). *Let $\mathbf{v}_1, \dots, \mathbf{v}_k$ be a set of linearly independent vectors in $\mathbb{R}^n$. There exists a second set of linearly independent vectors $\mathbf{u}_1, \dots, \mathbf{u}_k$ 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 any of* biorthogonal, dual *or* sister sets *(or bases if* $k = n$*).*

We present a simple observation to do with dual bases which will be useful in later sections. As usual, the reader can find the proof in Appendix A.1.

OBSERVATION 2.1. *Let* $\{\mathbf{v}_1, \dots, \mathbf{v}_n\} \subseteq \mathbb{R}^n$ *be a set of linearly independent vectors. The sister basis given by Lemma 2.1 is unique. Moreover, if we let* $\boldsymbol{M} \in \mathbb{R}^{n\times n}$ *have as columns the vectors* $\mathbf{v}_i$*, and* $\boldsymbol{Q}$ *have as columns the vectors of the sister basis, then* $\boldsymbol{Q}^t = \boldsymbol{M}^{-1}$*.*

Let $\boldsymbol{M} \in \mathbb{R}^{n\times n}$. We recall that a vector $\boldsymbol{\varphi}$ satisfying $\boldsymbol{M}\boldsymbol{\varphi} = \lambda\boldsymbol{\varphi}$ is an *eigenvector* (or *eigenfunction*) of $\boldsymbol{M}$, and call λ the associated *eigenvalue*. If $\boldsymbol{M}$ is real and symmetric, then the spectral theorem dictates that there exists an orthonormal basis consisting of eigenvectors $\{\boldsymbol{\varphi}_1, \boldsymbol{\varphi}_2, \dots, \boldsymbol{\varphi}_n\}$ of $\boldsymbol{M}$ whose corresponding eigenvalues $\{\lambda_1, \dots, \lambda_n\}$ are all real. Let $\boldsymbol{\Phi} = (\boldsymbol{\varphi}_1, \boldsymbol{\varphi}_2, \dots, \boldsymbol{\varphi}_n)$ be the matrix whose i-th column is the i-th eigenvector of $\boldsymbol{M}$, and set $\boldsymbol{\Lambda} = \mathrm{diag}(\lambda_1, \dots, \lambda_n)$. Observe that

$$\boldsymbol{M}\boldsymbol{\Phi} = \boldsymbol{M}(\boldsymbol{\varphi}_1, \dots, \boldsymbol{\varphi}_n) = (\boldsymbol{M}\boldsymbol{\varphi}_1, \dots, \boldsymbol{M}\boldsymbol{\varphi}_n) = (\lambda_1\boldsymbol{\varphi}_1, \dots, \lambda_n\boldsymbol{\varphi}_n) = \boldsymbol{\Phi}\boldsymbol{\Lambda}. \tag{2.2}$$

Moreover, if $\{\boldsymbol{\varphi}_i\}_i$ are assumed to be orthonormal then $\boldsymbol{\Phi}^t\boldsymbol{\Phi} = \mathbf{I}$ from which it follows from (2.2) that

$$\boldsymbol{M} = \boldsymbol{\Phi}\boldsymbol{\Lambda}\boldsymbol{\Phi}^t = \sum_{i\in[n]} \lambda_i \boldsymbol{\varphi}_i \boldsymbol{\varphi}_i^t, \tag{2.3}$$

which is called the *eigendecomposition* of $\boldsymbol{M}$. If $\boldsymbol{M}$ obeys $\boldsymbol{x}^t\boldsymbol{M}\boldsymbol{x} \geq 0$ for all $\boldsymbol{x} \in \mathbb{R}^n$, then we call $\boldsymbol{M}$ *positive semidefinite (PSD)*. Importantly, if $\boldsymbol{M}$ is PSD, then its eigenvalues are non-negative. Indeed, with the eigendecomposition of $\boldsymbol{M}$ as above,

$$0 \leq \boldsymbol{\varphi}_k^t\boldsymbol{M}\boldsymbol{\varphi}_k = \sum_{i\in[n]} \lambda_i \boldsymbol{\varphi}_k^t\boldsymbol{\varphi}_i\boldsymbol{\varphi}_i^t\boldsymbol{\varphi}_k = \lambda_k\boldsymbol{\varphi}_k^t\boldsymbol{\varphi}_k\boldsymbol{\varphi}_k^t\boldsymbol{\varphi}_k = \lambda_k,$$

for any k since $\{\boldsymbol{\varphi}_i\}$ are orthonormal. Thus, if $\boldsymbol{M}$ is PSD we define

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

It's easily verified that $(\boldsymbol{M}^{1/2})^2 = \boldsymbol{M}$. The following basic result will be useful.

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

We conclude with a formula for the determinant of a minor of an invertible matrix. It is often referred to as (a special case of) *Sylvester's identity* [Syl]. We state the version described by Viktor Prasolov [Pra94].

LEMMA 2.3. *Let* $\boldsymbol{Q} \in \mathbb{R}^{n\times n}$ *have a non-zero determinant, and let* $\emptyset \neq U \subsetneq [n]$*. Then*

$$\det\big(\boldsymbol{Q}^{-1}[U, U]\big)\det(\boldsymbol{Q}) = \pm\det(\boldsymbol{Q}[U^c, U^c]). \tag{2.4}$$

2.2.1. Pseudoinverse

If $\boldsymbol{M}$ is a singular matrix (has no inverse), 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 $\boldsymbol{M} \in \mathbb{R}^{n\times m}$ for some $n, m \in \mathbb{N}$. If $\boldsymbol{M}^+ \in \mathbb{R}^{m\times n}$ is such that

(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., $\boldsymbol{M}\boldsymbol{M}^+ = (\boldsymbol{M}\boldsymbol{M}^+)^t$, $\boldsymbol{M}^+\boldsymbol{M} = (\boldsymbol{M}^+\boldsymbol{M})^t$,

we call $\boldsymbol{M}^+$ 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 2.4 ([BH12]). *Let $\boldsymbol{M} \in \mathbb{R}^{n\times m}$. 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 2.4 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 2.5. *Suppose $\boldsymbol{M} \in \mathbb{R}^{m\times m}$ 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 $\boldsymbol{\varphi}_1, \dots, \boldsymbol{\varphi}_k$. Then the pseudoinverse of $\boldsymbol{M}$ is*

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

§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 $G = (V, E, w_G)$ where V is the *vertex set*, $E \subseteq V \times V$ is the *edge set* and $w_G : V \times V \to \mathbb{R}_{\geq 0}$ (the non-negative reals) a *weight function*. We will always drop the subscript on w_G unless we are dealing with multiple graphs. We let the domain of $w = w_G$ 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 $G = (V, E)$. We typically denote by $\boldsymbol{w}$ the vector $(w(1), \ldots, w(n))$ of weights. Throughout this manuscript, G will always be undirected (edges do not have directions), connected (each vertex is reachable from every other vertex), and simple ($w(i, i) = 0$ for all i). We will usually take $V = [n]$ for simplicity. For a vertex $i \in V$, we denote the set of its neighbours by

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

a set we call the *neighbourhood* of i. The *degree of* i is $\deg(i) \stackrel{\text{def}}{=} |\partial(i)|$. The *weight of* i is $w(i) \stackrel{\text{def}}{=} \sum_{j\in\partial(i)} w(i, j)$. 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*. For G unweighted, we call it *regular* if it is k-regular for some k. If G is weighted, then we say it is regular if each vertex has the same weight, i.e., $w(i) = w(j)$ for all i, j. If $U \subseteq V$ contains only vertices with the same degree (resp., weight), we call it *degree (resp., weight) homogeneous.* For a 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 $\mathrm{vol}(G) \stackrel{\text{def}}{=} \mathrm{vol}_G(V(G))$. 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, $w(U) = \mathrm{vol}(U)$, 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 always 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: $\sum_{(i,j)\in E} = \frac{1}{2}\sum_i \sum_{j\in\partial(i)}$. 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 the 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 associated to graphs, including the combinatorial and normalized Laplacians. See the survey by Merris [Mer94] for an excellent overview of the combinatorial Laplacian, and that by Mohar [MACO91] for an overview of its spectrum.

Let $G = (V, E, w)$ be a graph, with $V = [n]$ and $|E| = m$. Let $\boldsymbol{W}_G$ be the *weight matrix* of G, i.e., $\boldsymbol{W}_G = \text{diag}(w(1), w(2), \ldots, w(n))$. The *degree matrix* of G is the diagonal matrix $\text{diag}(\deg(1), \deg(2), \ldots, \deg(n))$. 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 $\boldsymbol{A}_G$ is symmetric and 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 $\boldsymbol{L}_{i,j} = w(i,j)(\boldsymbol{\chi}_i - \boldsymbol{\chi}_j)(\boldsymbol{\chi}_i - \boldsymbol{\chi}_j)^t \in \mathbb{R}^{V \times V}$, 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

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

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, 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

$$\mathcal{L}_G(\boldsymbol{f}) = \boldsymbol{f}^t \left(\sum_{i \sim j} \boldsymbol{L}_{i,j} \right) \boldsymbol{f} = \sum_{i \sim j} \boldsymbol{f}^t \boldsymbol{L}_{i,j} \boldsymbol{f} = \sum_{i \sim j} w(i,j)(\boldsymbol{f}(i) - \boldsymbol{f}(j))^2. \tag{2.10}$$

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

$$\widehat{\boldsymbol{L}}_G = \boldsymbol{W}_G^{-1/2} \boldsymbol{L}_G \boldsymbol{W}_G^{-1/2} = \mathbf{I} - \boldsymbol{W}_G^{-1/2} \boldsymbol{A}_G \boldsymbol{W}_G^{-1/2}. \tag{2.11}$$

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:

$$\widehat{\boldsymbol{L}}_G = \sum_{i \sim j} \widehat{\boldsymbol{L}}_{i,j}. \tag{2.12}$$

As we've done here, we will typically emphasize the associate of elements associated to the normalized Laplacian with a hat. Using Equation (2.12), we see that the quadratic form $\widehat{\mathcal{L}}_G$

associated with $\widehat{\boldsymbol{L}}_G$ acts as

$$\widehat{\mathcal{L}}_G(\boldsymbol{f}) = \sum_{i\sim j} w(i,j)\left(\frac{\boldsymbol{f}(i)}{\sqrt{w(i)}} - \frac{\boldsymbol{f}(j)}{\sqrt{w(j)}}\right)^2. \tag{2.13}$$

We now discuss the spectrum of $\boldsymbol{L}_G$ and $\widehat{\boldsymbol{L}}_G$. 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.

LEMMA 2.6. *Let $G = ([n], E)$ be a connected graph. Then* $\ker \boldsymbol{L}_G = \mathrm{span}(\mathbf{1})$ *and* $\ker \widehat{\boldsymbol{L}}_G = \mathrm{span}(\sqrt{\boldsymbol{w}})$*, where $\sqrt{\boldsymbol{w}} = (\sqrt{w(1)}, \dots, \sqrt{w(n)})$. Moreover, both $\boldsymbol{L}_G$ and $\widehat{\boldsymbol{L}}_G$ have a single zero eigenvalue (with corresponding eigenvector $\mathbf{1}$ and $\sqrt{\boldsymbol{w}}$, respectively); all other eigenvalues are strictly positive.*

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, $\mathrm{range}(\boldsymbol{L}^t) = \mathrm{range}(\boldsymbol{L}_G) = \mathbb{R}^n \setminus \ker(\boldsymbol{L}_G) = \mathbb{R}^n \setminus \mathrm{span}(\{\mathbf{1}\})$, and $\mathrm{range}(\widehat{\boldsymbol{L}}_G^t) = \mathrm{range}(\widehat{\boldsymbol{L}}_G) = \mathbb{R}^n \setminus \ker(\widehat{\boldsymbol{L}}_G) = \mathbb{R}^n \setminus \mathrm{span}(\{\sqrt{\boldsymbol{w}}\})$. It follows by Lemma 2.4 that the product of $\boldsymbol{L}_G$ and $\boldsymbol{L}_G^+$ is the projection

$$\boldsymbol{L}_G\boldsymbol{L}_G^+ = \boldsymbol{L}_G^+\boldsymbol{L}_G = \mathbf{I} - \frac{1}{n}\mathbf{1}\mathbf{1}^t, \tag{2.14}$$

i.e., onto $\mathrm{span}(\mathbf{1})^\perp$ (the orthogonal complement of $\mathrm{span}(\mathbf{1})$). The product of $\widehat{\boldsymbol{L}}_G$ and $\widehat{\boldsymbol{L}}_G^+$ meanwhile, is

$$\widehat{\boldsymbol{L}}_G\widehat{\boldsymbol{L}}_G^+ = \widehat{\boldsymbol{L}}_G^+\widehat{\boldsymbol{L}}_G = \mathbf{I} - \frac{1}{\mathrm{vol}(G)}\boldsymbol{W}_G^{1/2}\mathbf{1}(\boldsymbol{W}_G^{1/2}\mathbf{1})^t = \mathbf{I} - \frac{1}{\mathrm{vol}(G)}\sqrt{\boldsymbol{w}}\sqrt{\boldsymbol{w}}^t, \tag{2.15}$$

the projection onto $\mathrm{span}(\boldsymbol{w})^\perp$. Note that the denominator in (2.15) is $\mathrm{vol}(G)$ instead of n to ensure the result is a projection matrix.[1]

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* or the matrix 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].

[1]Indeed, put $\mathbf{P} = \mathbf{I} - \frac{1}{\mathrm{vol}(G)}\sqrt{\boldsymbol{w}}\sqrt{\boldsymbol{w}}^t$. Then $\mathbf{P}^2 = \mathbf{I} - \frac{2}{\mathrm{vol}(G)}\sqrt{\boldsymbol{w}}\sqrt{\boldsymbol{w}}^t + \frac{1}{\mathrm{vol}(G)^2}\sqrt{\boldsymbol{w}}\sqrt{\boldsymbol{w}}^t\sqrt{\boldsymbol{w}}\sqrt{\boldsymbol{w}}^t = \mathbf{P}$, since $\sqrt{\boldsymbol{w}}^t\sqrt{\boldsymbol{w}} = \mathrm{vol}(G)$.

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

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

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 $\boldsymbol{L}_G$, 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

$$\Gamma_G = \sum_{T\in\mathfrak{T}}\prod_{i\in V(T)} w_G(i). \tag{2.16}$$

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

One of the most successful physical interpretations of a graph arises from considering it as an electrical network [Ell11, Tet91]. We imagine placing a resistor of resistance $1/w(i, j)$ on each edge $(i, j) \in E(G)$. Injecting current at one or more of the vertices results in an *electrical flow* in the graph. While this physical interpretation is intuitively useful, it is not necessary for understanding the notion of electrical flows. Consequently, we move a more involved discussion on electrical flows to Appendix B and present only the required definitions and results here. The key concept is that of the "effective resistance" between two vertices:

DEFINITION 2.2. The *effective resistance* between nodes i and j is $r^{\text{eff}}(i, j) \stackrel{\text{def}}{=} \mathcal{L}_G^+(\boldsymbol{\chi}_i - \boldsymbol{\chi}_j)$, and the *effective resistance matrix of G* is the matrix $\boldsymbol{R}_G$ with entries $\boldsymbol{R}_G(i, j) = r^{\text{eff}}(i, j)$. The *total effective resistance in the graph* is the quantity $R_G^{\text{tot}} \stackrel{\text{def}}{=} \frac{1}{2}\mathbf{1}^t\boldsymbol{R}_G\mathbf{1}$.

We can relate the entries of the pseudoinverse Laplacian with the effective resistance as follows.

LEMMA 2.7. *For any graph G, $\boldsymbol{R}_G = \mathbf{1}\boldsymbol{\Delta}^t + \boldsymbol{\Delta}\mathbf{1}^t - 2\boldsymbol{L}_G^+$ where $\boldsymbol{\Delta} = diag(\boldsymbol{L}_G^+(i, i))$. Moreover, for all i, j (including $i = j$),*

$$\boldsymbol{L}_G^+(i, j) = \frac{1}{2n}\left(\sum_{k\in[n]} r^{\text{eff}}(i, k) + r^{\text{eff}}(j, k)\right) - \frac{1}{2}r^{\text{eff}}(i, j) - \frac{R_G^{\text{tot}}}{n^2}. \tag{2.17}$$

Later, we will demonstrate that the inverse combinatorial simplex of a graph G is intimately related to the effective resistance. The following block matrix equation will help us generate statements concerning the geometry of this simplex, and eventually, all simplices.

The following equation was first given in the following form by Van Mieghem *et al.* [VMDC17] and follows from a more general version proven by Fiedler [Fie93, Fie11].

LEMMA 2.8. *For a weighted graph G, let $\boldsymbol{\Delta} = diag(\boldsymbol{L}_G^+(i,i))$ be the vector containing the diagonal elements of $\boldsymbol{L}_G^+$. Then,*

$$-\frac{1}{2}\begin{pmatrix} 0 & \mathbf{1}_n^t \\ \mathbf{1}_n & \boldsymbol{R}_G \end{pmatrix} = \begin{pmatrix} \boldsymbol{\Delta}^t \boldsymbol{L}_G \boldsymbol{\Delta} + \frac{4}{n^2} R_G^{\text{tot}} & -(\boldsymbol{L}_G\boldsymbol{\Delta} + \frac{2}{n}\mathbf{1})^t \\ -(\boldsymbol{L}_G\boldsymbol{\Delta} + \frac{2}{n}\mathbf{1}) & \boldsymbol{L}_G \end{pmatrix}^{-1}. \tag{2.18}$$

Moreover, $\boldsymbol{L}_G\boldsymbol{R}_G\boldsymbol{L}_G = -2\boldsymbol{L}_G$ and for all $\boldsymbol{x} \in \operatorname{span}(\mathbf{1})^\perp$, $\boldsymbol{R}_G\boldsymbol{L}_G\boldsymbol{R}_G\boldsymbol{x} = -2\boldsymbol{R}_G\boldsymbol{x}$.

The proofs of Lemmas 2.7 and 2.8 are, as usual, found in Appendix A.1.

§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 those sets of three points which describe a triangle. See Figure 2.1b for an illustration of affine dependence and independence.

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 $\sum_{i\in[n]} \alpha_i \boldsymbol{x}_i = \mathbf{0}$ 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 2.9. *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.*

The following lemma demonstrates that if we form a matrix of size $(n-1)\times n$ whose columns are n affinely independent vectors, then this matrix has full rank. Moreover, we may assume that the linear combination of the vectors which generate any point in the image space is in fact an *affine combination*, in the following sense.

LEMMA 2.10. *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 $\boldsymbol{y} = \sum_{i\in[n]} \alpha_i \boldsymbol{x}_i$.*

The simplex. We jump straight into the definition; see Figure 2.1a for several examples.

DEFINITION 2.4. A *simplex* $\mathcal{T}$ in $\mathbb{R}^{n-1}$ is the convex hull of n affinely independent vectors $\boldsymbol{\sigma}_1, \dots, \boldsymbol{\sigma}_n$. That is, $\mathcal{T} = \operatorname{conv}(\gamma_1, \dots, \gamma_n)$.

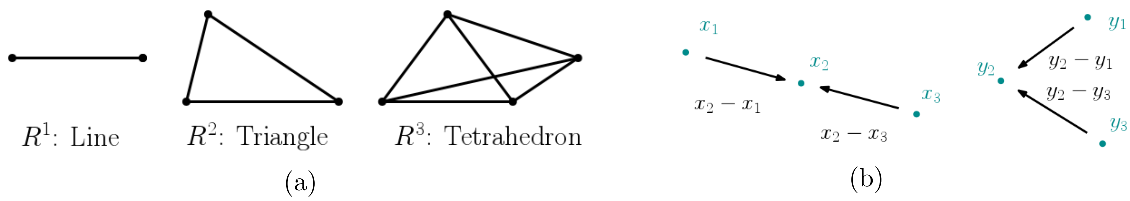

Figure 2.1: (a) Simplices in dimensions one, two, and three. (b) Example of affine dependence and independence. Here x_1, x_2, x_3 are not affinely independent, as evidenced by the fact that $x_2 - x_1$ and $x_2 - x_3$ are parallel. y_1, y_2, y_3 on the other hand, are affinely independent; one can easily visualize the triangle formed by their convex hull. We emphasize that the arrows representing the difference between two vectors, e.g., $x_2 - x_1$, represent their *direction only* and not their absolute position.

If we gather the vertices of the simplex $\mathcal{T}$ into the *vertex matrix* $\boldsymbol{\Sigma} = (\boldsymbol{\gamma}_1, \ldots, \boldsymbol{\gamma}_n)$ 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

$$\mathcal{T} \restriction_U \stackrel{\text{def}}{=} \{\boldsymbol{\Sigma x} : \boldsymbol{x} \geq 0,\ \|\boldsymbol{x}\|_1 = 1,\ x(i) = 0 \text{ for all } i \in U^c\}. \tag{2.19}$$

If $|U| = n - 1$, we call $\mathcal{T} \restriction_U$ a *facet*. Figure 2.2b illustrates a two-dimensional facet and one-dimensional face of a simplex in $\mathbb{R}^3$. If $\boldsymbol{x}$ is the barycentric coordinate for a point $\boldsymbol{p} \in \mathcal{T} \restriction_U$, we may write $\boldsymbol{x}_U$ to emphasize that $\boldsymbol{x}(U^c) = 0$. The following observation demonstrates that $\mathcal{T} \restriction_U$ is a well-defined simplex.

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

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 identify simplices which share the same relative properties, but are simply rotated and/or translated versions of one another. We will call such simplices *congruent*. Unfortunately for notational simplicity's sake, 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*, and the latter *rotational congruence*. We use the symbol $\cong$ to denote translational congruency between simplices; so $\mathcal{T}_1 \cong \mathcal{T}_2$ iff $\boldsymbol{\Sigma}(\mathcal{S}_1) = \boldsymbol{\Sigma}(\mathcal{S}_2) + \boldsymbol{\alpha}\boldsymbol{1}^t$ for some $\boldsymbol{\alpha} \in \mathbb{R}^{n-1}$. We

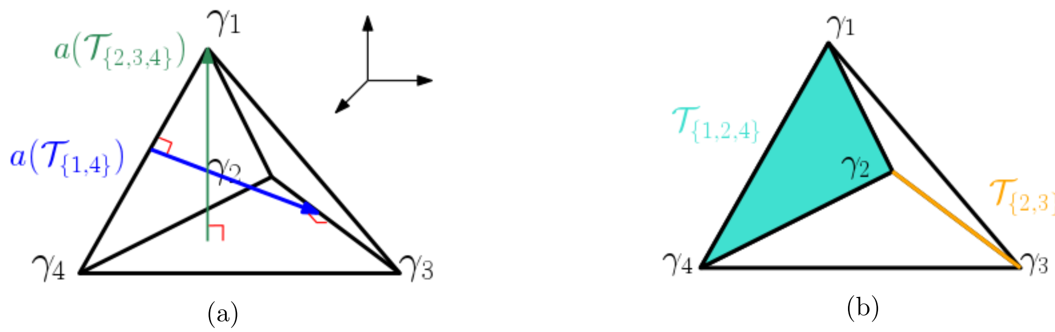

Figure 2.2: (a) The *directions* of altitudes in a simplex. We emphasize that the arrows do not represent the actual altitudes themselves, which are vectors and hence originate at the origin. (b) One and two-dimensional faces ($\mathcal{T}_{\{2,3\}}$ and $\mathcal{T}_{\{1,2,4\}}$, respectively) of a three dimensional simplex.

will also occasionally make use of the following *translational congruence class of simplices*:

$$[\mathcal{T}] \overset{\text{def}}{=} \{\mathcal{T}' : \mathcal{T}' \cong \mathcal{T}\}. \tag{2.20}$$

We will not require such notation for rotational congruence.

Two brief notes now on nomenclature. First, 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. Secondly, due possibly to lack of sleep and apparent lack of conscientiousness, we may write the vertex matrix $\boldsymbol{\Sigma}$ of a simplex $\mathcal{T}$ as $(\gamma_1, \dots, \gamma_n)$, (γ_i), or $\{\gamma_i\}$ as the case may be. Of course, they should be taken to mean the same thing.

Centroids and altitudes. Two fundamental objects related to a simplex are its centroids and altitudes (Figure 2.2). The *centroid* of a simplex is the point

$$\boldsymbol{c}(\mathcal{T}) \overset{\text{def}}{=} \frac{1}{n}\boldsymbol{\Sigma}\mathbf{1} = \frac{1}{n}\sum_{i\in[n]} \gamma_i. \tag{2.21}$$

The centroid of a simplex can be thought of as its centre of mass, assuming that weight is distributed evenly across its surface. We can also of course discuss the centroid of a face $\mathcal{T}_U$, which is $\boldsymbol{c}(\mathcal{T}_U) = |U|^{-1}\boldsymbol{\Sigma}\boldsymbol{\chi}_U$. 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 $\boldsymbol{a}(\mathcal{T}_U)$. We can write the altitude as $\boldsymbol{a}(\mathcal{T}_U) = \boldsymbol{p} - \boldsymbol{q}$ 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.

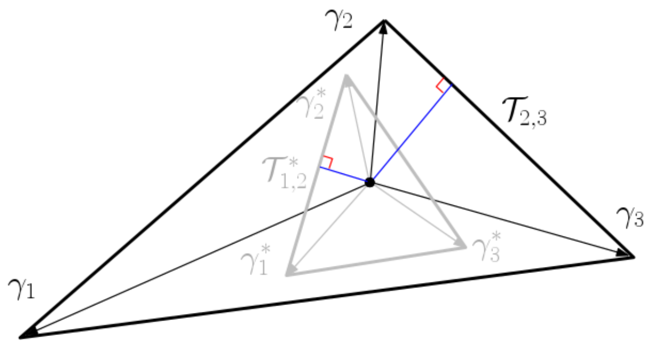

Figure 2.3: An example of a simplex $\mathcal{T} \subseteq \mathbb{R}^2$ (in black) and its dual, $\mathcal{T}^*$ (in gray). The blue lines serve to emphasize the fact that the dual vertex $\boldsymbol{\gamma}_1^*$ is orthogonal to the face $\mathcal{T}_{2,3}$ just as $\boldsymbol{\gamma}_3$ is to $\mathcal{T}_{1,2}^*$.

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 $\mathcal{T}_0 \in [\mathcal{T}]$. 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 $\boldsymbol{\Sigma}(\mathcal{T}) - (\boldsymbol{c}(\mathcal{T})\ \dots\ \boldsymbol{c}(\mathcal{T}))$ 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

Here we introduce the notion of the dual simplex of a given simplex. The inspiration for the construction comes from Fiedler's treatment of what he calls the "Gramian of a Graph" [Fie93]. The proofs in this section are relatively elementary. As such, most of them have been moved to Appendix A.1.

Let $\boldsymbol{\Sigma} = (\boldsymbol{\gamma}_1, \dots, \boldsymbol{\gamma}_n) \in \mathbb{R}^{n-1\times n}$ be the vertex matrix of a simplex $\mathcal{T} \subseteq \mathbb{R}^{n-1}$. For each $i \in [n-1]$, put $\mathbf{v}_i = \boldsymbol{\gamma}_n - \boldsymbol{\gamma}_i$. 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.*

Therefore, the set $\{\boldsymbol{\gamma}_1^*, \ldots, \boldsymbol{\gamma}_n^*\}$ 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 $\{\boldsymbol{\gamma}_i - \boldsymbol{\gamma}_n\}$. It is not clear a priori whether the vertices of the dual simplex would change were we to relabel the indices of $\{\boldsymbol{\gamma}_i\}$. In fact, they do not—the demonstration of which is the purpose of the following lemma.

LEMMA 2.11. *Let $\{\boldsymbol{\gamma}_1, \ldots, \boldsymbol{\gamma}_n\}$ be a set of affinely independent vectors. Fix $k \in [n-1]$ and define $\mathbf{v}_i = \boldsymbol{\gamma}_i - \boldsymbol{\gamma}_n$ for $i \in [n-1]$ and $\mathbf{u}_i = \boldsymbol{\gamma}_i - \boldsymbol{\gamma}_k$ 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 $\{\mathbf{u}_1, \ldots, \mathbf{u}_{k-1}, \mathbf{u}_{k+1}, \ldots, \mathbf{u}_n\}$.*

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 $\mathbf{v}_i = \boldsymbol{\gamma}_k - \boldsymbol{\gamma}_i$ and defined $\boldsymbol{\gamma}_k^* = -\sum_{i\neq k} \boldsymbol{\gamma}_i^*$ (as we did for $k = n$), Lemma 2.11 demonstrates that we would produce the same set of vectors for the dual simplex. What a relief! We honour the fact that the dual simplex is independent of labelling with the following definition.

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

We emphasize that the dual simplex is unique due to Observation 2.1.

Figure 2.3 illustrates a simplex and its dual. We remark that in light of the previous lemma, in order to determine whether the vertices $\{\boldsymbol{\gamma}_i^*\}$ are the dual vertices to $\{\boldsymbol{\gamma}_i\}$ it suffices to check whether $\langle \boldsymbol{\gamma}_i^*, \boldsymbol{\gamma}_j - \boldsymbol{\gamma}_k\rangle = \delta_{ij}$ 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 each congruence class $[\mathcal{T}]$ a centred simplex. Indeed, let $\mathcal{T}_1 \in [\mathcal{T}]$ and let $\boldsymbol{\Sigma}(\mathcal{T}^*) = (\boldsymbol{\gamma}_1^*, \ldots, \boldsymbol{\gamma}_n^*)$. We claim that the vertices $\boldsymbol{\Sigma}(\mathcal{T}^*)$ are also dual to $\boldsymbol{\Sigma}(\mathcal{T}_1) = (\boldsymbol{\sigma}_1, \ldots, \boldsymbol{\sigma}_n)$. As usual, let $\boldsymbol{\Sigma}(\mathcal{T}) = (\boldsymbol{\gamma}_i)$. Let $\boldsymbol{\alpha} \in \mathbb{R}^{n-1}$ be such that $\boldsymbol{\sigma}_i = \boldsymbol{\gamma}_i + \boldsymbol{\alpha}$ (such an $\boldsymbol{\alpha}$ exists by definition of $[\mathcal{T}]$). Then,

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

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., $\mathcal{T}^* = \mathcal{T}_0^*$.*

We can also characterize the pairwise interaction between the vertices of $\mathcal{T}$ and $\mathcal{T}^*$.

Lemma 2.12. *Let $\mathcal{T} \subseteq \mathbb{R}^{n-1}$ be centred and have vertices $\{\boldsymbol{\sigma}_i\}$. Then $\langle \boldsymbol{\gamma}_i, \boldsymbol{\gamma}_j^* \rangle = \delta_{ij} - 1/n$ for all $i, j \in [n]$, where $\{\boldsymbol{\gamma}_i^*\}$ are the dual vertices.*

Proof. By definition, we have $\langle \boldsymbol{\gamma}_i^*, \boldsymbol{\gamma}_j - \boldsymbol{\gamma}_k \rangle = \delta_{ij}$ for any k and all $i, j \neq k$. Fix such an i, j and k. Using that $\mathcal{T}$ is centred,

$$\langle \boldsymbol{\gamma}_i^*, \boldsymbol{\gamma}_k \rangle = -\sum_{\ell \neq k} \langle \boldsymbol{\gamma}_i^*, \boldsymbol{\gamma}_\ell \rangle = -\sum_{\ell \neq k} (\delta_{i\ell} + \langle \boldsymbol{\gamma}_i^*, \boldsymbol{\gamma}_k \rangle) = -1 - (n-1)\langle \boldsymbol{\gamma}_i^*, \boldsymbol{\gamma}_k \rangle.$$

Rearranging demonstrates that $\langle \boldsymbol{\gamma}_i^*, \boldsymbol{\gamma}_n \rangle = -1/n$, implying that $\langle \boldsymbol{\gamma}_i^*, \boldsymbol{\gamma}_j \rangle = \delta_{ij} + \langle \boldsymbol{\gamma}_i^*, \boldsymbol{\gamma}_k \rangle = \delta_{ij} - 1/n$. ⊠

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 2.13. *Let the simplex $\mathcal{T} \subseteq \mathbb{R}^{n-1}$ be centred. Then $\mathcal{T} = (\mathcal{T}^*)^*$.*

Proof. As usual, let $\{\boldsymbol{\gamma}_i\}$ be the vertices of $\mathcal{T}$ and $\{\boldsymbol{\gamma}_i^*\}$ those of $\mathcal{T}^*$. Let $\{\boldsymbol{\sigma}_i\}$ be the vertices of $(\mathcal{T}^*)^*$. We claim that, after possibly re-indexing, $\boldsymbol{\sigma}_i = \boldsymbol{\gamma}_i$ for all $i \in [n]$. By definition, the vertices $\{\boldsymbol{\sigma}_i\}_{i=1}^{n-1}$ are dual to $\{\boldsymbol{\gamma}_i^* - \boldsymbol{\gamma}_n^*\}$. Since the dual set is unique, to show that $\boldsymbol{\sigma}_i = \boldsymbol{\gamma}_i$ for $i \in [n-1]$, it suffices to show that $\{\boldsymbol{\gamma}_i\}$ obey this relationship. But by the previous lemma this follows readily:

$$\langle \boldsymbol{\gamma}_i, \boldsymbol{\gamma}_j^* - \boldsymbol{\gamma}_n^* \rangle = \langle \boldsymbol{\gamma}_i, \boldsymbol{\gamma}_j^* \rangle - \langle \boldsymbol{\gamma}_i, \boldsymbol{\gamma}_n^* \rangle = \delta_{ij} - \frac{1}{n} - \delta_{in} + \frac{1}{n} = \delta_{ij}.$$

For $i = n$ moreover, we have $\boldsymbol{\sigma}_n = -\sum_{\ell<n} \boldsymbol{\sigma}_\ell = -\sum_{\ell<n} \boldsymbol{\gamma}_i = \boldsymbol{\gamma}_n$ since $\mathcal{T}$ is centred. ⊠

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 $\langle \mathbf{u}_i, \boldsymbol{\gamma}_j - \boldsymbol{c} \rangle = \delta_{ij} - 1/n$, where $\boldsymbol{c} = \boldsymbol{c}(\mathcal{S})$. Such vectors then satisfy $\langle \mathbf{u}_i, \boldsymbol{\sigma}_j - \boldsymbol{\gamma}_k \rangle = \langle \mathbf{u}_i, \boldsymbol{\gamma}_j - \boldsymbol{c} - (\boldsymbol{\gamma}_k - \boldsymbol{c}) \rangle = \delta_{ij} - \delta_{ik} = \delta_{ij}$ 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 $\mathcal{T}_0$ is the dual of $\mathcal{T}^*$, where $\mathcal{T}_0 \cong \mathcal{T}$ is centred.*

Proof. Existence follows from Lemma 2.1 using the construction above. Uniqueness follows from Observation 2.1 and Lemma 2.11. The second part of the statement follows from Lemma 2.13. ⊠

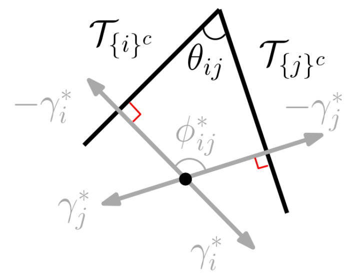

Figure 2.4: The angles in a simplex and its dual. The angle ϕ^*_{ij} between $\boldsymbol{\gamma}^*_i$ and $\boldsymbol{\gamma}^*_j$ is the same as that between $-\boldsymbol{\gamma}^*_i$ and $-\boldsymbol{\gamma}^*_j$. From here we see that $\theta_{ij} + \phi^*_{ij} = \pi$.

We end this section on dual simplices by giving a necessary condition of the relationship between a simplex and its dual. The following lemma also illustrates that the vertices $\boldsymbol{\gamma}^*_i$ are the "outer-normals" of $\mathcal{T}$ ($\boldsymbol{\gamma}^*_i$ is perpendicular to the face $\mathcal{T}_{\{i\}^c}$) and likewise, $\boldsymbol{\gamma}_i$ are the outer-normals of $\mathcal{T}^*$.

LEMMA 2.14. *Let $\mathcal{T}^*$ be the dual of the simplex $\mathcal{T} \subseteq \mathbb{R}^{n-1}$. For all $U \subseteq [n]$, $\emptyset \neq U \neq [n]$, $\mathcal{T}_U$ is orthogonal to $\mathcal{T}^*_{U^c}$.*

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 $\mathcal{T}_{\{i\}^c}$ and $\mathcal{T}_{\{j\}^c}$. 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

$$\cos\phi^*_{ij}(\mathcal{T}) = \frac{\langle \boldsymbol{\gamma}^*_i, \boldsymbol{\gamma}^*_j \rangle}{\|\boldsymbol{\gamma}^*_i\|_2 \cdot \left\|\boldsymbol{\gamma}^*_j\right\|_2},$$

where $\{\boldsymbol{\gamma}^*_i\}$ are the vertices of $\mathcal{T}^*$. The superscript represents the fact that the angle is between the vertices of the dual simplex. 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,

$$\cos\theta_{ij}(\mathcal{T}) = -\frac{\langle \boldsymbol{\gamma}^*_i, \boldsymbol{\gamma}^*_j \rangle}{\|\boldsymbol{\gamma}^*_i\|_2 \cdot \left\|\boldsymbol{\gamma}^*_j\right\|_2}, \tag{2.22}$$

where we've used that $\cos\left(\phi^*_{ij}\right) = \cos(\pi - \theta_{ij}) = -\cos(\theta_{ij})$. This allows us to define the notion of hyperacuteness in simplices as follows.

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*.

To summarize, a simplex $\mathcal{T}$ in $\mathbb{R}^{n-1}$ is the convex hull of n affinely independent vectors. We can assign to $\mathcal{T}$ a centred simplex $\mathcal{T}^*$ whose vertex vectors are normal to the facets of $\mathcal{T}$. We call $\mathcal{T}^*$ the dual simplex. It is unique up to translation.

Chapter 3

The Graph-Simplex Correspondence

> *The right understanding of any matter and a misunderstanding of the same matter do not wholly exclude each other.*
>
> — Franz Kafka, *The Trial*

> *Why, sometimes I've believed as many as six impossible things before breakfast.*
>
> — Lewis Carroll, *Alice's Adventures in Wonderland*

In this chapter we introduce the graph-simplex correspondence and explore its mathematical foundations. While the focus of this dissertation is specifically on the simplices arising from the Laplacian matrices of graphs, 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 polytope associated with a given matrix (we will use the words polyhedron and polytope interchangeably throughout this manuscript). Let $\boldsymbol{M} \in \mathbb{R}^{n\times n}$ be PSD and admitting of the eigendecomposition $\boldsymbol{M} = \sum_{i=1}^{d} \lambda_i \boldsymbol{\varphi}_i \boldsymbol{\varphi}_i^t$ for some $d \le n$ (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 absences of $\boldsymbol{\varphi}_{d+1}, \dots, \boldsymbol{\varphi}_n$ and $\lambda_{d+1}, \dots, \lambda_n$ respectively), 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.,

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

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

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

Letting $\boldsymbol{\Sigma} = \boldsymbol{\Sigma}(\mathcal{P}_{\boldsymbol{M}}) = (\boldsymbol{\sigma}_1, \ldots, \boldsymbol{\sigma}_n) \in \mathbb{R}^{d\times n}$ 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 $\boldsymbol{\Sigma} = \boldsymbol{\Lambda}_M^{1/2}\boldsymbol{\Phi}_M^t = (\boldsymbol{\Phi}_M\boldsymbol{\Lambda}_M^{1/2})^t$, and

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

Observe that the polytope $\mathcal{T}_{\boldsymbol{M}}$ is d-dimensional, i.e., its vertices span a d-dimensional subspace, since $\operatorname{rank}(\boldsymbol{\Sigma}) = \operatorname{rank}(\boldsymbol{\Sigma}^t\boldsymbol{\Sigma}) = \operatorname{rank}(\boldsymbol{M}) = d$, where we've employed Lemma 2.2 and the fact that $\boldsymbol{M}$ has rank d due to its eigendecomposition. We thus conceptualize $\mathcal{P}_{\boldsymbol{M}}$ as a polytope in $\mathbb{R}^d$.

Remark 3.1. The ordering of the non-zero eigenvalues did not enter our considerations when defining $\mathcal{P}_{\boldsymbol{M}}$. 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 $\operatorname{conv}(\boldsymbol{\sigma}_1^\tau, \ldots, \boldsymbol{\sigma}_n^\tau)$ and $\operatorname{conv}(\boldsymbol{\sigma}_1, \ldots, \boldsymbol{\sigma}_n)$ 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 $\boldsymbol{M}^{-1}$ if $\boldsymbol{M}$ is invertible, or with its pseudoinverse $\boldsymbol{M}^+$ more generally. As illustrated in Section 2.2.1, with the eigendecomposition of $\boldsymbol{M}$ as above, we can write the pseudoinverse as

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

We can thus associate with $\boldsymbol{M}^+$ a polytope $\mathcal{P}_{\boldsymbol{M}^+}$, which has as its vertex matrix $\boldsymbol{\Sigma}(\mathcal{P}_{\boldsymbol{M}^+}) = (\boldsymbol{\Phi}_M\boldsymbol{\Lambda}_M^{-1/2})^t$; 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 $\mathcal{P}_{\boldsymbol{M}}$ and $\mathcal{P}_{\boldsymbol{M}^+}$. In what follows we drop the subscript M from the eigenvalue and eigenvector matrix. Note that because of the orthogonality relationships among eigenvectors of $\boldsymbol{M}$,

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

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 $\mathcal{P}_{\boldsymbol{M}}$ and $\mathcal{P}^+_{\boldsymbol{M}}$ satisfy the same pseudoinverse relation:

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

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

LEMMA 3.1. *Let $\boldsymbol{\Sigma} = \boldsymbol{\Sigma}(\boldsymbol{M})$ and $\boldsymbol{\Sigma}^+ = \boldsymbol{\Sigma}(\boldsymbol{M}^+)$ be the vertex matrices of $\mathcal{P}_M$ and $\mathcal{P}_{M^+}$ where $\boldsymbol{M}$ is a real and symmetric matrix. The matrices $\boldsymbol{\Sigma}^t\boldsymbol{\Sigma}^+$ and $(\boldsymbol{\Sigma}^+)^t\boldsymbol{\Sigma}$ are equal and act as the orthogonal projection onto* $\mathrm{range}(\boldsymbol{M})$*. Moreover, $(\mathbf{I}-\boldsymbol{\Sigma}^t\boldsymbol{\Sigma}^+)$ acts as the orthogonal projection onto* $\ker(\boldsymbol{M})$.

Proof. Apply Lemma 2.4. ⊠

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

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

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

and likewise,

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

In summary, any real PSD matrix $\boldsymbol{M} \in \mathbb{R}^{n\times n}$ of rank d yields a d-dimensional convex polytope $\mathcal{P}_{\boldsymbol{M}}$ in $\mathbb{R}^{d\times d}$. The vertex matrices of $\mathcal{P}_{\boldsymbol{M}}$ and $\mathcal{P}_{\boldsymbol{M}^+}$—the polytope of the pseudoinverse of $\boldsymbol{M}$—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 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 a (connected, undirected, and) weighted graph $G = (V, E, w)$. The previous section yields several polytopes related to G by means of its Laplacian matrices. In particular, we obtain the polytopes $\mathcal{S}_G \overset{\text{def}}{=} \mathcal{P}_{\boldsymbol{L}_G}$ 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 $\boldsymbol{\Sigma} = \boldsymbol{\Sigma}(\mathcal{S}_G) = (\boldsymbol{\sigma}_1, \ldots, \boldsymbol{\sigma}_n)$ and $\widehat{\boldsymbol{\Sigma}} = \boldsymbol{\Sigma}(\widehat{\mathcal{S}}_G) = (\widehat{\boldsymbol{\sigma}}_1, \ldots, \widehat{\boldsymbol{\sigma}}_n)$ 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., $\widehat{\boldsymbol{\Phi}}$) the matrix of the corresponding (normalized) eigenvectors. Since $\text{rank}(\boldsymbol{L}_G) = \text{rank}(\widehat{\boldsymbol{L}}_G) = n - 1$, 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. 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 $\ker(\boldsymbol{\Sigma}) = \ker(\boldsymbol{\Sigma}^t\boldsymbol{\Sigma}) = \ker(\boldsymbol{L}) = \text{span}(\{\boldsymbol{1}\})$, 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 $\boldsymbol{\alpha} \in \ker(\widehat{\boldsymbol{\Sigma}}) = \ker(\widehat{\boldsymbol{L}}) = \text{span}(\{\sqrt{\boldsymbol{w}}\})$, then $\boldsymbol{\alpha} = k\sqrt{\boldsymbol{w}}$. But $\langle k\sqrt{\boldsymbol{w}}, \boldsymbol{1}\rangle = k\sum_i \sqrt{w(i)} = 0$, so $\boldsymbol{\alpha} = \boldsymbol{0}$. As above, this implies that $\{\widehat{\boldsymbol{\sigma}}_i\}$ is affinely independent. ⊠

We will 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 may 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 $\boldsymbol{\Sigma}^+ = \boldsymbol{\Lambda}^{-1/2}\boldsymbol{\Phi}^t$ and $\widehat{\boldsymbol{\Sigma}}^+ = \widehat{\boldsymbol{\Lambda}}^{-1/2}\widehat{\boldsymbol{\Phi}}^t$.

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 explicitly 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 $\langle \boldsymbol{\sigma}_i^+, \boldsymbol{\sigma}_j \rangle = \delta_{i,j} - 1/n$, 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 (2.22) 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 our attention now to the normalized simplices. Double orthogonality also holds for the eigenvectors of the normalized Laplacian and so, recalling that $\boldsymbol{\varphi}_n \in \text{span}(\boldsymbol{W}_G^{1/2}\mathbf{1})$, (Section 2.3.1) we can write

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

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

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

and so

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

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 centred 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 (2.22) from the discussion in Section 2.5.2, we can write the entries of $\boldsymbol{Q}_2$ as

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

where $\{\boldsymbol{\gamma}_i^*\}$ are the vertices of $\mathcal{T}^*$ (note that this holds for $i = j$ as well). Lemma 2.14 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:

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

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 $i \neq j$, $\boldsymbol{Q}(i,j) \leq 0$ since $\theta_{i,j} \leq \pi/2$ 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 $G = (V, E, w)$ on n vertices with edge weights $w(i,j) = -\boldsymbol{Q}(i,j)$, 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 $\{\boldsymbol{\sigma}_i^*\}$ 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 $\mathcal{T}^*$. We 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 however, we would require that $\|\boldsymbol{\sigma}_i^*\|_2 = 1$. This only holds for a very restricted class of simplex.

§3.3. Examples & Simplices of Special Graphs

In this section we provide several examples of simplices of graphs in order to give the reader a more intuitive feeling of the correspondence. In Appendix C, we also give visualizations of all four simplices of all unweighted graphs on 4 vertices.

Fix a 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 $\boldsymbol{A}^c \overset{\text{def}}{=} \boldsymbol{A}_{G^c} = \boldsymbol{1}\boldsymbol{1}^t - \mathbf{I} - \boldsymbol{A}_G$ and degree matrix $\boldsymbol{D}^c \overset{\text{def}}{=} \boldsymbol{D}_{G^c} =$

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

$(n-1)\mathbf{I} - \boldsymbol{D}_G$ 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 4.2.

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 denoted $G \times H$.

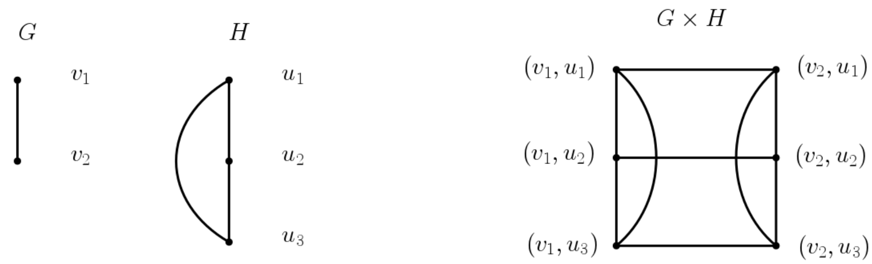

Figure 3.1: Two graphs and their product graph.

In order to investigate the simplex of a product graph, we must better understand its eigenstructure. The proof can be found in Appendix A.2.

LEMMA 3.4. *Let graphs G and H be given. 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 $\boldsymbol{\psi}_1, \ldots, \boldsymbol{\psi}_m$. Then $G \times H$ 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 $f_{i,j}(k, \ell) = \boldsymbol{\varphi}_i(k)\boldsymbol{\psi}_j(\ell)$.*

Consequently, with G and H as in Lemma 3.4, we see that 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

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

since $\sum_i \boldsymbol{\varphi}(i) = \langle \boldsymbol{\varphi}, \mathbf{1}\rangle = 0$. Let $\boldsymbol{Q}$ be the matrix which rotates each vector by $\pi/4$ about each axis. Thus $\boldsymbol{Q}\boldsymbol{e}_1 = \mathbf{1}$, and $n-1$ orthogonal eigenvectors are given by $\boldsymbol{Q}\boldsymbol{e}_2, \ldots, \boldsymbol{Q}\boldsymbol{e}_n$. Hence the vertices of $\mathcal{S}$ are 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. One can verify by direct computation that the eigenvalues and eigenvectors of $\boldsymbol{L}_{C_n}$ are given by

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

for $i = 1, \ldots, n/2+1$, 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 $i = n/2+2, \ldots, n$. 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 $\widetilde{\mathcal{S}}_p = \operatorname{conv}(\{\boldsymbol{\chi}_i\}_{i=1}^n \cup \{\mathbf{0}\})$. 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

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

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

$$\cos\theta_{ij}(\mathcal{S}_p) = -\frac{\langle \boldsymbol{\chi}_i, \boldsymbol{\chi}_j \rangle}{\|\boldsymbol{\chi}_i\|_2 \|\boldsymbol{\chi}_j\|_2} = -\delta_{ij},$$

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

$$\cos\theta_{in}(\mathcal{S}_p) = -\frac{\langle \boldsymbol{\chi}_i, -\mathbf{1} \rangle}{\|\boldsymbol{\chi}_i\|_2 \|\mathbf{1}\|_2} = 1/\sqrt{n},$$

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 $\boldsymbol{\Sigma}(\mathcal{S}_p^*)^t \boldsymbol{\Sigma}(\mathcal{S}_p^*)$, where $\boldsymbol{\Sigma}(\mathcal{S}_p^*) = (\boldsymbol{\sigma}_1^*, \ldots, \boldsymbol{\sigma}_n^*)$. 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 observations.

Lemma 3.5. *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),

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

The third property follows as a result of the fact that $\mathcal{S}_G^+$ is dual to $\mathcal{S}_G$ (Observation 3.1) and Lemma 2.14. ⊠

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

Proof. Using Equation (2.22) 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 $\langle \boldsymbol{\sigma}_i^+, \boldsymbol{\sigma}_j^+\rangle \le 0$. In this case $\boldsymbol{L}_G^+(i,j) \le 0$, 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 $\boldsymbol{L}_G^+(i,i) \ge 0$). ⊠

Corollary 3.1. *The combinatorial simplex $\mathcal{S}_{K_n}$ of the complete graph 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 $\operatorname{sign}(\boldsymbol{L}(k,\ell)) = \operatorname{sign}(\boldsymbol{L}^+(k,\ell))$ 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, $\operatorname{sign}(\boldsymbol{L}(k,\ell)) = \operatorname{sign}(n\sum_{i<n}\boldsymbol{\varphi}_i(k)\boldsymbol{\varphi}_i(\ell)) = \operatorname{sign}(\sum_{i<n}\boldsymbol{\varphi}_i(k)\boldsymbol{\varphi}_i(\ell)) = \operatorname{sign}(\boldsymbol{L}^+(k,\ell))$ which implies the result. ⊠

Before continuing, we make a brief detour to demonstrate how this result combined with the link between $\mathcal{S}_G^+$ and the effective resistance of G allows us to uncover the total effective resistance of certain graphs. Recalling that R_G^{tot} is the total effective resistance in G, apply Lemma 3.5 and write

$$\begin{aligned} R_G^{\text{tot}} &= \frac{1}{2}\sum_{i,j\in[n]} r^{\text{eff}}(i,j) = \frac{1}{2}\sum_{i,j\in[n]}\left\|\boldsymbol{\sigma}_i^+ - \boldsymbol{\sigma}_j^+\right\|_2^2 \\ &= \frac{n}{2}\sum_{in[n]}\|\boldsymbol{\sigma}_i^+\|_2^2 + \frac{n}{2}\sum_{j\in[n]}\left\|\boldsymbol{\sigma}_j^+\right\|_2^2 - 2\sum_{i,j\in[n]}\langle\boldsymbol{\sigma}_i^+,\boldsymbol{\sigma}_j^+\rangle \\ &= n\sum_{i\in[n]}\|\boldsymbol{\sigma}_i^+\|_2^2 - 2\sum_{i\in[n]}\langle\boldsymbol{L}_G(i,\cdot),\mathbf{1}\rangle = n\sum_{i\in[n]}\|\boldsymbol{\sigma}_i^+\|_2^2. \end{aligned}$$

Let K_n^α denote the complete graph on n vertices where each edge has weight α. By Corollary 3.1, $\boldsymbol{L}_{K_n^\alpha}^+ = \boldsymbol{L}_H$ for some graph H. Therefore, $\boldsymbol{L}_{K_n^\alpha} = \boldsymbol{L}_H^+$ and $\left\|\boldsymbol{\sigma}_i^+(H)\right\|_2^2 = \left\|\boldsymbol{\sigma}_i(\boldsymbol{L}_{K_n^\alpha})\right\|_2^2$. If K_n is the unweighted complete graph, we see that $\boldsymbol{L}_{K_n^\alpha} = \alpha\boldsymbol{L}_{K_n}$. Using that L_{K_n} has eigenvalue n with multiplicity $n-1$ (Section 3.3.1) gives $L_{K_n^\alpha} = \alpha n\sum_{i<n}\boldsymbol{\varphi}_i\boldsymbol{\varphi}_i^t$, meaning that $\boldsymbol{L}_{K_n^\alpha} = \boldsymbol{L}_H^+$ has eigenvalue αn with multiplicity $n-1$. The effective resistance of H is then

$$R_H^{\text{tot}} = n\operatorname{Tr}\big(\boldsymbol{L}_H^+\big) = \alpha(n-1).$$

Moreover, $\boldsymbol{L}_H$ has eigenvalue $(\alpha n)^{-1}$ with multiplicity $n-1$, and is therefore a complete graph with weights $(\alpha n^2)^{-1}$. We have proven the following:

Lemma 3.7. *For any complete graph H on n vertices with uniform edge weights $(\alpha n^2)^{-1}$ for any α, $R_H^{\text{tot}} = \alpha(n-1)$.*

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

Lemma 3.8. *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

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

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. As our proof is similar to theirs, we move it to Appendix A.2.

Lemma 3.9 ([DVM18]). *For a simplex $\mathcal{S}$ of a graph G,*

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

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* (i.e., a linear subspace shifted by some constant[2]) of dimension $|U| - 1$. The following lemma helps characterize these flats.

Lemma 3.10. *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 $\boldsymbol{\Sigma x} \in \mathcal{S}_U$ be arbitrary. For any $i \in U^c$ we have $\langle \boldsymbol{\Sigma x}, \boldsymbol{\sigma}_i^+ \rangle = \boldsymbol{x}^t \boldsymbol{\Sigma}^t \boldsymbol{\Sigma}^+ \boldsymbol{\chi}_i = -1/n$ because $\boldsymbol{x}$ is a barycentric coordinate with $x(i) = 0$. 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 3.10 gives us an alternate way to prove Lemma 3.9. For any i, taking $U = N \setminus \{i\}$ and $E = \{i\}$, it implies that $\mathcal{S}_{\{i\}^c}$ is a subset of the hyperplane

$$\mathcal{H}_i \stackrel{\text{def}}{=} \{ \boldsymbol{x} \in \mathbb{R}^{n-1} : \langle \boldsymbol{x}, \boldsymbol{\sigma}_i^+ \rangle + 1/n = 0 \}. \tag{3.7}$$

See Figure 3.2 for an illustration. All points in the simplex $\mathcal{S}$ lie to one side of $\mathcal{S}_{\{i\}^c}$, i.e., they lie in the halfspace

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

[2] Also called an affine subspace.

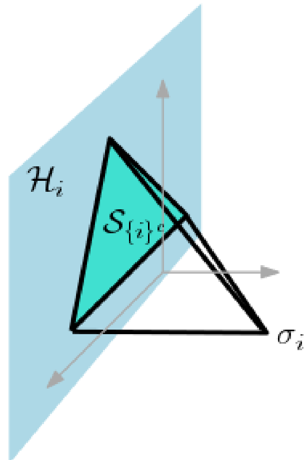

Figure 3.2: An illustration of the combinatorial simplex $\mathcal{S}_G \subseteq \mathbb{R}^3$ and its face $\mathcal{S}_{\{i\}^c}$ contained in the hyperplane $\mathcal{H}_i$.

(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.,

$$\mathcal{S} = \bigcap_i \mathcal{H}_i^{\geq}. \tag{3.8}$$

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., $(\langle \boldsymbol{x}, \boldsymbol{\sigma}_1^+ \rangle, \dots, \langle \boldsymbol{x}, \boldsymbol{\sigma}_n^+ \rangle) + \mathbf{1}/n \geq \mathbf{0}$, meaning $\boldsymbol{x}$ satisfies (3.6). We emphasize that a very similar discussion applies to $\mathcal{S}^+$, in which case one has

$$\mathcal{S}^+ = \bigcap_i (\mathcal{H}_i^+)^{\geq}, \tag{3.9}$$

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 3.11.

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 3.11 ([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 originating from the face generated by U in the dual simplex. First however, we require the following technical result.

Lemma 3.12. *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 $\boldsymbol{f}_{U^c}(U) = \mathbf{0}$.*

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 $\boldsymbol{f}(U) = \mathbf{0}$. 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 $\boldsymbol{x}(U^c) = \boldsymbol{y}(U^c) = \mathbf{0}$,

$$\begin{aligned} 0 &= \langle \boldsymbol{y}, \boldsymbol{\Sigma}\boldsymbol{x}_U - \boldsymbol{\Sigma}\boldsymbol{y}_u\rangle \\ &= \sum_{i\in U^c} z(i)\langle\boldsymbol{\sigma}_i^+, \boldsymbol{\Sigma}(\boldsymbol{x}_U - \boldsymbol{y}_U)\rangle + \sum_{j\in U} z(j)\langle\boldsymbol{\sigma}_j^+, \boldsymbol{\Sigma}(\boldsymbol{x}_U - \boldsymbol{y}_U)\rangle \\ &= \sum_{j\in U} z(j)\langle\boldsymbol{\sigma}_j^+, \boldsymbol{\Sigma}(\boldsymbol{x}_U - \boldsymbol{y}_U)\rangle, \end{aligned} \tag{3.10}$$

where the final inequality follows because $\boldsymbol{\sigma}_i^+$ is orthogonal to $\mathcal{S}_U$ for $i \in U^c$ by Lemma 3.5. Now, for $j \in U$,

$$\langle\boldsymbol{\sigma}_j^+, \boldsymbol{\Sigma}(\boldsymbol{x}_U - \boldsymbol{y}_U)\rangle = \boldsymbol{\chi}_j^t\boldsymbol{\Sigma}^+\boldsymbol{\Sigma}(\boldsymbol{x}_U - \boldsymbol{y}_U) = \boldsymbol{\chi}_j^t\left(\mathbf{I} - \frac{\mathbf{J}}{n}\right)(\boldsymbol{x}_U - \boldsymbol{y}_U) = \boldsymbol{\chi}_j^t(\boldsymbol{x}_U - \boldsymbol{y}_U). \tag{3.11}$$

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 (3.11) write (3.10) 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 3.13. *For a simplex $\mathcal{S}$ of a graph $G = (V, E)$ and any $U \subseteq V$, $U \neq \emptyset$,*

$$\frac{\boldsymbol{a}(\mathcal{S}_U)}{\|\boldsymbol{a}(\mathcal{S}_U)\|_2} = \frac{\boldsymbol{c}(\mathcal{S}_{U^c}^+)}{\left\|\boldsymbol{c}(\mathcal{S}_{U^c}^+)\right\|_2} = -\frac{\boldsymbol{c}(\mathcal{S}_U^+)}{\left\|\boldsymbol{c}(\mathcal{S}_U^+)\right\|_2}, \tag{3.12}$$

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 3.12 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 $\boldsymbol{f}(U) = \boldsymbol{0}$ and $\boldsymbol{g}(U^c) = \boldsymbol{0}$. In particular then,

$$\frac{\boldsymbol{\Sigma}^+(\boldsymbol{f} + \alpha\boldsymbol{\chi}_U)}{\|\boldsymbol{\Sigma}^+(\boldsymbol{f} + \alpha\boldsymbol{\chi}_U)\|_2} = \frac{\boldsymbol{\Sigma}^+(\boldsymbol{g} + \beta\boldsymbol{\chi}_{U^c})}{\|\boldsymbol{\Sigma}^+(\boldsymbol{g} + \beta\boldsymbol{\chi}_{U^c})\|_2}. \tag{3.13}$$

By Lemma 3.11, 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 (3.12) 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,

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

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,

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

which is Equation (3.12). ⊠

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

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

so $f - \beta\boldsymbol{\chi}_{U^c} + \alpha\boldsymbol{\chi} - g \in \ker(\boldsymbol{\Sigma}^+) = \operatorname{span}(\mathbf{1})$, 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

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

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

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

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

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

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

$$\left\|\boldsymbol{c}(\mathcal{S}_U^+)\right\|_2^2 = \frac{w(\partial^+ U)}{|U|^2}, \tag{3.15}$$

where we follow the notation of [DVM18] and define

$$w(\partial^+ U) \stackrel{\text{def}}{=} \langle \boldsymbol{\Sigma}^+\boldsymbol{\chi}_U, \boldsymbol{\Sigma}^+\boldsymbol{\chi}_U\rangle = \langle \boldsymbol{\chi}_U, \boldsymbol{L}^+\boldsymbol{\chi}_U\rangle = \mathcal{L}^+(\boldsymbol{\chi}_U). \tag{3.16}$$

Equations (3.14) and (3.15) 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 3.14. *For any non-empty $U \subseteq V$, $\left\|\boldsymbol{a}_U^+\right\|_2^2 = 1/w(\partial U)$ 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 $\boldsymbol{a}_U^+ = \boldsymbol{\Sigma}^+(\boldsymbol{x}_U - \boldsymbol{x}_{U^c})$. Combining this representation of $\boldsymbol{a}_U^+$ with that given by Lemma 3.13, write

$$\left\|\boldsymbol{a}_U^+\right\|_2 = \frac{\langle \boldsymbol{a}_U^+, \boldsymbol{a}_U^+\rangle}{\left\|\boldsymbol{a}_U^+\right\|_2} = \frac{\langle \boldsymbol{\Sigma}^+(\boldsymbol{x}_{U^c} - \boldsymbol{x}_U), \boldsymbol{c}_{U^c}\rangle}{\|\boldsymbol{c}_{U^c}\|_2} = \frac{\langle \boldsymbol{\Sigma}^+(\boldsymbol{x}_{U^c} - \boldsymbol{x}_U), \boldsymbol{\Sigma}\boldsymbol{\chi}_{U^c}\rangle}{\sqrt{w(\partial U^c)}},$$

where the final equality comes from using the definition of the centroid in the numerator, and Equation (3.14) 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

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

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

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

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

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

Proof. This is a consequence of identities (3.14) and (3.15) and Lemmas 3.13 and 3.14. Applying the latter and then the former, observe that

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

where we've once against used that $w(\partial^+ U^c) = w(\partial^+ U)$. 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

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

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

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

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,

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

which proves the first equality. The second is shown similarly by employing Lemma 3.15 and the previous identity:

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

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 3.5) and (ii) the lengths of the altitudes and centroids of $\mathcal{S}$ and $\mathcal{S}^+$ are proportional to the weights of cuts (Equations (3.14), (3.15), Lemmas 3.14, 3.15, 3.16).

§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 (recall that here, regular refers to *weight-regular*: each vertex has the same weight, not only the same degree). 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 $\langle\boldsymbol{\varphi}_i,\mathbf{1}\rangle\neq0$. In this case then,

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

Since $\ker(\widehat{\boldsymbol{L}}_G^+)=\ker(\widehat{\boldsymbol{L}}_G)$, the same reasoning applies to $\widehat{\mathcal{S}}_G^+$. This argument proves the following.

LEMMA 3.17. *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 $\mathbf{u} = \sqrt{\boldsymbol{w}}/\|\sqrt{\boldsymbol{w}}\|_1$, 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 $\mathbf{0} = \widehat{\mathbf{\Sigma}}\mathbf{u} \in \widehat{\mathcal{S}}$.

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. Since dual simplices are centred by definition, Lemma 3.17 demonstrates that $\widehat{\mathcal{S}}_G^+$ cannot be the dual of $\widehat{\mathcal{S}}_G$ unless G is regular. However, we might suspect that the centred simplex corresponding to $\widehat{\mathcal{S}}_G^+$ is dual to $\widehat{\mathcal{S}}_G$. The following lemma dashes these hopes.

Lemma 3.18. *The centred simplex $(\widehat{\mathcal{S}}_G^+)_0$ is the dual of $\widehat{\mathcal{S}}_G$ iff G is regular.*

Proof. First note that for any i, j,

$$\langle \widehat{\boldsymbol{\sigma}}_i^+, \widehat{\boldsymbol{\sigma}}_j \rangle = \boldsymbol{\chi}_i^t (\widehat{\mathbf{\Sigma}}^+)^t \widehat{\mathbf{\Sigma}} \boldsymbol{\chi}_j = \boldsymbol{\chi}_i^t \left(\mathbf{I} - \frac{\sqrt{\boldsymbol{w}}\sqrt{\boldsymbol{w}}}{\text{vol}(G)} \right) \boldsymbol{\chi}_j = \delta_{ij} - \frac{\sqrt{w(i)w(j)}}{\text{vol}(G)}.$$

Now if G is regular then $\widehat{\mathcal{S}}_0^+ = \widehat{\mathcal{S}}^+$ by Lemma 3.17. In this case, for all $i, j \neq k$,

$$\langle \widehat{\boldsymbol{\sigma}}_i^+, \widehat{\boldsymbol{\sigma}}_j - \widehat{\boldsymbol{\sigma}}_k \rangle = \delta_{ij} - \delta_{ij} + \frac{\sqrt{w(i)w(k)}}{\text{vol}(G)} - \frac{\sqrt{w(i)w(j)}}{\text{vol}(G)} = \delta_{ij},$$

since $w(i) = w(j) = w(k)$. This proves duality. Now suppose that G is not regular. For any j, k note that,

$$\begin{aligned} \frac{1}{n} \sum_{\ell \in [n]} \langle \widehat{\boldsymbol{\sigma}}_\ell^+, \widehat{\boldsymbol{\sigma}}_j - \widehat{\boldsymbol{\sigma}}_k \rangle &= \frac{1}{n} \sum_{\ell \in [n]} \left(\delta_{\ell j} - \delta_{\ell k} + \frac{\sqrt{w(\ell)}}{\text{vol}(G)} (\sqrt{w(k)} - \sqrt{w(j)}) \right) \\ &= \frac{\sqrt{w(k)} - \sqrt{w(j)}}{n\text{vol}(G)} \sum_{\ell \in [n]} \sqrt{w(\ell)} = \frac{\sqrt{w(k)} - \sqrt{w(j)}}{n\text{vol}(G)} \|\sqrt{\boldsymbol{w}}\|_1. \end{aligned}$$

Recall that the simplex $\widehat{\mathcal{S}}_0^+$ has vertices $\{\widehat{\boldsymbol{\sigma}}_i^+ - \boldsymbol{c}\}$ where $\boldsymbol{c} = \boldsymbol{c}(\widehat{\mathcal{S}}_G^+)$. For any $i, j \neq k \in \mathbb{N}$ compute

$$\begin{aligned} \langle \widehat{\boldsymbol{\sigma}}_i^+ - \boldsymbol{c}, \widehat{\boldsymbol{\sigma}}_j - \widehat{\boldsymbol{\sigma}}_k \rangle &= \langle \widehat{\boldsymbol{\sigma}}_i^+, \widehat{\boldsymbol{\sigma}}_j - \widehat{\boldsymbol{\sigma}}_k \rangle - \frac{1}{n} \sum_{\ell \in [n]} \langle \widehat{\boldsymbol{\sigma}}_\ell^+, \widehat{\boldsymbol{\sigma}}_j - \widehat{\boldsymbol{\sigma}}_k \rangle \\ &= \delta_{ij} + \left(\frac{\sqrt{w(i)}}{\text{vol}(G)} - \frac{\|\sqrt{\boldsymbol{w}}\|_1}{n\text{vol}(G)} \right) \left(\sqrt{w(k)} - \sqrt{w(j)} \right) \end{aligned}$$

Choose j, k such that $w(j) \neq w(k)$ (this is possible if G is not regular). Then the above is equal to δ_{ij} (which is necessary if $\widehat{\mathcal{S}}_0^+$ is dual to $\widehat{\mathcal{S}}$) iff

$$\sqrt{w(i)} = \frac{1}{n} \|\sqrt{\boldsymbol{w}}\|_1.$$

Thus, we see that $\{\widehat{\boldsymbol{\sigma}}_i^+ \boldsymbol{c}\}$ 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 2.14 (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 homogenous if each vertex in the set has the same weight.

LEMMA 3.19. *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 $\widehat{\mathcal{S}}[U_2]$.

$$\begin{aligned}
\langle \widehat{\boldsymbol{\Sigma}}^+ \boldsymbol{x}_{U_1}, \widehat{\boldsymbol{\Sigma}} \boldsymbol{x}_{U_2} \rangle &= \boldsymbol{x}_{U_1}^t \left(\mathbf{I} - \frac{\sqrt{\boldsymbol{w}}\sqrt{\boldsymbol{w}}^t}{\mathrm{vol}(G)} \right) \boldsymbol{x}_{U_2} \\
&= \boldsymbol{x}_{U_1}^t \boldsymbol{x}_{U_2} - \frac{1}{\mathrm{vol}(G)} \sum_{i \in U_1} \boldsymbol{x}_{U_1}(i) \sqrt{w(i)} \sum_{j \in U_2} \boldsymbol{x}_{U_2}(j) \sqrt{w(j)} \\
&= -\frac{1}{\mathrm{vol}(G)} \sqrt{w_1 w_2} \sum_{i \in U_1} \boldsymbol{x}_{U_1}(i) \sum_{j \in U_2} \boldsymbol{x}_{U_2}(j) = -\frac{\sqrt{w_1 w_2}}{\mathrm{vol}(G)},
\end{aligned}$$

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 3.20. *Suppose $U_1 \subseteq V(G)$ is not degree homogeneous. Then for all $U_2 \subseteq V(G)$ the 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

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

We state a consequence of Lemmas 3.19 and 3.20 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 3.19 $\widehat{\mathcal{S}}[\{i\}] = \widehat{\boldsymbol{\sigma}}_i$ (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 3.20 $\widehat{\boldsymbol{\sigma}}_i$ (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 $\mathcal{S}_G^+$. Let $U \subseteq V$. For the normalized Laplacian we have

$$\begin{aligned}
\widehat{\mathcal{L}}(\boldsymbol{\chi}_U) &= \sum_{i\sim j} w(i,j)\left(\frac{\boldsymbol{\chi}_U(i)}{\sqrt{w(i)}} - \frac{\boldsymbol{\chi}_U(j)}{\sqrt{w(j)}}\right)^2 \\
&= \sum_{i,j\in U} w(i,j)\left(\frac{1}{\sqrt{w(i)}} - \frac{1}{\sqrt{w(j)}}\right)^2 + \sum_{i\in U, j\in U^c} w(i,j)\left(\frac{\boldsymbol{\chi}_U(i)}{\sqrt{w(i)}}\right)^2 \\
&= \sum_{i,j\in U} \frac{w(i,j)}{w(i)w(j)}(\sqrt{w(i)} - \sqrt{w(j)})^2 + \sum_{i\in U, j\in U^c} \frac{w(i,j)}{w(i)} \\
&= \sum_{i\in U} \frac{1}{w(i)}\left\{\sum_{j\in U}\frac{w(i,j)}{w(j)}(\sqrt{w(i)} - \sqrt{w(j)})^2 + \sum_{j\in U^c} w(i,j)\right\}.
\end{aligned} \tag{3.17}$$

Admittedly, this lends itself much less easily to interpretation than in the case of the combinatorial simplex. However, we will see in Chapter 5 that when U is an independent set this formula has a more elegant form.

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 3.10 for the normalized simplex.

Lemma 3.21. *Let $U \subseteq V$ be non-empty and $F \subseteq U^c$. Setting*

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

for any set S, we have

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

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 $i \in U^c$,

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

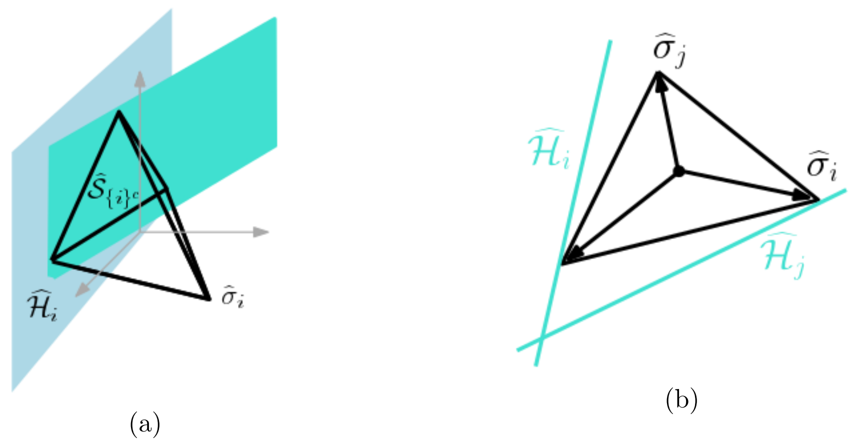

Figure 3.3: An illustration of the fact that, in general, $\widehat{\mathcal{S}}_{\{i\}^c}$ is not contained in $\widehat{\mathcal{H}}_i = \{\boldsymbol{x} : \langle \boldsymbol{x}, \widehat{\boldsymbol{\sigma}}_i^+\rangle + \beta_i = 0\}$.

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 3.21 yields a hyperplane representation of the normalized simplex, as did Lemma 3.10 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 $\widehat{\mathcal{H}}_i$:

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

by assumption. The other way to see this is to note that $\widehat{\boldsymbol{\sigma}}_i^+$ is not perpendicular to $\widehat{\mathcal{S}}_{\{i\}^c}$ 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 $\widehat{\mathcal{S}}_G^*$ and and $(\widehat{\mathcal{S}}_G^+)^*$? 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?". The question has an interesting implicit answer when asked of $\widehat{\mathcal{S}}_G^+$, as demonstrated by the following lemma.

LEMMA 3.22. *For any graph G, there exists a graph H such that the dual of $\widehat{\mathcal{S}}_G^+$ is the combinatorial simplex of H.*

Proof. Using the same reasoning which was applied to $\mathcal{S}_G^+$, we see that $\widehat{\mathcal{S}}_G^+$ is also hyperacute. This implies, by Theorem 3.1, that its centred version is the inverse *combinatorial* simplex of some graph H. That is, $(\widehat{\mathcal{S}}_G^+)_0 = \mathcal{S}_H^+$. Since all translationally congruent simplices share the same dual, we have

$$(\widehat{\mathcal{S}}_G^+)^* = (\widehat{\mathcal{S}}_G^+)_0^* = (\mathcal{S}_H^+)^* = \mathcal{S}_H. \qquad \boxtimes$$

Unfortunately, this result is purely existential and does not yield much insight as to actual structure of $(\widehat{\mathcal{S}}_G^+)^*$. In the case of $\widehat{\mathcal{S}}_G$, somewhat surprisingly, the 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

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

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 halfspaces, 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 sufficient conditions as to when this is the case.

LEMMA 3.23. *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 $\mathcal{T}^*$.*

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 3.23 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 3.24. *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 3.23 and 3.24 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 3.24 and to the dual of its centred version by Lemma 3.23. Since the dual is common to all congruent simplices by Observation 2.3, this would yield $\mathcal{S}_G^*$. Unfortunately, obtaining such a representation is not trivial. We leave the question as an open problem.

Chapter 4

Further Properties of the Correspondence

Everything is funny, if you can laugh at it.

— Lewis Carroll

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 (but perhaps more complicated) properties. We begin, however, by demonstrating that some of the interplay between $\mathcal{S}_G$ and $\mathcal{S}_G^+$ generalizes to an arbitrary simplex and its dual.

§4.1. A General Property of the Dual Simplex

Given that $\mathcal{S}_G^+$ is the dual of $\mathcal{S}_G$, it is natural to wonder whether some aspects of their relationship are common to that between any simplex and its dual. Here we demonstrate that this is indeed the case; in particular, the Gram matrix of any (centred) simplex and its dual enjoy the same pseudoinverse relationship. As we explained in Section 3.5, this relationship is crucial to many of the proofs pertaining to the combinatorial simplices. That an equivalent property holds for arbitrary simplices is therefore highly beneficial for their study.

Lemma 4.1. *Let $\mathcal{T} \subseteq \mathbb{R}^{n-1}$ be an arbitrary centred simplex, and $\mathcal{T}^*$ its dual. Put $\mathbf{\Sigma} = \mathbf{\Sigma}(\mathcal{T}) = (\boldsymbol{\gamma}_i)$ and $\mathbf{\Sigma}^* = \mathbf{\Sigma}(\mathcal{T}) = (\boldsymbol{\gamma}_i^*)$ as usual. Then $\mathbf{\Sigma}^*\mathbf{\Sigma}^t = \mathbf{\Sigma}(\mathbf{\Sigma}^*)^t = \mathbf{I}$ and $(\mathbf{\Sigma}^*)^t\mathbf{\Sigma}^*$ is the Moore-Penrose pseudoinverse of $\mathbf{\Sigma}^t\mathbf{\Sigma}$.*

Proof. First we inquire into the relationship between $\mathbf{\Sigma}$ and $\mathbf{\Sigma}^*$. Put $\boldsymbol{M} = (\boldsymbol{\gamma}_i - \boldsymbol{\gamma}_n)$, $i \in [n-1]$, and $\boldsymbol{Q} = (\boldsymbol{\gamma}_1^*, \dots, \boldsymbol{\gamma}_{n-1}^*)$. By definition, $\{\boldsymbol{\gamma}_i^*\}$ is the dual basis to $\{\boldsymbol{\gamma}_i - \boldsymbol{\gamma}_n\}$. Thus, by Observation 2.1, $\boldsymbol{Q}^t = \boldsymbol{M}^{-1}$ (we are working in $\mathbb{R}^{n-1}$), so $\boldsymbol{M}\boldsymbol{Q}^t = \mathbf{I}$. The (i,j)-th component of this matrix product can therefore be expressed as

$$\delta_{ij} = \boldsymbol{M}\boldsymbol{Q}^t(i,j) = \sum_{\ell=1}^{n-1}(\boldsymbol{\gamma}_\ell(i) - \boldsymbol{\gamma}_n(i))\boldsymbol{\gamma}_\ell^*(j) = \sum_{\ell=1}^{n-1}\boldsymbol{\gamma}_\ell(i)\boldsymbol{\gamma}_\ell^*(j) - \boldsymbol{\gamma}_n(i)\sum_{\ell=1}^{n-1}\boldsymbol{\gamma}_\ell^*(j). \tag{4.1}$$

Now, since $\mathcal{T}^*$ is centred,

$$0 = (\boldsymbol{\Sigma}^*\mathbf{1})(j) = \sum_{\ell\in[n]} \boldsymbol{\gamma}_\ell^*(j),$$

implying that $\sum_{\ell=1}^{n-1}\boldsymbol{\gamma}_\ell^*(j) = -\boldsymbol{\gamma}_n^*(j)$. Equation (4.1) can then be written $\sum_{\ell=1}^{n}\boldsymbol{\gamma}_\ell(i)\boldsymbol{\gamma}_\ell^*(j) = \delta_{ij}$, implying that the components of $\boldsymbol{\Sigma}^*\boldsymbol{\Sigma}^t$ are

$$(\boldsymbol{\Sigma}^*\boldsymbol{\Sigma}^t)(i,j) = \sum_{\ell=1}^{n}\boldsymbol{\gamma}_\ell^*(i)\boldsymbol{\gamma}_\ell(j) = \delta_{ij},$$

so that $\boldsymbol{\Sigma}^*\boldsymbol{\Sigma}^t = \mathbf{I}$. A similar argument holds for $\boldsymbol{\Sigma}(\boldsymbol{\Sigma}^*)^t$, *mutatis mutandis.*

We now proceed to demonstrating the pseudoinverse relation between $\boldsymbol{\Sigma}^t\boldsymbol{\Sigma}$ and $(\boldsymbol{\Sigma}^*)^t\boldsymbol{\Sigma}^*$. Recall that to demonstrate that a matrix $\boldsymbol{B}_1$ is the pseudoinverse of $\boldsymbol{B}_2$, we need to show that (i) $\boldsymbol{B}_1\boldsymbol{B}_2\boldsymbol{B}_1 = \boldsymbol{B}_1$, (ii) $\boldsymbol{B}_2\boldsymbol{B}_1\boldsymbol{B}_2 = \boldsymbol{B}_2$, (iii) $(\boldsymbol{B}_1\boldsymbol{B}_2)^t = \boldsymbol{B}_1\boldsymbol{B}_2$ and (iv) $(\boldsymbol{B}_2\boldsymbol{B}_1)^t = \boldsymbol{B}_2\boldsymbol{B}_1$ (Definition 2.4). Using the relationship between $\boldsymbol{\Sigma}^*$ and $\boldsymbol{\Sigma}$ given above, these become simple computations. For instance,

$$\boldsymbol{\Sigma}^t\boldsymbol{\Sigma}(\boldsymbol{\Sigma}^*)^t\boldsymbol{\Sigma}^*\boldsymbol{\Sigma}^t\boldsymbol{\Sigma} = \boldsymbol{\Sigma}^t\mathbf{I}^2\boldsymbol{\Sigma} = \boldsymbol{\Sigma}^t\boldsymbol{\Sigma},$$

and,

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

Conditions (i) and (iii) therefore hold between $\boldsymbol{\Sigma}^t\boldsymbol{\Sigma}$ and $(\boldsymbol{\Sigma}^*)^t\boldsymbol{\Sigma}^*$; conditions (ii) and (iv) follow similarly. ⊠

In the next section, we will demonstrate that this insight allows us to generalize results pertaining to hyperacute simplices to all simplices. We thus witness another benefit of the correspondence: By leveraging knowledge of $\mathcal{S}_G$ and $\mathcal{S}_G^+$ we can gain insights into the behaviour of general simplices.

§4.2. Block Matrix Equations

In this section we are finally able to satisfy those readers who have wondered about the applicability of electrical networks to the graph-simplex correspondence. Applying Lemma 2.8, we are able to develop block matrix equations which relate the structure of $\mathcal{S}_G$ and $\mathcal{S}_G^+$. Then, using the results of the previous section we generalize these equations to arbitrary simplices.

Before we begin, a brief remark on the relationship of the following results and Fiedler's work. Fiedler's derivation of the graph-simplex correspondence relied on a matrix equation—an equation equivalent to (4.4), in fact [Fie93, Theorem 3.1]. Conversely, we are obtaining such equations as a *consequence* of the correspondence. It is our hope that different treatments of the material shed light on its different—and hopefully complementary—implications.

Let a centred, hyperacute simplex $\mathcal{T}$ be given, with $\boldsymbol{\Sigma}(\mathcal{T}) = \{\boldsymbol{\gamma}_i\}$. Let $\bar{d}$ be the average squared distance between all the vertices of $\mathcal{T}$, that is

$$\bar{d} \overset{\text{def}}{=} \frac{1}{n^2} \sum_{i \leq j} \|\boldsymbol{\gamma}_i - \boldsymbol{\gamma}_j\|_2^2. \tag{4.2}$$

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

$$\xi(i) \overset{\text{def}}{=} \frac{1}{n} \sum_{j} \|\boldsymbol{\gamma}_i - \boldsymbol{\gamma}_j\|_2^2 - \bar{d}, \tag{4.3}$$

and put $\boldsymbol{\xi} = (\xi(1), \ldots, \xi(n))$. The following results relate the distance matrix of $\mathcal{T}$ to the vertex matrix of its dual.

Lemma 4.2. *Let $\mathcal{T} \subseteq \mathbb{R}^{n-1}$ be a hyperacute simplex with squared distance matrix $\boldsymbol{D}_{\mathcal{T}}$, and average squared distance vector $\boldsymbol{\xi}$. Let $\boldsymbol{Q} = (\boldsymbol{\Sigma}^*)^t \boldsymbol{\Sigma}^*$ where $\boldsymbol{\Sigma}^*$ is the vertex matrix of $\mathcal{T}^*$. Then,*

$$-\frac{1}{2}\begin{pmatrix} 0 & \mathbf{1}_n^t \\ \mathbf{1}_n & \boldsymbol{D}_{\mathcal{T}} \end{pmatrix} = \begin{pmatrix} \boldsymbol{\xi}^t \boldsymbol{Q} \boldsymbol{\xi} + 4\bar{d} & -(\boldsymbol{Q}\boldsymbol{\xi} + 2\mathbf{1}/n)^t \\ -(\boldsymbol{Q}\boldsymbol{\xi} + 2\mathbf{1}/n) & \boldsymbol{Q} \end{pmatrix}^{-1}. \tag{4.4}$$

Moreover, the vertices of $\mathcal{T}^*$ and the distance matrix of $\mathcal{T}$ are related by the equation

$$\boldsymbol{Q}\boldsymbol{D}_{\mathcal{T}}\boldsymbol{Q} = -2\boldsymbol{Q}, \tag{4.5}$$

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

$$\boldsymbol{D}_{\mathcal{T}}\boldsymbol{Q}\boldsymbol{D}_{\mathcal{T}} = -2\boldsymbol{D}_{\mathcal{T}}.$$

Proof. By Theorem 3.1, $\mathcal{T}$ is the inverse simplex of some graph G and therefore $\boldsymbol{D} = \boldsymbol{D}_{\mathcal{T}} = \boldsymbol{R}$, where $\boldsymbol{R}$ is the effective resistance matrix (Lemma 3.5). Therefore, we can rewrite $\xi(i)$ as

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

whence,

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

Meanwhile, the dual simplex to $\mathcal{T}$ is the simplex of the graph G, and hence obeys $\boldsymbol{Q} = \boldsymbol{L}_G$. Consequently, letting $\boldsymbol{\Delta} = \frac{1}{n}\boldsymbol{R}\mathbf{1} - \frac{1}{n^2}\mathbf{J}\boldsymbol{R}\mathbf{1}$, we can rewrite Equation (4.4) as the purely graph theoretic statement

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

This equation is verified by Lemma 2.8. The final two equations in the lemma translate to $\boldsymbol{L}_G\boldsymbol{R}_G\boldsymbol{L}_G = -2\boldsymbol{L}_G$ and $\boldsymbol{R}_G\boldsymbol{L}_G\boldsymbol{R}_G = -2\boldsymbol{R}_G$ on $\operatorname{span}(\mathbf{1})^\perp$. Both of these also hold via Lemma 2.8. ⊠

While Lemma 4.2 may be interesting, it is unfortunately restricted in its scope. In what follows we demonstrate that it can be generalized to hold for all simplices. Before we begin, we require a generalization of the statement $\boldsymbol{R} = \boldsymbol{\Delta}\mathbf{1}^t + \mathbf{1}\boldsymbol{\Delta}^t - 2\boldsymbol{L}_G^+$ to all distance matrices (recall that $\boldsymbol{R}$ is the distance matrix of $\mathcal{S}_G^+$). This is accomplished by the following lemma.

LEMMA 4.3. *For any centred simplex $\mathcal{T} \subseteq \mathbb{R}^{n-1}$ with distance matrix $\boldsymbol{D}_{\mathcal{T}}$ and vertex matrix $\boldsymbol{\Sigma}$, it holds that $\boldsymbol{D}_{\mathcal{T}} = \mathbf{1}\boldsymbol{\xi}^t + \boldsymbol{\xi}\mathbf{1}^t - 2\boldsymbol{\Sigma}^t\boldsymbol{\Sigma}$.*

Proof. Fix $k, \ell \in [n]$. The proof is purely computational. We have

$$(\boldsymbol{\xi}\mathbf{1}^t)(k,\ell) = \frac{1}{n}\sum_j \left\|\boldsymbol{\gamma}_k - \boldsymbol{\gamma}_j\right\|_2^2 - \bar{d}, \quad (\mathbf{1}\boldsymbol{\xi}^t)(k,\ell) = \frac{1}{n}\sum_j \left\|\boldsymbol{\gamma}_\ell - \boldsymbol{\gamma}_j\right\|_2^2 - \bar{d},$$

and $-2\boldsymbol{\Sigma}^t\boldsymbol{\Sigma} = -2\langle\boldsymbol{\gamma}_k, \boldsymbol{\gamma}_\ell\rangle$. Expanding the norm in terms of dot products, write

$$\begin{aligned}
(\boldsymbol{\xi}\mathbf{1}^t + \mathbf{1}\boldsymbol{\xi}^t - 2\boldsymbol{\Sigma}^t\boldsymbol{\Sigma})(k,\ell) &= \frac{1}{n}\left(\sum_j \left\|\boldsymbol{\gamma}_k - \boldsymbol{\gamma}_j\right\|_2^2 + \sum_j \left\|\boldsymbol{\gamma}_\ell - \boldsymbol{\gamma}_j\right\|_2^2\right) \\
&\quad - \frac{2}{n^2}\sum_{i<j}\left\|\boldsymbol{\gamma}_i - \boldsymbol{\gamma}_j\right\|_2^2 - 2\langle\boldsymbol{\gamma}_k, \boldsymbol{\gamma}_\ell\rangle \\
&= \frac{1}{n}\sum_j \left(\|\boldsymbol{\gamma}_k\|_2^2 + \left\|\boldsymbol{\gamma}_j\right\|_2^2 + \|\boldsymbol{\gamma}_\ell\|_2^2 + \left\|\boldsymbol{\gamma}_j\right\|_2^2 - 2\langle\boldsymbol{\gamma}_k, \boldsymbol{\gamma}_j\rangle - 2\langle\boldsymbol{\gamma}_\ell, \boldsymbol{\gamma}_j\rangle\right) \\
&\quad - \frac{1}{n^2}\sum_{i,j}\left(\|\boldsymbol{\gamma}_i\|_2^2 + \left\|\boldsymbol{\gamma}_j\right\|_2^2 - 2\langle\boldsymbol{\gamma}_i, \boldsymbol{\gamma}_j\rangle\right) - 2\langle\boldsymbol{\gamma}_k, \boldsymbol{\gamma}_\ell\rangle. \\
&= \|\boldsymbol{\gamma}_k\|_2^2 + \|\boldsymbol{\gamma}_\ell\|_2^2 - 2\langle\boldsymbol{\gamma}_k, \boldsymbol{\gamma}_\ell\rangle + 2\left(\frac{1}{n}\sum_j \left\|\boldsymbol{\gamma}_j\right\|_2^2 - \frac{1}{n^2}\sum_{i,j}\left\|\boldsymbol{\gamma}_j\right\|_2^2\right) \\
&\quad + \frac{1}{n^2}\sum_{i,j}\langle\boldsymbol{\gamma}_i, \boldsymbol{\gamma}_j\rangle - \frac{2}{n}\sum_j(\langle\boldsymbol{\gamma}_k, \boldsymbol{\gamma}_j\rangle - \boldsymbol{\gamma}_\ell, \boldsymbol{\gamma}_j\rangle).
\end{aligned}$$

Note that in the second line we removed the factor of two from $\bar{d}$ by summing over all i, j rather than simply $i < j$. Now, the first three terms in the final equation are equal to $\|\boldsymbol{\gamma}_k - \boldsymbol{\gamma}_\ell\|_2^2 = \boldsymbol{D}_{\mathcal{T}}(k,\ell)$. Therefore, it remains to show that the final three terms are zero. The first of these, $\frac{1}{n}\sum_j \left\|\boldsymbol{\gamma}_j\right\|_2^2 - \frac{1}{n^2}\sum_{i,j}\left\|\boldsymbol{\gamma}_j\right\|_2^2$, is clearly zero after noticing that the final summand is independent of i. As for the final two, we write them in terms of the centroid of $\mathcal{T}$ (which is $\mathbf{0}$), as

$$\begin{aligned}
&\frac{1}{n^2}\sum_{i,j}\langle\boldsymbol{\gamma}_i, \boldsymbol{\gamma}_j\rangle - \frac{2}{n}\sum_j(\langle\boldsymbol{\gamma}_k, \boldsymbol{\gamma}_j\rangle - \boldsymbol{\gamma}_\ell, \boldsymbol{\gamma}_j\rangle) \\
&= \frac{1}{n^2}\left\langle\sum_i \boldsymbol{\gamma}_i, \sum_j \boldsymbol{\gamma}_j\right\rangle - \frac{2}{n}\left(\left\langle\boldsymbol{\gamma}_k, \sum_j \boldsymbol{\gamma}_j\right\rangle - \left\langle\boldsymbol{\gamma}_\ell, \sum_j \boldsymbol{\gamma}_j\right\rangle\right) \\
&= \frac{1}{n^2}\langle n\boldsymbol{c}(\mathcal{T}), n\boldsymbol{c}(\mathcal{T})\rangle - \frac{2}{n}(\langle\boldsymbol{\gamma}_k, n\boldsymbol{c}(\mathcal{T})\rangle - \langle\boldsymbol{\gamma}_\ell, n\boldsymbol{c}(\mathcal{T})\rangle) \\
&= 0,
\end{aligned}$$

as was to be shown. ⊠

We can now strengthen Lemma 4.2 to all simplices, even those which are not centred.

THEOREM 4.1. *The equations of Lemma 4.2 hold for* any *simplex* $\mathcal{T} \subseteq \mathbb{R}^{n-1}$.

Proof. Let us first assume that $\mathcal{T}$ is centred. The proof proceeds very much as does that of Lemma 2.8, by computing the matrix product

$$\begin{pmatrix} 0 & \mathbf{1}^t \\ \mathbf{1} & \boldsymbol{D}_{\mathcal{T}} \end{pmatrix} \begin{pmatrix} \boldsymbol{\xi}^t \boldsymbol{Q} \boldsymbol{\xi} + 4\bar{d} & -(\boldsymbol{Q}\boldsymbol{\xi} + \frac{2}{n}\mathbf{1})^t \\ -(\boldsymbol{Q}\boldsymbol{\xi} + \frac{2}{n}\mathbf{1}) & \boldsymbol{Q} \end{pmatrix},$$

and demonstrating that it equals $-2\mathbf{I}$. Instead of leveraging the relationship $\boldsymbol{R}_G = \mathbf{1}\boldsymbol{\Delta}^t + \boldsymbol{\Delta}\mathbf{1}^t - 2\boldsymbol{L}_G^+$ as was done in that case, we use the more general equation $\boldsymbol{D}_{\mathcal{T}} = \mathbf{1}\boldsymbol{\xi}^t + \boldsymbol{\xi}\mathbf{1}^t - 2\boldsymbol{\Sigma}^t\boldsymbol{\Sigma}$ given by Lemma 4.3. However, since that proof was given in the appendix we will give this one here. The top left corner of the product of these two matrices is $-\mathbf{1}^t\boldsymbol{Q}\boldsymbol{\xi} - 2/n\mathbf{1}^t\mathbf{1} = -2$ as $\mathbf{1}^t\boldsymbol{Q} = \mathbf{1}^t(\boldsymbol{\Sigma}^*)^t\boldsymbol{\Sigma}^*$ since $\mathcal{T}^*$ is centred by definition. Likewise, the top right hand corner is zero. After expanding $\boldsymbol{D}_{\mathcal{T}}$ in accordance with Lemma 4.3 the bottom left corner becomes

$$\mathbf{1}\boldsymbol{\xi}^t\boldsymbol{Q}\boldsymbol{\xi} + 4\bar{d}\mathbf{1} - (\mathbf{1}\boldsymbol{\xi}^t + \boldsymbol{\xi}\mathbf{1}^t - 2\boldsymbol{\Sigma}^t\boldsymbol{\Sigma})\boldsymbol{Q}\boldsymbol{\xi} - \frac{2}{n}\boldsymbol{D}_{\mathcal{T}}\mathbf{1} = 4\bar{d}\mathbf{1} + 2\boldsymbol{\Sigma}^t\boldsymbol{\Sigma}\boldsymbol{Q}\boldsymbol{\xi} - \frac{2}{n}\boldsymbol{D}_{\mathcal{T}}\mathbf{1}. \tag{4.6}$$

Lemma 4.1 dictates that $\boldsymbol{Q}$ is the pseudoinverse of $\boldsymbol{\Sigma}^t\boldsymbol{\Sigma}$ so, by Lemma 2.4, $\boldsymbol{\Sigma}^t\boldsymbol{\Sigma}\boldsymbol{Q} = \mathbf{I} - \mathbf{J}/n$ (of course, we're implicitly using that $\text{span}(\mathbf{1})^\perp = \ker(\boldsymbol{\Sigma}) = \ker(\boldsymbol{\Sigma}^t\boldsymbol{\Sigma})$). Moreover, after noting that

$$\boldsymbol{\xi} = \frac{1}{n}\boldsymbol{D}_{\mathcal{T}}\mathbf{1} - \bar{d}\mathbf{1}, \quad \text{and} \quad \bar{d} = \frac{1}{2n^2}\mathbf{1}^t\boldsymbol{D}\mathbf{1},$$

we can rewrite the right hand side of Equation (4.6) as

$$\begin{aligned} &4\bar{d}\mathbf{1} + 2\left(\mathbf{I} - \frac{\mathbf{J}}{n}\right)\left(\frac{1}{n}\boldsymbol{D}_{\mathcal{T}}\mathbf{1} - \bar{d}\mathbf{1}\right) - \frac{2}{n}\boldsymbol{D}_{\mathcal{T}}\mathbf{1} \\ &= 2\bar{d}\mathbf{1} - \frac{2}{n^2}\mathbf{J}\boldsymbol{D}_{\mathcal{T}}\mathbf{1} + \frac{2}{n}\mathbf{J}\bar{d}\mathbf{1} \\ &= \frac{1}{n^2}\mathbf{J}\boldsymbol{D}_{\mathcal{T}}\mathbf{1} - \frac{2}{n^2}\mathbf{J}\boldsymbol{D}_{\mathcal{T}}\mathbf{1} + \frac{1}{n^3}\mathbf{J}^2\boldsymbol{D}_{\mathcal{T}}\mathbf{1} \\ &= \frac{1}{n^2}\mathbf{J}\boldsymbol{D}_{\mathcal{T}}\mathbf{1} - \frac{2}{n^2}\mathbf{J}\boldsymbol{D}_{\mathcal{T}}\mathbf{1} + \frac{1}{n^2}\mathbf{J}\boldsymbol{D}_{\mathcal{T}}\mathbf{1} = \mathbf{0}. \end{aligned}$$

Carrying out a similar procedure for the bottom right corner, we obtain

$$\begin{aligned} -\mathbf{1}\boldsymbol{\xi}^t\boldsymbol{Q} - \frac{2}{n}\mathbf{J} + \boldsymbol{D}_{\mathcal{T}}\boldsymbol{Q} &= -\mathbf{1}\boldsymbol{\xi}^t\boldsymbol{Q} - \frac{2}{n}\mathbf{J} + (\mathbf{1}\boldsymbol{\xi}^t + \boldsymbol{\xi}\mathbf{1}^t - 2\boldsymbol{\Sigma}^t\boldsymbol{\Sigma})\boldsymbol{Q} \\ &= -\frac{2}{n}\mathbf{J} - 2\left(\mathbf{I} - \frac{\mathbf{J}}{n}\right) = -2\mathbf{I}. \end{aligned}$$

The final two equations follow via similar computations:

$$\boldsymbol{Q}\boldsymbol{D}_{\mathcal{T}}\boldsymbol{Q} = \boldsymbol{Q}(\mathbf{1}\boldsymbol{\xi}^t + \boldsymbol{\xi}\mathbf{1}^t - 2\boldsymbol{\Sigma}^t\boldsymbol{\Sigma})\boldsymbol{Q} = -2\boldsymbol{Q}\boldsymbol{\Sigma}^t\boldsymbol{\Sigma}\boldsymbol{Q} = -2\boldsymbol{Q},$$

due to properties of the pseudoinverse (Definition 2.1), and if $\boldsymbol{x} \perp \mathbf{1}$ then

$$\boldsymbol{D}_{\mathcal{T}}\boldsymbol{Q}\boldsymbol{D}_{\mathcal{T}}\boldsymbol{x} = \boldsymbol{D}_{\mathcal{T}}\boldsymbol{Q}(\mathbf{1}\boldsymbol{\xi}^t + \boldsymbol{\xi}\mathbf{1}^t - 2\boldsymbol{\Sigma}^t\boldsymbol{\Sigma})\boldsymbol{x} = -2\boldsymbol{D}_{\mathcal{T}}\boldsymbol{Q}\boldsymbol{\Sigma}^t\boldsymbol{\Sigma}\boldsymbol{x} = -2\boldsymbol{D}_{\mathcal{T}}\left(\mathbf{I} - \frac{\mathbf{J}}{n}\right)\boldsymbol{x} = -2\boldsymbol{D}_{\mathcal{T}},$$

which completes the proof if $\mathcal{T}$ is centred. If $\mathcal{T}$ is not centred, then we need only apply the relationship to its centred version $\mathcal{T}_0$, and note that the quantities $\boldsymbol{D}_{\mathcal{T}}, \boldsymbol{\xi}, \bar{d}$ and $\boldsymbol{Q}$ are the same for $\mathcal{T}_0$ and $\mathcal{T}$. The first three are the same because they deal with distances between vertices, which are invariant under linear transformations. $\boldsymbol{Q}$ is the same due to Observation 2.3. ⊠

Remark 4.1. We have thus recovered Fiedler's block matrix relation [Fie93], although he does not give the same explicit interpretation of the entries as we do. As discussed above, it is interesting that Fiedler used the equation as the basis for the correspondence while our approach is the reverse.

4.2.1. Applications

We now discuss several uses of the equations developed above. One consequence is a relation between the volume of the simplex and 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

$$\begin{pmatrix} 0 & \mathbf{1}^t \\ \mathbf{1} & \boldsymbol{D}(\mathcal{X}) \end{pmatrix} \in \mathbb{R}^{(d+1)\times(d+1)}, \tag{4.7}$$

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

$$\mathrm{vol}^2(\mathrm{conv}(\mathcal{X})) = \frac{(-1)^d}{((d-1)!)^2 2^{d-1}} \det \begin{pmatrix} 0 & \mathbf{1}^t \\ \mathbf{1} & \boldsymbol{D}(\mathcal{X}) \end{pmatrix}. \tag{4.8}$$

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 fact was first pointed out by Van Mieghem *et al.* [VMDC17].

Lemma 4.5. *Let $\mathcal{S}^+ \subseteq \mathbb{R}^{n-1}$ be the inverse combinatorial simplex of G. The $n-1$ dimensional volume of $\mathcal{S}^+$ is*

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

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

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

We remind the reader that Γ_G was discussed in Section 2.3.1; see Equation (2.16) in particular. The proof of Lemma 4.5 may be found in Appendix A.3.

We can use these results to produce an equation relating the diagonal entries of the Laplacian to the volume of $\mathcal{S}_G^+$ and its facets.

LEMMA 4.6. *Let G be a connected graph and fix $i \in V(G)$. Put $G_{\{i\}^c} = G[V \setminus \{i\}]$. If $\mathcal{S}^+ \subseteq \mathbb{R}^{n-1}$ is the inverse combinatorial simplex of G then the volumes of $\mathcal{S}^+_{\{i\}^c}$ and $\mathcal{S}^+$ are related as*

$$\frac{\mathrm{vol}^2(\mathcal{S}^+_{\{i\}^c})}{\mathrm{vol}^2(\mathcal{S}^+)} = (n-1)^2 \boldsymbol{L}_G(i,i) = (n-1)^2 w(i). \tag{4.10}$$

Proof. Let $\mathcal{S}^+$ have vertices $\boldsymbol{\sigma}_1^+, \dots, \boldsymbol{\sigma}_n^+$, and let $\boldsymbol{M}$ be the Menger matrix associated with $\mathcal{S}^+$. Sylvester's formula (Lemma 2.3) gives us that

$$\boldsymbol{M}^{-1}(i+1,i+1) = \det \boldsymbol{M}^{-1}(i+1,i+1) = \pm \frac{\det \boldsymbol{M}(U,U)}{\det \boldsymbol{M}},$$

where $U = \{i+1\}^c$. Observe that $\boldsymbol{M}(U,U)$ is the Menger matrix of the simplex $\mathcal{S}^+_{\{i\}^c}$; we are simply removing the row and column corresponding to the i-th vertex. Translating the determinants of Menger matrices into statements about volumes of simplices via Equation (4.9) gives

$$\begin{aligned}\boldsymbol{M}^{-1}(i+1,i+1) &= \pm \frac{[(n-2)!]^2 2^{n-2}}{(-1)^{n-1}} \mathrm{vol}^2(\mathcal{S}^+_{\{i\}^c}) \Big/ \frac{[(n-1)!]^2 2^{n-1}}{(-1)^n} \mathrm{vol}^2(\mathcal{S}^+) \\ &= \mp \frac{1}{2(n-1)^2} \frac{\mathrm{vol}^2(\mathcal{S}^+_{\{i\}^c})}{\mathrm{vol}^2(\mathcal{S}^+)}.\end{aligned}$$

Via the block matrix equation (2.18) we have $\boldsymbol{M}^{-1}(i+1,i+1) = -\frac{1}{2}\boldsymbol{L}_G(i,i)$ (since the distance matrix of $\mathcal{S}^+$ is the effective resistance matrix of G). Plugging this into the above equation and noting that both $\boldsymbol{L}_G(i,i)$ and $\mathrm{vol}^2(\mathcal{S}^+_{\{i\}^c})/(2(n-1)^2\mathrm{vol}^2(\mathcal{S}^+))$ are positive gives the desired result. ⊠

Remark 4.2. The facet $\mathcal{S}^+_{\{i\}^c}$ is distinct from the inverse combinatorial simplex of the graph $G_{\{i\}^c}$. However, if one could relate their volumes then this would yield an equation for $\boldsymbol{L}_G(i,i)$ in terms of the spanning trees of G and $G_{\{i\}^c}$ by combining Lemma 4.5 and Equation (4.10).

Given that Lemma 4.5 uses the block matrix equation for hyperacute simplices, it is natural to wonder whether we can generalize the result by appealing instead to generalized matrix equation which holds for all simplices (Theorem 4.1). We can in fact, but first we need to prove several results concerning the Gram matrix of a general dual simplex. We begin with two technical lemmas which will later prove useful.

LEMMA 4.7. *For any simplex $\mathcal{T} \subseteq \mathbb{R}^{n-1}$, let $\boldsymbol{Q} = \boldsymbol{\Sigma}(\mathcal{T}^*)^t \boldsymbol{\Sigma}(\mathcal{T}^*)$ be the Gram matrix of the dual simplex. The volume of $\mathcal{T}$ is related to the cofactors of $\boldsymbol{Q}$ as*

$$\mathrm{vol}^2(\mathcal{T}) = \frac{4}{[(n-1)!]^2} \Bigg(\sum_{i\in[n]} \sum_{j\in[n]} \boldsymbol{r}(i)\boldsymbol{r}(j)(-1)^{i+j} \det\big(\boldsymbol{Q}_{-i,-j}\big) \Bigg)^{-1},$$

where $\boldsymbol{r} = -\boldsymbol{Q}\boldsymbol{\xi} - \frac{2}{n}\mathbf{1}$.

Proof. The statement is essentially extracted from the proof of Lemma 4.5, so we do not reformulate it here. We do note, however, that this lemma makes use of the block matrix equation for general simplices, whereas the proof of Lemma 4.5 relies only on Lemma 4.2. ⊠

The following second technical lemma will help with our eventual aim of demonstrating that all cofactors of a Gram matrix (of a centred simplex) are constant. The previous lemma will then enable us to relate this value to the volume.

Lemma 4.8. *Let* $\boldsymbol{M} \in \mathbb{R}^{n\times n}$ *have real eigenvalues* $\mu_1, \ldots, \mu_n$. *Then*

$$\sum_{i=1}^{n} \prod_{j\neq i} \mu_i = \sum_{i=1}^{n} \det(\boldsymbol{M}_{-i,-j}). \tag{4.11}$$

Proof. We make use of technique used by Godsil and Royle [GR13] to prove Kirchoff's matrix tree theorem. For $\boldsymbol{M}'$ and $\boldsymbol{M}''$ square, it holds that $\det(\boldsymbol{M}' + \boldsymbol{M}'') = \sum_{U\subseteq[n]} \det \boldsymbol{M}'_U$, where $\boldsymbol{M}'_U$ is the matrix obtained by replacing row i in $\boldsymbol{M}'$ with row i of $\boldsymbol{M}''$ for all $i \in U$. We will apply this to the sum $t\mathbf{I} - \boldsymbol{M}$. Fix $U \subseteq [n]$ and let us consider $\det(t\mathbf{I})_U$ for a moment. Letting S_n denote the set of all permutations on n vertices, recall that the determinant obeys

$$\det((t\mathbf{I})_U) = \sum_{\tau\in S_n} \operatorname{sgn}(\tau) \prod_{i\in[n]} (t\mathbf{I})_U(i, \tau(i)),$$

where $\operatorname{sgn}(\tau)$ is the sign of the permutation. Now, for $i \notin U$, the i-th row of $t\mathbf{I}$ is $t\boldsymbol{e}_i$, so $(t\mathbf{I})_U(i, \tau(i)) = t\delta_{i,\tau(i)}$. Consequently, we can restrict our attention to those permutations which fix each $i \notin U$:

$$\begin{aligned}
\det((t\mathbf{I})_U) &= \sum_{\substack{\tau\in S_n\\ \tau(i)=i, i\in U^c}} \operatorname{sgn}(\tau) \prod_{j\in U} (t\mathbf{I})_U(j, \tau(j)) \prod_{i\notin U} (t\mathbf{I})_U(i, \tau(i)) \\
&= \sum_{\substack{\tau\in S_n\\ \tau(i)=i, i\in U^c}} \operatorname{sgn}(\tau) \bigg(\prod_{j\in U} (t\mathbf{I})_U(j, \tau(j)) \bigg) t^{n-|U|} \\
&= t^{n-|U|} \sum_{\tau\in S_U} \operatorname{sgn}(\tau) \prod_{j\in U} (-\boldsymbol{M})(j, \tau(j)) \\
&= t^{n-|U|} \det(-\boldsymbol{M}(U, U)),
\end{aligned}$$

where we recall that $\boldsymbol{M}(U, U)$ denotes the submatrix of $\boldsymbol{M}$ indexed by the rows and columns of U. It is worth remarking that the penultimate inequality follows because the set of all permutations in S_n which fix the elements of U^c (i.e., do not change their positions) is in one-to-one correspondence with the set of all permutations on U. The final equality then uses the definition of the determinant. Returning to the characteristic polynomial, and noting that $\det(-\boldsymbol{M}(U,U)) = (-1)^{|U|}\det(\boldsymbol{M}(U,U))$ write

$$\begin{aligned}\det(t\mathbf{I}-\boldsymbol{M}) &= \sum_{U\subseteq[n]}\det((t\mathbf{I})_U) = \sum_{U\subseteq[n]} t^{n-|U|}(-1)^{|U|}\det(\boldsymbol{M}(U,U)) \\ &= \sum_{k=1}^{n}\sum_{U\subseteq[n],|U|=k} t^{n-k}(-1)^k\det(\boldsymbol{M}(U,U)).\end{aligned} \tag{4.12}$$

On the other hand, we can of course write the characteristic polynomial in terms of the eigenvalues of $\boldsymbol{M}$ [Bro06]:

$$\det(t\mathbf{I}-\boldsymbol{M}) = \sum_{k=0}^{n}(-1)^{n-k}\bigg(\sum_{U\subseteq[n],|U|=k}\prod_{i\in U}\mu_i\bigg)t^{n-k}. \tag{4.13}$$

Matching the coefficients of the term involving t in Expressions (4.12) and (4.13) gives

$$\begin{aligned}(-1)^{n-1}\sum_{U\subseteq[n],|U|=n-1}\prod_{i\in U}\mu_i &= (-1)^{n-1}\sum_{U\subseteq[n],|U|=n-1}\det(\boldsymbol{M}(U,U)) \\ &= (-1)^{n-1}\sum_{i=1}^{n}\det(\boldsymbol{M}_{-i,-i}),\end{aligned}$$

which is equivalent to the desired expression. ⊠

We are now almost ready to prove that all cofactors of Gram matrices of dual simplices are equal. We require one final tool, however. Let $\boldsymbol{M}\in\mathbb{R}^{n\times n}$. The *adjugate* of $\boldsymbol{M}$, denoted by $\operatorname{adj}(\boldsymbol{M})$, is the matrix whose (i,j)-th entry is equal to the (j,i)-th cofactor of $\boldsymbol{M}$, i.e.,

$$\operatorname{adj}(\boldsymbol{M})(i,j) = (-1)^{i+j}\det(\boldsymbol{M}_{-i,-j}),$$

where $\boldsymbol{M}_{-i,-j}\in\mathbb{R}^{(n-1)\times(n-1)}$ is the matrix obtained by removing the i-th row and column of $\boldsymbol{M}$. The adjugate obeys the following equation (see e.g., [GR13])

$$\boldsymbol{M}\operatorname{adj}(\boldsymbol{M}) = \det(\boldsymbol{M})\mathbf{I}. \tag{4.14}$$

Lemma 4.9. *Let $\boldsymbol{\Gamma}$ be the vertex matrix of n affinely independent points in $\mathbb{R}^{n-1}$ whose centroid is $\mathbf{0}$, i.e., $\boldsymbol{\Gamma}\mathbf{1}=\mathbf{0}$. Then (i) the cofactors of the Gram matrix $\boldsymbol{Q}=\boldsymbol{\Gamma}^t\boldsymbol{\Gamma}$ are all equal to some number $\kappa(\boldsymbol{Q})$ and (ii) $\prod_{i<n}\mu_i = n\cdot\kappa(\boldsymbol{Q})$ where $\mu_1,\dots,\mu_{n-1}$ are the non-zero eigenvalues of $\boldsymbol{Q}$.*

Proof. Note that $\det\boldsymbol{Q}=\mathbf{0}$ since $\mathbf{1}\in\ker\boldsymbol{Q}$. Hence, using Equation (4.14), $\boldsymbol{Q}\operatorname{adj}\boldsymbol{Q} = \det(\boldsymbol{Q})\mathbf{I} = \mathbf{0}_{n\times n}$. Each column of $\operatorname{adj}\boldsymbol{Q}$ is thus in $\ker\boldsymbol{Q}=\ker\boldsymbol{\Gamma}=\operatorname{span}(\mathbf{1})$ (here we're using both Lemma 2.2 and the fact that $\dim\ker\boldsymbol{\Gamma}=1$ due to affine independence). Therefore, $\operatorname{adj}\boldsymbol{Q} = (\alpha_1\mathbf{1},\alpha_2\mathbf{1},\dots,\alpha_n\mathbf{1})$ for some $\alpha_i\in\mathbb{R}$. However, since $\boldsymbol{Q}$ is symmetric, $\boldsymbol{Q}_{-i,-j} = \boldsymbol{Q}_{-j,-i}$ for each $i,j\in[n]$, implying that $\operatorname{adj}\boldsymbol{Q} = (\operatorname{adj}\boldsymbol{Q})^t$. This in turn implies that $\alpha_i=\alpha_j$ for all i,j, meaning that $\operatorname{adj}\boldsymbol{Q}$ is a constant matrix equal to, say, $\kappa(\boldsymbol{Q})\mathbf{J}$. This proves (i). (ii) now follows from applying Lemma 4.8 along with the fact that since $\boldsymbol{Q}$ has rank $n-1$, it has $n-1$ non-zero eigenvalues. Hence, if μ_n is the single zero eigenvalue,

$$\prod_{j<n}\mu_j = \sum_{i=1}^{n}\prod_{j\neq i}\mu_i = \sum_i \det\big(\boldsymbol{Q}_{-i,-i}\big) = n\kappa(\boldsymbol{Q}). \qquad \boxtimes$$

Finally, we can extract a general theorem about the volume of arbitrary simplices.

THEOREM 4.2. *For any simplex $\mathcal{T}\subseteq\mathbb{R}^{n-1}$,*

$$\mathrm{vol}(\mathcal{T}) = \frac{\sqrt{n}}{(n-1)!}\prod_{i<n}\frac{1}{\mu_i^{1/2}},$$

where $\mu_1,\dots,\mu_{n-1}$ are the non-zero eigenvalues of the matrix $\boldsymbol{Q}=\boldsymbol{\Sigma}(\mathcal{T}^*)^t\boldsymbol{\Sigma}(\mathcal{T})$, the Gram matrix of the dual simplex.

Proof. As per Lemma 4.9, let the cofactors of $\boldsymbol{Q}$ be equal to $\kappa(\boldsymbol{Q})$. Take $\boldsymbol{r}=-\boldsymbol{Q}\boldsymbol{\xi}-\frac{2}{n}\boldsymbol{1}$ as usual. Combining Lemmas 4.7 and 4.8 gives

$$\begin{aligned}\mathrm{vol}^2(\mathcal{T}) &= \frac{4}{[(n-1)!]^2}\left(\kappa(\boldsymbol{Q})\sum_{i,j\in[n]}r(i)r(j)\right)^{-1}\\ &= \frac{4}{[(n-1)!]^2\kappa(\boldsymbol{Q})}(\langle\boldsymbol{r},\boldsymbol{1}\rangle^2)^{-1} = \frac{n}{[(n-1)!]^2\prod_{i<n}\mu_i},\end{aligned}$$

where we've written $\kappa(\boldsymbol{Q})$ in terms of the eigenvalues by Lemma 4.9 and used that $\langle\boldsymbol{r},\boldsymbol{1}\rangle = -2$. $\boxtimes$

As an immediate consequence of this theorem, we obtain the volume of the combinatorial simplex of a graph. Our result matches that obtained by Van Mieghem *et al.* [VMDC17], but is gleaned in a different manner.

COROLLARY 4.1. *For a connected graph G,*

$$\mathrm{vol}(\mathcal{S}_G) = \frac{\sqrt{n}}{(n-1)!}\prod_{i<n}\lambda_i^{1/2} = \frac{n\cdot\Gamma_G^{1/2}}{(n-1)!}$$

where $\lambda_1\geq\lambda_2\geq\cdots\geq\lambda_{n-1}>\lambda_n=0$ are the eigenvalues of $\boldsymbol{L}_G$.

Proof. The Gram matrix of the dual simplex of $\mathcal{S}_G$ is $\boldsymbol{L}_G^+$, which has eigenvalues λ_i^{-1}. Apply Theorem 4.2. The second inequality follows from applying the matrix tree theorem. $\boxtimes$

Another consequence relates the volumes of the combinatorial simplices to the weight of all spanning trees of G.

COROLLARY 4.2. *The ratio of G's combinatorial simplices obeys*

$$\frac{\mathrm{vol}(\mathcal{S}_G)}{\mathrm{vol}(\mathcal{S}_G^+)} = n\Gamma_G.$$

Proof. We have $\mathrm{vol}(\mathcal{S}_G) = \frac{\sqrt{n}}{(n-1)!}\prod_{i<n}\lambda_i^{1/2}$ and $\mathrm{vol}(\mathcal{S}_G^+) = \frac{\sqrt{n}}{(n-1)!}\prod_{i<n}\lambda_i^{-1/2}$. Take the ratio and recall that $\Gamma_G = \prod_{i<n}\lambda_i$. ⊠

Unfortunately, it is difficult to garner similar insights regarding the normalized simplices. Indeed, because we do not know what the duals of the normalized simplices are in general, we cannot relate their volumes to the eigenvalues of $\widehat{\boldsymbol{L}}_G$. We can however, relate the eigenvalues of $\widehat{\boldsymbol{L}}_G$ to the volumes of $\mathcal{S}_G$ and $\mathcal{S}_G^+$. To do this, we first need to make a detour to study the adjugate the normalized Laplacian.

It is well-known that the adjugate is commutative with matrix multiplication [GR13]: $\mathrm{adj}(\boldsymbol{MQ}) = \mathrm{adj}(\boldsymbol{M})\,\mathrm{adj}(\boldsymbol{Q})$ for any $\boldsymbol{M}$ and $\boldsymbol{Q}$. Applying this to $\widehat{\boldsymbol{L}}$ (we drop the subscript), we have

$$\begin{aligned}\mathrm{adj}(\widehat{\boldsymbol{L}}) &= \mathrm{adj}(\boldsymbol{W}^{-1/2}\boldsymbol{L}_G\boldsymbol{W}^{-1/2})\\ &= \mathrm{adj}(\boldsymbol{W}^{-1/2})\,\mathrm{adj}(\boldsymbol{L}_G)\,\mathrm{adj}(\boldsymbol{W}^{-1/2})\\ &= \Gamma_G\cdot\mathrm{adj}(\boldsymbol{W}^{-1/2})\,\mathbf{J}\,\mathrm{adj}(\boldsymbol{W}^{-1/2}),\end{aligned}$$

where we've used that each cofactor of $\boldsymbol{L}_G$ is equal to Γ_G by Theorem 2.2. Using Equation (4.14) to compute $\mathrm{adj}(\boldsymbol{W}^{-1/2})$ yields

$$\mathrm{adj}(\boldsymbol{W}^{-1/2}) = \boldsymbol{W}^{1/2}\det\Big(\boldsymbol{W}^{-1/2}\Big)\mathbf{I} = \left(\prod_i w(i)^{-1/2}\right)\boldsymbol{W}^{1/2},$$

therefore,

$$\mathrm{adj}(\widehat{\boldsymbol{L}}) = \Gamma_G\left(\prod_i w(i)^{-1/2}\right)^2\boldsymbol{W}^{1/2}\mathbf{J}\boldsymbol{W}^{1/2} = \Gamma_G\left(\prod_i\frac{1}{w(i)}\right)\sqrt{\boldsymbol{w}}\sqrt{\boldsymbol{w}}^t. \tag{4.15}$$

From the above we gather that each cofactor of $\widehat{\boldsymbol{L}}$ is not constant. This can, however, be remedied by weighting each cofactor judiciously:

Lemma 4.10. *For each $i,j\in[n]$, $(-1)^{i+j}\det\Big(\widehat{\boldsymbol{L}}_{-i,-j}\Big))(w(i)w(j))^{-1/2}$ is independent of i and j and equal to the constant $\kappa(\widehat{\boldsymbol{L}}) = \Gamma_G\prod_k 1/w(k)$.*

Proof. Equation (4.15) implies that

$$(-1)^{i+j}\det(\boldsymbol{L}_{-i,-j}) = \mathrm{adj}(\widehat{\boldsymbol{L}})(j,i) = \Gamma_G\left(\prod_k\frac{1}{w(k)}\right)(w(i)w(j))^{1/2}.$$

Rearranging gives the result. ⊠

This allows us to relate the eigenvalues of $\widehat{\boldsymbol{L}}$ to those of $\boldsymbol{L}_G$, and consequently to the volume of $\mathcal{S}_G$ and $\mathcal{S}_G^+$ as follows.

Lemma 4.11. *If $\widehat{\lambda}_1 \geq \cdots \geq \lambda_{n-1} > \widehat{\lambda}_0$ are the eigenvalues of $\widehat{\boldsymbol{L}}_G$, then*

$$\prod_{i<n} \widehat{\lambda}_i = \Gamma_G \left(\prod_j \frac{1}{w(j)} \right) \mathrm{vol}(G) = \frac{\mathrm{vol}(\mathcal{S}_G)}{n \mathrm{vol}(\mathcal{S}_G^+)} \left(\prod_j \frac{1}{w(j)} \right) \mathrm{vol}(G). \tag{4.16}$$

Proof. We apply Lemma 4.8. Observe that the only non-zero product of $n-1$ eigenvalues is $\prod_{i<n} \widehat{\lambda}_i$ since $\widehat{\lambda}_n = 0$. Applying Lemma 4.10 to Equation (4.11) yields

$$\begin{aligned} \prod_{i<n} \widehat{\lambda}_i &= \sum_{i \in [n]} \det\left(\widehat{\boldsymbol{L}}_{-i,-i} \right) = \sum_{i \in [n]} (-1)^{i+i} \det\left(\widehat{\boldsymbol{L}}_{-i,-i} \right) w(i) \cdot w(i)^{-1} \\ &= \kappa(\widehat{\boldsymbol{L}}) \sum_{i \in [n]} w(i) = \Gamma_G \ \mathrm{vol}(G) \prod_k \frac{1}{w(k)}. \end{aligned}$$

This proves the first equality. The second follows from writing Γ_G in terms of the volumes of the combinatorial simplices as per Corollary 4.2. ⊠

Finally, we remark that the previous lemma provides an explicit relationship between the eigenvalues of $\widehat{\boldsymbol{L}}_G$ and those of $\boldsymbol{L}_G$. Indeed, combining Kirchoff's matrix tree theorem—Theorem 2.2—with Equation (4.16) gives

$$\prod_{i<n} \widehat{\lambda}_i \lambda_i = \frac{\mathrm{vol}(G)}{n} \prod_{j \in [n]} \frac{1}{w(j)}.$$

We now turn to investigating the relationships between the volumes of the facets of a simplex. Several of the following results are given by Fiedler in his most recent work on the subject [Fie11], but he does not prove them by means of the correspondence.

Lemma 4.12. *For any hyperacute simplex $\mathcal{T} \subseteq \mathbb{R}^{n-1}$ and $i \in [n]$, the following equations hold:*

1. $\mathrm{vol}(\mathcal{T}_{\{i\}^c}) = \sum_{j \neq i} \mathrm{vol}(\mathcal{T}_{\{j\}^c}) \cos \theta_{ij}(\mathcal{T})$;
2. $\mathrm{vol}^2(\mathcal{T}_{\{i\}^c}) = \sum_{j \neq i} \mathrm{vol}^2(\mathcal{T}_{\{j\}^c}) - \sum_{j,k \neq i, j \neq k} \mathrm{vol}(\mathcal{T}_{\{j\}^c}) \mathrm{vol}(\mathcal{T}_{\{k\}^c}) \cos \theta_{jk}(\mathcal{T})$; *and*
3. $(n-1)\mathrm{vol}(\mathcal{T}_{\{i,j\}^c}) \mathrm{vol}(\mathcal{T}) = (n-2) \mathrm{vol}(\mathcal{T}_{\{i\}^c}) \mathrm{vol}(\mathcal{T}_{\{j\}^c}) \sin \theta_{ij}(\mathcal{T})$ *for all $j \neq i$.*

Here, as usual, $\theta_{ij}(\mathcal{T})$ is the angle between $\mathcal{T}_{\{i\}^c}$ and $\mathcal{T}_{\{j\}^c}$.

Remark 4.3. One might expect that the second equation in the above lemma follows immediately from squaring the first. However, performing the computation demonstrates that this is not the case. Hence the second equation is in fact providing new information.

Proof. It suffices to take $\mathcal{T} = \mathcal{S}^+$, the inverse combinatorial simplex of some graph G. Let $\{\boldsymbol{\sigma}_i\}$ be the vertices of $\mathcal{S}_G$, the combinatorial simplex of G. We have $\boldsymbol{L}_G(i,j) = \langle \boldsymbol{\sigma}_i, \boldsymbol{\sigma}_j \rangle = \|\boldsymbol{\sigma}_i\|_2 \|\boldsymbol{\sigma}_j\|_2 \cos \phi_{ij}$, where ϕ_{ij} is the angle between $\boldsymbol{\sigma}_i$ and $\boldsymbol{\sigma}_j$. Since the vertices $\{\boldsymbol{\sigma}_i\}$ are dual to those of $\mathcal{S}_G^+$, we have $\cos \phi_{ij} = -\cos \theta_{ij}^+$ where θ_{ij}^+ is the angle between $\mathcal{S}_{\{i\}^c}^+$ and

$\mathcal{S}^+_{\{j\}^c}$. (We are applying the same reasoning here as in Sections 2.5.2 and 3.2.2.) Combining this with the fact that $\boldsymbol{L}_G\mathbf{1} = \mathbf{0}$ and Equation (4.10) gives

$$\begin{aligned}
0 = \sum_{j\in[n]} \boldsymbol{L}_G(i,j) &= \|\boldsymbol{\sigma}_i\|_2^2 - \sum_{j\neq i} \|\boldsymbol{\sigma}_i\|_2 \|\boldsymbol{\sigma}_j\|_2 \cos\theta^+_{ij} \\
&= \frac{\mathrm{vol}(\mathcal{S}^+_{\{i\}^c})}{(n-1)^2\mathrm{vol}^2(\mathcal{S}^+)}\bigg(\mathrm{vol}(\mathcal{S}^+_{\{i\}^c}) - \sum_{j\neq i}\mathrm{vol}(\mathcal{S}^+_{\{j\}^c})\cos\theta^+_{ij}\bigg),
\end{aligned}$$

implying that $\mathrm{vol}(\mathcal{S}^+_{\{i\}^c}) - \sum_{j\neq i}\mathrm{vol}(\mathcal{S}^+_{\{j\}^c})\cos\theta^+_{ij} = 0$ which proves the first equation. To see the second, note that $\boldsymbol{L}_G(i,k) = -\sum_{j\neq k}\boldsymbol{L}_G(i,k)$ (again using that $\boldsymbol{L}_G\mathbf{1} = \mathbf{0}$). Applying this twice, we obtain

$$\boldsymbol{L}_G(i,i) = -\sum_{j\neq i}\boldsymbol{L}_G(i,j) = \sum_{j\neq i}\sum_{k\neq i}\boldsymbol{L}_G(k,j) = \sum_{j\neq i}\boldsymbol{L}_G(j,j) + \sum_{j,k\neq i,k\neq j}\boldsymbol{L}_G(k,j).$$

As above, translating this to expressions involving the volumes of facets of $\mathcal{S}^+$ and then multiplying through by $n^2\mathrm{vol}(\mathcal{S}^+)$ gives

$$\mathrm{vol}^2(\mathcal{S}^+_{\{j\}^c}) = \sum_{j\neq i}\mathrm{vol}^2(\mathcal{S}^+_{\{j\}^c}) - \sum_{j,k\neq i,k\neq j}\mathrm{vol}(\mathcal{S}^+_{\{k\}^c})\mathrm{vol}(\mathcal{S}^+_{\{j\}^c})\cos\theta^+_{kj}.$$

It remains to prove the third equation. Let $\boldsymbol{M}$ be the Menger matrix of $\mathcal{S}^+$, and let $U = \{i,j\}$ and $U_1 = \{i+1, j+1\}$ for any $i \neq j$. Without loss of generality assume $i < j$. Notice that $\boldsymbol{M}(U_1^c, U_1^c)$ is the Menger matrix of the vertices $\{\boldsymbol{\sigma}_k\}_{k\neq i,j}$. Combining Sylvester's equation and our usual block matrix relation gives

$$\begin{aligned}
\frac{\det \boldsymbol{M}(U_1^c, U_1^c)}{\det \boldsymbol{M}} &= \pm\det\bigg(-\frac{1}{2}\boldsymbol{L}_G(U,U)\bigg) \\
&= \pm\frac{1}{4}\det\begin{pmatrix} \|\boldsymbol{\sigma}_i\|_2^2 & \langle\boldsymbol{\sigma}_i,\boldsymbol{\sigma}_j\rangle \\ \langle\boldsymbol{\sigma}_i,\boldsymbol{\sigma}_j\rangle & \|\boldsymbol{\sigma}_j\|_2^2\end{pmatrix} \\
&= \pm\frac{1}{4}\bigg(\|\boldsymbol{\sigma}_i\|_2^2\|\boldsymbol{\sigma}_j\|_2^2 - \langle\boldsymbol{\sigma}_i,\boldsymbol{\sigma}_j\rangle^2\bigg) \\
&= \pm\frac{1}{4}\|\boldsymbol{\sigma}_i\|_2^2\|\boldsymbol{\sigma}_j\|_2^2(1-\cos^2\phi_{ij})
\end{aligned}$$

where ϕ_{ij} is the angle between $\boldsymbol{\sigma}_i$ and $\boldsymbol{\sigma}_j$ (Section 2.5.2). Since the vertices $\{\boldsymbol{\sigma}_i\}$ are the duals to those in $\mathcal{S}^+$, we have $\cos\phi_{ij} = -\cos\theta^+_{ij}$ so

$$\|\boldsymbol{\sigma}_i\|_2^2\|\boldsymbol{\sigma}_j\|_2^2(1-\cos^2\phi_{ij}) = \|\boldsymbol{\sigma}_i\|_2^2\|\boldsymbol{\sigma}_j\|_2^2(1-\cos^2\theta^+_{ij}) = \|\boldsymbol{\sigma}_i\|_2^2\|\boldsymbol{\sigma}_j\|_2^2\sin^2\theta^+_{ij}.$$

Writing $\det\boldsymbol{M}(U_1^c, U_1^c)$ in terms of $\mathrm{vol}(\mathcal{S}^+_{U^c})$ and $\det\boldsymbol{M}$ in terms of $\mathrm{vol}(\mathcal{S}^+)$ by means of Equation (4.8), and using (4.10) to relate $\|\boldsymbol{\sigma}_i\|_2^2 = \boldsymbol{L}_G(i,i)$ and $\|\boldsymbol{\sigma}_j\|_2^2 = \boldsymbol{L}_G(j,j)$ to the volumes of $\mathcal{S}^+_{\{i\}^c}$ and $\mathcal{S}^+_{\{j\}^c}$ then yields

$$\frac{1}{4(n-1)^2(n-2)^2}\frac{\mathrm{vol}^2(\mathcal{S}^+_{U^c})}{\mathrm{vol}^2(\mathcal{S}^+)} = \frac{\mathrm{vol}^2(\mathcal{S}^+_{\{i\}^c})}{(n-1)^2\mathrm{vol}^2(\mathcal{S}^+)}\frac{\mathrm{vol}^2(\mathcal{S}^+_{\{j\}^c})}{(n-1)^2\mathrm{vol}^2(\mathcal{S}^+)}\sin^2\theta^+_{ij}.$$

Notice that we have rid ourselves of the ambiguity in sign because we see that both sides are the square of some quantity, hence are positive. Simplying and taking the square root of both sides of the above expression gives the third equation. ⊠

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

LEMMA 4.13. *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 $i=v_1,v_2,\dots,v_k=j$ is the unique path between i and j. Then,*

$$-\frac{1}{2}\begin{pmatrix}0 & \mathbf{1}^t\\ \mathbf{1} & \boldsymbol{S}_T\end{pmatrix}\begin{pmatrix}\sum_{i\sim j}1/w(i,j) & (\boldsymbol{d}-2\mathbf{1})^t\\ \boldsymbol{d}-2\mathbf{1} & \boldsymbol{L}_T\end{pmatrix}=\mathbf{I}, \tag{4.17}$$

where $\boldsymbol{d}=(\deg(1),\dots,\deg(n))$.

This result is interesting insofar as it lets us generate new statements concerning the effective resistance in trees. For example:

COROLLARY 4.3. *Let T be a weighted and connected tree. Then*

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

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

Proof. Let $\boldsymbol{S}_T$ be as it was in Lemma 4.13. 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 (4.17) and (2.18) yields

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

from which the claim follows. ⊠

§4.3. Inequalities

In this section we demonstrate how the correspondence 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. As usual, omitted proofs are found in the appendix.

LEMMA 4.14. *For any f with $\langle f, \mathbf{1}\rangle = 0$, $\mathcal{L}(f) \geq \|f\|_1^2/4w(\partial^+ F^+)$, for $F^+ \overset{def}{=} \{i : f(i) \geq 0\}$.*

Next we give an (admittedly, somewhat undecipherable) inequality relating the centroids of $\mathcal{S}_G$ to the vertex matrix of $\widehat{\mathcal{S}}$. The motivation is simply to demonstrate the potential uses of known graph-theoretic inequalities in the simplex domain.

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,

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

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

OBSERVATION 4.1.

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

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. ⊠

We can also translate several of the results obtained in the previous section on volumes and spanning trees into inequalities.

LEMMA 4.15. *For any hyperacute simplex $\mathcal{T} \subseteq \mathbb{R}^{n-1}$ and $i \in [n]$, the following equations hold:*

1. $\text{vol}(\mathcal{T}_{\{i\}^c}) \leq \sum_{j\neq i} \text{vol}(\mathcal{T}_{\{j\}^c})$;
2. $\sum_{j\neq i} \text{vol}^2 \mathcal{T}_{\{j\}^c} \geq \text{vol}^2 \mathcal{T}_{\{i\}^c} \geq \sum_{j\neq i} \text{vol}^2(\mathcal{T}_{\{j\}^c}) - \sum_{j,k\neq i, j\neq k} \text{vol}(\mathcal{T}_{\{j\}^c})\text{vol}(\mathcal{T}_{\{k\}^c})$; *and*
3. $(n-1)\text{vol}\mathcal{T}_{\{i,j\}^c}\text{vol}(\mathcal{T}) \leq (n-2)\text{vol}(\mathcal{T}_{\{i\}^c})\text{vol}(\mathcal{T}_{\{j\}^c})$ *for all $j \neq i$.*

Proof. Follows immediately from Lemma 4.12 after recalling that because $\mathcal{T}$ is hyperacute all interior angles are at most $\pi/2$. We remark that for the second equation we have simply provided the easy upper bound provided by Equation (2) of Lemma 4.12. ⊠

§4.4. Quadrics

Here we explore several quadrics associated with the simplices of G. Again, proofs which are found elsewhere are typically omitted and found in Appendix A.3.

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 $\mathcal{T}$ with vertices $\{\boldsymbol{\gamma}_i\}$ is a quadric which contains the vertices and whose tangent plane at $\boldsymbol{\gamma}_i$ is parallel to the affine plane spanned by $\{\boldsymbol{\gamma}_j\}_{j\neq i}$.

Figure 4.1 illustrates the Steiner ellipsoid of a generic simplex. Its existence and uniqueness is guaranteed by the following theorem.

Theorem 4.3 ([Fie05]). *The Steiner ellipsoid of a simplex $\mathcal{T}$ is unique and moreover, is the ellipsoid with minimum volume which contains $\mathcal{T}$.*

Owing to its uniqueness, we denote the Steiner ellipsoid of the simplex $\mathcal{T}$ by $\mathcal{E}(\mathcal{T})$. 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 4.16 ([Fie05]). *The Steiner circumscribed ellipsoid of G and its inverse are described by*

$$\mathcal{E}(\mathcal{S}_G) = \left\{\boldsymbol{x} : \boldsymbol{x}^t\boldsymbol{\Sigma}^+(\boldsymbol{\Sigma}^+)^t\boldsymbol{x} - \frac{n-1}{n} = 0\right\}, \tag{4.18}$$

and

$$\mathcal{E}(\mathcal{S}_G^+) = \left\{\boldsymbol{x} : \boldsymbol{x}^t\boldsymbol{\Sigma}\boldsymbol{\Sigma}^t\boldsymbol{x} - \frac{n-1}{n} = 0\right\}. \tag{4.19}$$

Perhaps more insightful representations of $\mathcal{E}(\mathcal{S}_G)$ and $\mathcal{E}(\mathcal{S}_G^+)$ come from appealing to Equations (3.1) and (3.2), i.e., $\boldsymbol{\Sigma}^+(\boldsymbol{\Sigma}^+)^t = \boldsymbol{\Lambda}^{-1}$ and $\boldsymbol{\Sigma}\boldsymbol{\Sigma}^t = \boldsymbol{\Lambda}$. Applying these,

$$\mathcal{E}(\mathcal{S}_G) = \left\{\boldsymbol{x} : \boldsymbol{x}^t\boldsymbol{\Lambda}^{-1}\boldsymbol{x} = \frac{n-1}{n}\right\}, \quad \text{and} \quad \mathcal{E}(\mathcal{S}_G^+) = \left\{\boldsymbol{x} : \boldsymbol{x}^t\boldsymbol{\Lambda}\boldsymbol{x} = \frac{n-1}{n}\right\} \tag{4.20}$$

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 $\boldsymbol{x}^t\boldsymbol{S}^2\boldsymbol{x} = 1$ with $\boldsymbol{S} \in \mathbb{R}^{d\times d}$ a diagonal matrix are the d vectors $\boldsymbol{e}_i \cdot \boldsymbol{S}(i,i)^{-1}$. 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].

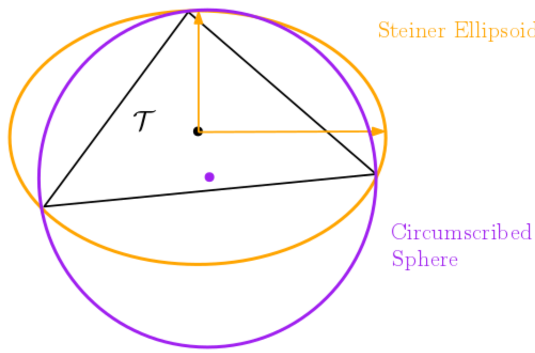

Figure 4.1: A simplex $\mathcal{T} \subseteq \mathbb{R}^2$ and its corresponding Steiner circumscribed ellipsoid in orange (light) and circumscribed sphere in purple (dark). The arrows illustrate the semi-axes of the ellipsoid. The purple point is the centre of the sphere—note that it does not necessarily coincide with the origin of the ellipsoid.

LEMMA 4.17. *The semi-axes of the Steiner Ellipsoids $\mathcal{E}(\mathcal{S}_G)$ and $\mathcal{E}(\mathcal{S}_G^+)$ are, respectively,*

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

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

Proof. Consider $\mathcal{E}(\mathcal{S}_G)$. The diagonal matrix $\boldsymbol{S} = \boldsymbol{\Lambda}^{-1/2}(\frac{n}{n-1})^{1/2}$ has entries $\boldsymbol{S}(i,i) = \boldsymbol{e}_i(\frac{n}{(n-1)\lambda_i})^{1/2}$, and equation (4.20) demonstrates that $\mathcal{E}(\mathcal{S}_G) = \{\boldsymbol{x} : \boldsymbol{x}^t\boldsymbol{S}^2\boldsymbol{x} = 1\}$. Apply the definition of semi-axes. The argument is similar for $\mathcal{E}(\mathcal{S}_G^+)$. ⊠

The appearance of the eigenvalues in the semi-axes allows us to relate the volumes of $\mathcal{E}(\mathcal{S}_G)$ and $\mathcal{E}(\mathcal{S}_G^+)$. The volume of an ellipsoid in $\mathbb{R}^{n-1}$ written in the standard form mentioned above is

$$\frac{\pi^{\frac{n-1}{2}}}{\Gamma(\frac{n+1}{2})}\det\big(\boldsymbol{S}^{-1}\big),$$

where $\Gamma(z)$ is the gamma function. We emphasize that the gamma function is distinct from Γ_G, the total weight of spanning trees in G. For $\mathcal{E}(\mathcal{S}_G)$, $\boldsymbol{S} = \sqrt{\frac{n}{n-1}}\boldsymbol{\Lambda}^{-1/2}$, so

$$\begin{aligned}
\operatorname{vol}(\mathcal{E}(\mathcal{S}_G)) &= \frac{\pi^{\frac{n-1}{2}}}{\Gamma(\frac{n+1}{2})}\left(\frac{n-1}{n}\right)^{\frac{n-1}{2}} \det \boldsymbol{\Lambda}^{1/2} \\
&= \frac{\pi^{\frac{n-1}{2}}}{\Gamma(\frac{n+1}{2})}\left(\frac{n-1}{n}\right)^{\frac{n-1}{2}} \left(\prod_{i<n}\lambda_i\right)^{1/2} \\
&= \frac{\pi^{\frac{n-1}{2}}}{\Gamma(\frac{n+1}{2})}\left(\frac{n-1}{n}\right)^{\frac{n-1}{2}} \sqrt{n}\Gamma_G^{1/2}.
\end{aligned}$$

Moreover, as was noticed by Devriendt and Van Mieghem [DVM18], the linear dependence of both $\mathrm{vol}(\mathcal{E}(\mathcal{S}_G)$ and $\mathrm{vol}(\mathcal{S}_G)$ on $\Gamma_G^{1/2}$ (recall Corollary 4.1) implies their ratio is independent of the particular graph G:

$$\frac{\mathrm{vol}(\mathcal{E}(\mathcal{S}_G))}{\mathrm{vol}(\mathcal{S}_G)} = \frac{\pi^{\frac{n-1}{2}}}{\Gamma(\frac{n+1}{2})}\left(\frac{n-1}{n}\right)^{\frac{n-1}{2}} \frac{(n-1)!}{\sqrt{n}}.$$

A similar procedure may be performed with $\mathrm{vol}(\mathcal{E}(\mathcal{S}_G^+))$ and $\mathrm{vol}(\mathcal{S}_G^+)$. In that case we have

$$\mathrm{vol}(\mathcal{E}(\mathcal{S}_G^+)) = \frac{\pi^{\frac{n-1}{2}}}{\Gamma(\frac{n+1}{2})}\left(\frac{n-1}{n}\right)^{\frac{n-1}{2}} \det \mathbf{\Lambda}^{-1/2} = \frac{\pi^{\frac{n-1}{2}}}{\Gamma(\frac{n+1}{2})}\left(\frac{n-1}{n}\right)^{\frac{n-1}{2}} (n\Gamma_G)^{-1/2}.$$

The ratio of $\mathrm{vol}(\mathcal{E}(\mathcal{S}_G^+))$ to $\mathrm{vol}(\mathcal{S}_G^+)$ is the same as above.

Next we investigate the circumscribed sphere of the combinatorial simplex. Similarly to the circumscribed ellipsoid, the *circumscribed 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 4.18 ([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 $\{\boldsymbol{x} : \boldsymbol{x} = \mathbf{\Sigma}\boldsymbol{\alpha},\ \langle \boldsymbol{\alpha}, \mathbf{1}\rangle = 1,\ \langle \boldsymbol{\alpha}, \boldsymbol{D}\boldsymbol{\alpha}\rangle = 0\}$, which is a sphere centred at the point $\frac{1}{2}\mathbf{\Sigma}(\boldsymbol{L}_G\mathbf{\Delta} + \mathbf{1}/n)$ with radius $\frac{1}{2}\sqrt{\mathbf{\Delta}^t \boldsymbol{L}_G \mathbf{\Delta} + 4R_G^{\mathrm{tot}}/n^2}$ where G is $\mathcal{S}^+$'s associated graph, and $\mathbf{\Delta} = \mathrm{diag}(\boldsymbol{L}_G^+(i,i))$.*

Remark 4.4. It is no coincidence that the radius of the sphere is related to the top left entry in the inverse of the Menger matrix associated with $\mathcal{S}^+$. This was noticed by Fiedler and is relied upon in the proof of Lemma 4.18.

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 $\boldsymbol{x}^t\widehat{\mathbf{\Sigma}}^+(\widehat{\mathbf{\Sigma}}^+)^t = 1 - 1/n$, as this is the natural analogue of (4.18). However, because $\widehat{\mathbf{\Sigma}}^+$ and $\widehat{\mathbf{\Sigma}}$ obey a non-constant pseudoinverse relation, this equation fails the first test: $\widehat{\boldsymbol{\sigma}}_i^t\widehat{\mathbf{\Sigma}}^+(\widehat{\mathbf{\Sigma}}^+)^t\widehat{\boldsymbol{\sigma}}_i = \boldsymbol{\chi}_i^t(\mathbf{I} - \sqrt{\boldsymbol{w}}\sqrt{\boldsymbol{w}}^t/\mathrm{vol}(G))\boldsymbol{\chi}_i = 1 - \sqrt{w(i)w(j)}/\mathrm{vol}(G)$ is not 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 $\widehat{\mathbf{\Sigma}}^*(\widehat{\mathbf{\Sigma}}^*)^t$, where $\widehat{\mathbf{\Sigma}}^*$ is the vertex matrix of $\widehat{\mathcal{S}}^*$. The following lemma confirms this hypothesis and, moreover, verifies that similar reasoning can be applied to the Steiner Ellipsoid of any simplex—not only those corresponding to graphs.

Lemma 4.19. *Let $\mathcal{T} \subseteq \mathbb{R}^{n-1}$ be a simplex whose dual has vertex matrix $\mathbf{\Sigma}^*$. Then the Steiner ellipsoid of $\mathcal{T}$ is*

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

Proof. The computation is almost identical to that in the proof of Lemma 4.16, except we take $\boldsymbol{M} = \boldsymbol{\Sigma}^*(\boldsymbol{\Sigma}^*)^t$ and use the general relationship between $\boldsymbol{\Sigma}^t\boldsymbol{\Sigma}$ and $\boldsymbol{\Sigma}^*(\boldsymbol{\Sigma}^*)^t$ given by Lemma 4.1. ⊠

§4.5. 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:

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

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 well known fact that the effective resistance is a metric (e.g., [KR93]). That being said however, while the mapping seems to be known [GBS08], there is very little literature on its properties.

Set

$$\mathcal{R}_G \stackrel{\text{def}}{=} \text{conv}(\{\boldsymbol{\mu}_i\}), \tag{4.21}$$

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 product between the vertices of $\mathcal{R}_G$ does respect the same relationships as those between the vertices of $\mathcal{S}_G^+$:

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

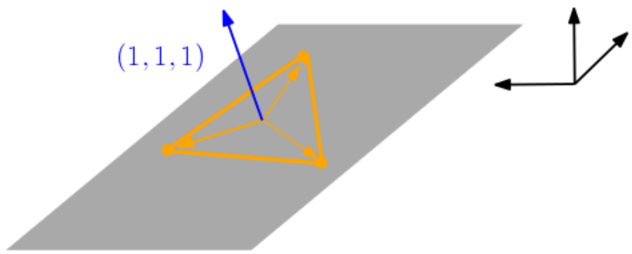

Figure 4.2: The resistive embedding (in orange; light) of a graph with three nodes sits in a plane (gray) which is parallel to the all ones vector.

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 $\|\boldsymbol{\mu}_i - \boldsymbol{\mu}_j\|_2^2 = r^{\text{eff}}(i,j)$ and $\|\boldsymbol{\mu}_i\|_2^2 = \boldsymbol{L}_G^{+}(i,i)$. 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 $\text{span}(\mathbf{1})$ as its orthogonal complement. See Figure 4.2 for an illustration.

Lemma 4.20. *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

(3.14): There exists an isometry[2] 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,

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

To conclude, there exists an isometry between the inverse combinatorial simplex of a graph G (which lies in $\mathbb{R}^{n-1}$) and the effective polytope, $\mathcal{R}_G$ of G (which lies in $\mathbb{R}^n$). The resistive polytope lies in a hyperplane orthogonal to the all-ones vector.

§4.6. Continuous Time Random Walks

This current section is for the reader who is less interested in the mathematics behind the graph-simplex correspondence, and is reading only for the vague hope that some of the underlying geometry will be aesthetically pleasing. While the content has certainly failed in this vein thus far, this section is the closest we will come to remedying the situation.

Consider a random walk on a graph. The probability distribution governing the dynamics is a barycentric coordinate: each coordinate is non-negative and they sum to one. Therefore, we can represent the probability distribution as a point in the simplex and the probability distribution as a function of time as a path in the simplex. See Figure 4.3 for an illustration. In what follows we give equations which determine the dynamics of the path in the simplex as a function of the eigenvalues and eigenvectors of the graph.

[2] A distance preserving map.

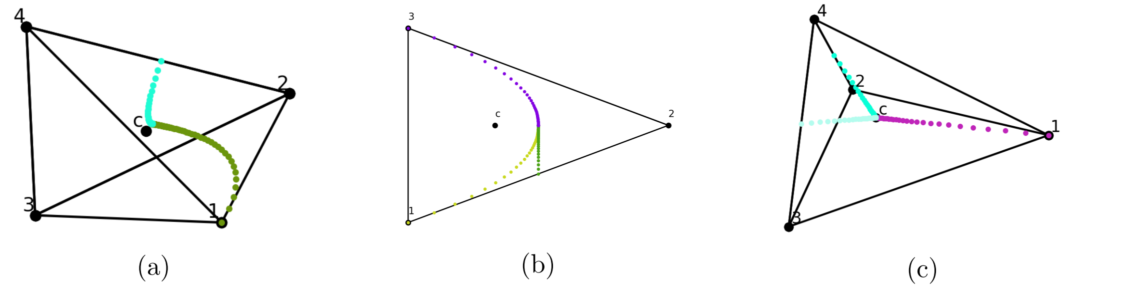

Figure 4.3: Random walk dynamics plotted as points in the simplex. Figures (a) and (b) are plotted using the normalized simplex; figure (c) uses the normalized simplex. The underlying graph of Figure (a) has edges $(1,2)$, $(2,3)$, $(3,4)$, $(2,4)$, that underlying (b) edges $(1,2)$ and $(2,3)$ and that of (c) is the complete graph K_4.

We will examine a continuous time random walk which obeys the equation

$$\frac{d\boldsymbol{\pi}(t)}{dt} = -\boldsymbol{L}_G\boldsymbol{W}_G^{-1/2}\boldsymbol{\pi}(t),$$

and has the solution $\boldsymbol{\pi}(t) = \exp\Big(-\boldsymbol{L}_G\boldsymbol{W}_G^{-1/2}t\Big)\boldsymbol{\pi}(0)$. This, however, is relatively unsightful in terms of analyzing the dynamics of $\boldsymbol{\pi}(t)$ in terms of the graph. Instead, in what follows we seek to develop a solution to $\boldsymbol{\pi}(t)$ in terms of the eigendecomposition of G. Define $\boldsymbol{\pi}_1(t) = \boldsymbol{W}^{-1/2}\boldsymbol{\pi}(t)$ and $\boldsymbol{\pi}_2(t) = \widehat{\boldsymbol{\Phi}}^t\boldsymbol{\pi}_1(t)$, where we recall that $\widehat{\boldsymbol{\Phi}}^t$ is the eigenvector matrix of $\widehat{\boldsymbol{L}}_G$. Then

$$\frac{d\boldsymbol{\pi}_1(t)}{dt} = \boldsymbol{W}^{-1/2}\frac{d\boldsymbol{\pi}(t)}{dt} = -\boldsymbol{W}^{-1/2}\boldsymbol{L}_G\boldsymbol{W}^{-1/2}\boldsymbol{W}^{-1/2}\boldsymbol{\pi}(t) = -\widehat{\boldsymbol{L}}_G\boldsymbol{\pi}_1(t),$$

and, using the eigendecomposition of $\widehat{\boldsymbol{L}}_G$,

$$\frac{d\boldsymbol{\pi}_2(t)}{dt} = \widehat{\boldsymbol{\Phi}}^t\frac{d\boldsymbol{\pi}_1(t)}{dt} = -\widehat{\boldsymbol{\Phi}}^t\widehat{\boldsymbol{L}}_G\boldsymbol{\pi}_1(t) = -\widehat{\boldsymbol{\Phi}}^t\widehat{\boldsymbol{\Phi}}\widehat{\boldsymbol{\Lambda}}\widehat{\boldsymbol{\Phi}}^t\boldsymbol{\pi}_1(t) = -\widehat{\boldsymbol{\Lambda}}\boldsymbol{\pi}_2(t),$$

since $\widehat{\boldsymbol{\Phi}}^t\widehat{\boldsymbol{\Phi}} = \mathbf{I}$. This equation has the solution

$$\boldsymbol{\pi}_2(t) = \exp\Big(-\widehat{\boldsymbol{\Lambda}}t\Big)\boldsymbol{\pi}_2(0) = \begin{pmatrix} e^{-\lambda_1 t} & & \\ & \ddots & \\ & & e^{-\lambda_{n-1}t}\end{pmatrix}\boldsymbol{\pi}_2(0).$$

Combining the definitions of $\boldsymbol{\pi}_1$ and $\boldsymbol{\pi}_2$ gives $\boldsymbol{\pi}_2(t) = \widehat{\boldsymbol{\Phi}}^t\boldsymbol{\pi}_1(t) = \widehat{\boldsymbol{\Phi}}^t\boldsymbol{W}^{-1/2}\boldsymbol{\pi}(t)$, hence $\boldsymbol{\pi}(t) = \boldsymbol{W}^{1/2}\widehat{\boldsymbol{\Phi}}\boldsymbol{\pi}_2(t)$. As a point in the simplex this gives

$$\boldsymbol{p}(t) = \boldsymbol{\Sigma}\boldsymbol{\pi}(t) = \boldsymbol{\Lambda}^{1/2}\boldsymbol{\Phi}^t\boldsymbol{W}^{1/2}\widehat{\boldsymbol{\Phi}}\boldsymbol{\pi}_2(t) = \boldsymbol{Y}\boldsymbol{\pi}_2(t),$$

after defining $\boldsymbol{Y} \overset{\text{def}}{=} \boldsymbol{\Lambda}^{1/2}\boldsymbol{\Phi}^t\boldsymbol{W}^{1/2}\widehat{\boldsymbol{\Phi}}$. As a point in the normalized simplex, we have

$$\boldsymbol{q}(t) = \widehat{\boldsymbol{\Sigma}}\boldsymbol{\pi}(t) = \widehat{\boldsymbol{\Lambda}}^{1/2}\widehat{\boldsymbol{\Phi}}^t\boldsymbol{W}^{1/2}\widehat{\boldsymbol{\Phi}}\boldsymbol{\pi}_2(t) = \widehat{\boldsymbol{Y}}\boldsymbol{\pi}_2(t),$$

where $\widehat{\boldsymbol{Y}} = \widehat{\boldsymbol{\Lambda}}^{1/2}\widehat{\boldsymbol{\Phi}}^t\boldsymbol{W}^{1/2}\widehat{\boldsymbol{\Phi}}$. We thus see that the matrices

$$\boldsymbol{Y} = \begin{pmatrix} \lambda_1^{1/2}\sum_{i\in[n]}\boldsymbol{\varphi}_1(i)\widehat{\boldsymbol{\varphi}}_1(i)w_i^{1/2} & \dots & \lambda_1^{1/2}\sum_{i\in[n]}\boldsymbol{\varphi}_1(i)\widehat{\boldsymbol{\varphi}}_{n-1}(i)w_i^{1/2} \\ \vdots & \ddots & \vdots \\ \lambda_{n-1}^{1/2}\sum_{i\in[n]}\boldsymbol{\varphi}_{n-1}(i)\widehat{\boldsymbol{\varphi}}_1(i)w_i^{1/2} & \dots & \lambda_{n-1}^{1/2}\sum_{i\in[n]}\boldsymbol{\varphi}_{n-1}(i)\widehat{\boldsymbol{\varphi}}_{n-1}(i)w_i^{1/2} \end{pmatrix},$$

and

$$\widehat{\boldsymbol{Y}} = \begin{pmatrix} \widehat{\lambda}_1^{1/2}\sum_{i\in[n]}\widehat{\boldsymbol{\varphi}}_1(i)\widehat{\boldsymbol{\varphi}}_1(i)w_i^{1/2} & \dots & \widehat{\lambda}_1^{1/2}\sum_{i\in[n]}\widehat{\boldsymbol{\varphi}}_1(i)\widehat{\boldsymbol{\varphi}}_{n-1}(i)w_i^{1/2} \\ \vdots & \ddots & \vdots \\ \widehat{\lambda}_{n-1}^{1/2}\sum_{i\in[n]}\widehat{\boldsymbol{\varphi}}_{n-1}(i)\widehat{\boldsymbol{\varphi}}_1(i)w_i^{1/2} & \dots & \widehat{\lambda}_{n-1}^{1/2}\sum_{i\in[n]}\widehat{\boldsymbol{\varphi}}_{n-1}(i)\widehat{\boldsymbol{\varphi}}_{n-1}(i)w_i^{1/2} \end{pmatrix},$$

govern the dynamics of the random walk in $\mathcal{S}_G$ and $\widehat{\mathcal{S}}_G$, respectively. More specifically, letting $\boldsymbol{Y} = (\boldsymbol{y}_1 \ \dots \ \boldsymbol{y}_n)$ we have

$$\boldsymbol{p}(t) = \sum_{i\in[n-1]}\boldsymbol{y}_i(\boldsymbol{\pi}_2(t))(i) = \sum_{i\in[n-1]}\boldsymbol{y}_i e^{-\lambda_i t}\widehat{\boldsymbol{\Phi}}^t\boldsymbol{W}^{-1/2}\boldsymbol{\pi}(0)(i),$$

and a similar equation for $\boldsymbol{q}(t)$.

Chapter 5

Algorithmics

I'm smart enough to know that I'm dumb.

— Richard Feynman

Beware of bugs in the above code; I have only proved it correct, not tried it.

— Donald Knuth

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, we will attempt to leverage knowledge we have in the hitherto mostly unrelated areas of computational graph theory and high-dimensional computational geometry to draw new conclusions about the complexity of several problems. For instance, if a graph theoretic problem has an analogue in the simplex, any fact regarding the problem's difficulty—whether it's NP-complete, say—translates to an immediate result concerning its geometric counterpart. In particular, since the simplex of a graph can be generated 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 time in either the simplex or graph domain translate to polynomially solvable (yet perhaps not optimal!) problems in the other domain. Likewise, problems which are NP-hard in one domain have analogues which are NP-hard in the other.

For the benefit of the 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.

[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.

§5.1. Preliminaries

Asymptotics. Asymptotic notation 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 $f = o(g)$ 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 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.

We end by remarking that when discussing general polytopes, we continue to work in $\mathbb{R}^{n-1}$ as a vector space. Thus, the vertices of the polytope are still vectors which begin at the origin.

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 is the runtime required to solve Q, since

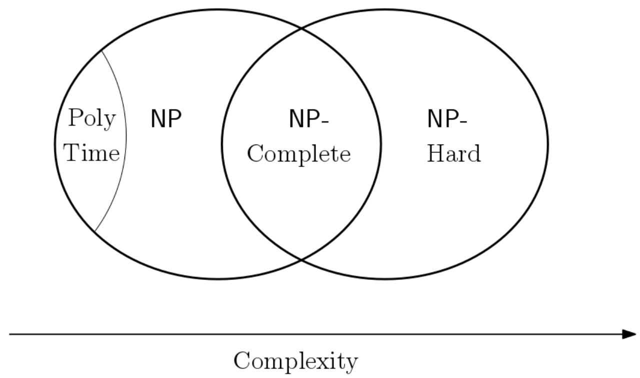

Figure 5.1: Illustration of the relationships between the classes NP, NP-hard, and NP-complete. “Poly-time” refers to problems with polynomial time solutions. Such algorithms can trivially be verified in polynomial time, hence are a subset of problems in NP. We emphasize that the diagram is for intuitive purposes only, and may not reflect the true relationships between these classes. For example, in the unlikely case that P=NP (i.e., all problems in NP are solvable in polynomail time), then the regions “Poly time”, NP and NP-complete coincide. Additionally, the relative sizes of the regions above say nothing about their true cardinalities.

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. In this case we say that P *has been reduced to* Q, or that Q *was reduced from* P. 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 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 in polynomial time [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, $P \in$ NP-hard iff for all $Q \in$ NP, Q can be reduced to P in polynomial time. Thus, to show that $P \in$ NP-hard, it suffices to reduce another problem $R \in$ 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.

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

§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 difficult to obtain (certainly more difficult than the following proof, at any rate). It was first stated by Devriendt and Van Mieghem [DVM18] for inverse combinatorial simplices, and can be slightly generalized as follows.

LEMMA 5.1. *Computing the altitude of minimum length in any simplex is* NP*-hard.*

Proof. The relationship $\left\|\boldsymbol{a}(\mathcal{S}_U^+)\right\|_2^2 = w(\partial U)^{-1}$ (Lemma 3.15) 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 all hyperacute simplices is contained in the class of all simplices, the result follows. (We note that formally, we have reduced the maximum cut problem to the minimum altitude problem.) ⊠

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 between the various descriptions. With regard to NP-completeness therefore, the description makes no difference. Consequently, we will continue to ignore this distinction for the remainder of this section.

Remark 5.2. Altitudes do not have an analogue in general polyhedra. However, for those problems which do have analogues, if they are NP-hard in hyperacute simplices then are so in general polyhedra (since simplices are a subclass of polyhedra). Henceforth, we might use this observation without justification.

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 $\partial(i) \cap I^c = \partial(i)$ for all $i \in I$; otherwise I would contain two vertices which share an edge. Therefore,

$$w(\delta I) = \sum_{i\in I}\sum_{j\in I^c} w(i,j) = \sum_{i\in I}\sum_{j\in\partial(i)\cap I^c} w(i,j) = \sum_{i\in I}\sum_{j\in\partial(i)} w(i,j) = \mathrm{vol}(I),$$

so

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

where the second inequality again follows from the fact that I is an independent set.

The INDEPENDENT-SET problem involves finding the largest independent set in a given graph or, in the decision variant, whether there exists an independent set of size at least

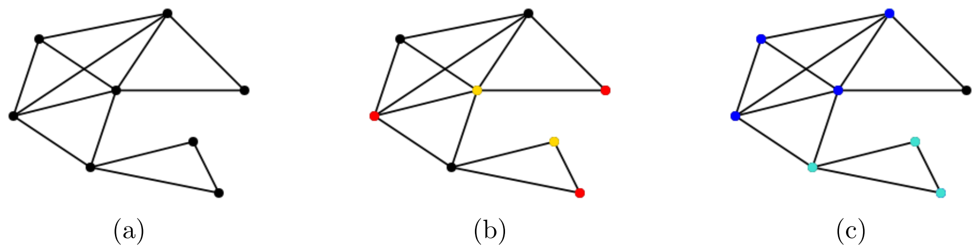

Figure 5.2: (a) A connected graph. (b) Two of its independent sets; one in red (dark) and one yellow (light). The red set constitutes a maximum sized independent set. (c) Two of its cliques; one in blue (dark), one turquoise (light). The blue set constitutes a maximum sized clique.

k for a given k. The decision variant is NP-complete while the optimization version is NP-hard [Kar72]. Suppose we assign each vertex i a weight $f(i) \geq 0$. The Max-Weight Independent-Set problem consists of maximizing $f(I) \stackrel{\text{def}}{=} \sum_{i \in I} f(i)$ 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 problem's tractability.

Lemma 5.2. Vertex-Weighted Independent-Set *in* NP*-complete.*

Proof. First we note that Vertex-Weighted Independent-Set is in NP. Indeed, the size of a given set I can be checked in $O(|I|)$ time and it can be verified to be an independent set by checking in time $O(|I|^2)$ whether any pair in $|I|$ has an edge in the graph.

To see that is it NP-hard, we reduce from Independent-Set. Let a graph G and a parameter k be given. The intuition behind the following reduction is the following. We construct a graph H with $V(H) \supseteq V(G)$ such that each vertex $v \in V(G)$ has constant degree in H. Each independent I in G therefore has volume proportional to $|I|$ in H. The trick is then to ensure that each independent set in H also corresponds to an independent set in I. Let us proceed with the formalities.

Let $m = \max_i \deg_G(i)$ be the maximum degree of any vertex in G. Construct H as follows. For each vertex $u \in V(G)$, define $\alpha(u) = m - \deg_G(u)$ new vertices $u_1, \ldots, u_\alpha$ and take

$$V(H) = V(G) \cup \bigcup_{u \in V(G)} \{u_1, \ldots, u_\alpha\}.$$

We call the vertices which were originally in $V(G)$ *real*, and the newly created vertices *fake*. We add to $E(H)$ the original edges in G and several sets of new edges. First, we add an edge between each real vertex and all its corresponding fake vertices ((u, u_i) for $i = 1, \ldots, \alpha(u)$ and all $u \in V(G)$), and between all fake vertices corresponding to a single vertex. Thus, each vertex u and its fake vertices $u_1, \ldots, u_\alpha$ form a clique. Next, we add an edge between every pair of fake vertices, i.e., (u_i, v_j) for all $u, v \in V(G)$ and $i \in [\alpha(u)]$, $j \in [\alpha(v)]$. Formally then,

$$V(H) = V(G) \cup \bigcup_{u \in V(G)} \{(u, u_i) : i \in [\alpha(u)]\} \cup \bigcup_{u,v \in V(G)} \{(u_i, v_j) : i \in [\alpha[u], j \in [\alpha(v)]\}.$$

We claim that G has an independent set of size k iff H has a vertex weighted independent set of size

$$mk + \sum_{i \in V(G)} \alpha(i).$$

Consider first an independent set $I \subseteq V(G)$ in G. Take any vertex $v \in V(G) \setminus I$ (this set is non-empty, else G has no edges), and let v_i be one of its fake vertices. Consider the set $J = I \cup \{v_i\} \subseteq V(H)$. We claim J is an independent set. Indeed, all added edges in H involve fake vertices. Hence the vertices in I still constitute an independent set in H. Moreover, the only real vertex with which v_i shares an edge is v, which is not in I by assumption. Hence J is an independent set in H. Its volume is

$$\begin{aligned}
\mathrm{vol}_H(J) &= \deg_H(u_i) + \sum_{i \in I} \deg_H(i) \\
&= \sum_{v \in V(G)} \alpha(v) + \sum_{i \in I} (\deg_G(i) + \alpha(i)) = \sum_{v \in V(G)} \alpha(v) + m|I|.
\end{aligned}$$

Now consider an independent set J in H. Observe that J contains at most a single fake vertex (since all fake vertices are connected). Moreover, if it has no fake vertices, we may add a fake vertex of one of the real vertices which is not in J. Consequently, without loss of generality we may write $J = I \cup \{v_i\}$ where $I \subseteq V(G)$ are real vertices and v_i a fake. The edges in H are a superset of those in G, hence I is an independent set in G. The volume of J in H is computed in the same way as above.

We conclude that G has an independent of size k iff H has an inpedendent set of size $mk + \sum_{i \in (V(G)} \alpha(i)$, which demonstrates that Max-Weight Independent-Set is NP-hard. ⊠

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 $\mathcal{P} = \mathcal{S}$ 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 (3.14) in Section 3.4 gives us

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

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*

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

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. As before, notice that for such an I, if $i \in I$ then $\partial(i) \cap I^c = \partial(i)$ (none of i's neighbours are in I). Moreover, for $i, j \in I$, $w(i,j) = 0$. Therefore, Equation (3.17) yields

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

The length of the centroid $\mathcal{P}_I$ is then

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

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. ⊠

A *clique* in a graph G is a complete subgraph of G. The MAX-CLIQUE problems asks, given G, what is the largest k such that G has a clique of size k? Its decision version variant, K-CLIQUE, has parameters G and k, and asks whether G has a clique of size k. Karp [Kar72] demonstrated that K-CLIQUE $\in$ NP and MAX-CLIQUE $\in$ NP-hard.

Lemma 5.5. *Given a polytope in either* V*-description or* H*-description, consider finding a subset* U *of the vertices such that none of the vertices in* U *are orthogonal. The optimization version of these problem is* NP*-hard while the decision variant is* NP*-complete, even in the case of hyperacute simplices.*

Proof. The optimization version corresponds to Max-Clique while the decision variant corresponds to k-Clique via the correspondence. ⊠

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 $\in \mathsf{NP}$, 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 in polynomial time, demonstrating that said problem is polynomial time equivalent to Graph-Isomorphism. 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.*

Proof. Let two graphs G_1 and G_2 be given. Compute their corresponding inverse simplices $\mathcal{S}_1^+$ and $\mathcal{S}_2^+$ (which takes cubic time by computing the eigencomposition of both graphs—see Section 5.3). We claim that $\mathcal{S}_1^+$ and $\mathcal{S}_2^+$ are congruent iff $G_1 \cong G_2$. If $\mathcal{S}_1^+$ and $\mathcal{S}_2^+$ are congruent, then they must be rotationally congruent since they are both centred at the origin. That is, there exists a rotation matrix $\boldsymbol{Q}$ such that $\boldsymbol{Q}\boldsymbol{\Sigma}_1^+ = \boldsymbol{\Sigma}_2^+$. Recalling that $\boldsymbol{Q}$ obeys $\boldsymbol{Q}^t\boldsymbol{Q} = \mathbf{I}$,

$$\boldsymbol{L}_{G_2}^+ = (\boldsymbol{\Sigma}_2^+)^t\boldsymbol{\Sigma}_2^+ = (\boldsymbol{Q}\boldsymbol{\Sigma}_1^+)^t(\boldsymbol{Q}\boldsymbol{\Sigma}_1^+) = (\boldsymbol{\Sigma}_1^+)^t\boldsymbol{Q}^t\boldsymbol{Q}\boldsymbol{\Sigma}_1^+ = (\boldsymbol{\Sigma}_1)^+\boldsymbol{\Sigma}_1^+ = \boldsymbol{L}_{G_1}^+,$$

so G_1 and G_2 share the same pseudoinverse Laplacian. Since the pseudoinverse is unique (Lemma 2.4), G_1 and G_2 share the same Laplacian and are therefore isomorphic. Conversely, if $G_1 \cong G_2$, then there exists a relabelling of the vertices such that their Laplacian matrices are identical, implying that the simplices are congruent. ⊠

Kaibel and Schwarz [KS08] investigated the problem of polytope isomorphism and demonstrate that it is Graph-Isomorphism-Hard. They define two polytopes as 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. As we will see, if we are prepared to compute eigendecompositions, then we can compute all the objects from one another. However, since solving the eigendecomposition is expensive in general (see below), we are mainly interested in circumstances in which a transition can be computed without resorting to this. Unfortunately, it will become clear that the complexity of computing a Laplacian eigendecomposition is actually a lower bound to computing 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[4] of $2^{-\epsilon}$, and there exist 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 (either the combinatorial or normalized)of a graph, i.e., computing its eigenvalues and eigenvectors. The complexity of Laplacian Eigendecomposion does not seem to be known in general, 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 $\tau > 2$.

Observe that given G, we can compute the combinatorial and normalized simplices (and their inverses) by first constructing the combinatorial or normalized Laplacian 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) in time $O(n^{2.3727})$, and from here 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 $O(n^\tau)$.

Besides the question of transitioning between various objects, we might be interested in the issue of *certification*. That is, verifying whether a given simplex is one of the combinatorial or normalized simplices of a graph. We will investigate this question at the end of this section.

Nota Bene: Throughout this section, when referring to the complexity of generating a graph, we mean the complexity of generating any data structure which describes its connectivity; that is, lists its edges (and their weights, if applicable). Formally, the edge weights should be accessible in $O(1)$ time. The Laplacian matrix, adjacency matrix, incidence matrix, etc., all suit this purpose. Similarly, when discussing the problem of generating a simplex *from* a graph, we assume access to such a data structure. We remark that the the normalized Laplacian matrix is *not* such a structure; it provides no immediate access to the edge weights.

We begin by investigating the relationship between $\mathcal{S}$ and $\widehat{\mathcal{S}}$, when either $\mathcal{S}$ or $\widehat{\mathcal{S}}$ are given

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

From/To			V				H			
		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 5.3: 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 or empty square indicates that no bounds are yet known.

and we are told a priori that they are the simplices of a graph. The results obtained in this section are summarized in Figure 5.3.

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

$$\cos\phi_{ij} = \frac{\langle \boldsymbol{\sigma}_i, \boldsymbol{\sigma}_j\rangle}{\|\boldsymbol{\sigma}_i\|_2\|\boldsymbol{\sigma}_j\|_2} = \frac{\boldsymbol{L}_G(i,j)}{\sqrt{w(i)w(j)}} = \widehat{\boldsymbol{L}}_G(i,j), \quad \text{and} \quad \cos\widehat{\phi}_{ij} = \frac{\langle \widehat{\boldsymbol{\sigma}}_i, \widehat{\boldsymbol{\sigma}}_j\rangle}{\|\widehat{\boldsymbol{\sigma}}_i\|_2\|\widehat{\boldsymbol{\sigma}}_j\|_2} = \widehat{\boldsymbol{L}}_G(i,j),$$

since $\|\widehat{\boldsymbol{\sigma}}_i\|_2 = 1$ 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 $\boldsymbol{\sigma}_j$:

$$\frac{\langle \boldsymbol{\gamma}_i, \boldsymbol{\gamma}_j\rangle}{\|\boldsymbol{\gamma}_i\|_2\|\boldsymbol{\gamma}_j\|_2} = \left\langle \frac{\boldsymbol{\sigma}_i}{\|\boldsymbol{\sigma}_i\|_2}, \frac{\boldsymbol{\sigma}_j}{\|\boldsymbol{\sigma}_j\|_2}\right\rangle = \cos(\phi_{ij}).$$

Therefore, the simplex $\text{conv}(\{\boldsymbol{\gamma}_i\})$ (the n vectors $\{\boldsymbol{\gamma}_i\}$ remain affinely independent) has all of its vertices on the unit sphere and the angle between each pair of vertices is the same as in $\widehat{\mathcal{S}}$. Thus, this simplex is rotationally congruent to $\widehat{\mathcal{S}}$. This yields the following.

LEMMA 5.6. *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 5.7. *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.*

$\mathcal{S}$ 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 $i < n$,

$$\lambda_i = \frac{\lambda_i^{1/2}\boldsymbol{\varphi}_j(i)}{\lambda_i^{-1/2}\boldsymbol{\varphi}_j(i)} = \frac{\boldsymbol{\sigma}_i(j)}{\boldsymbol{\sigma}_i^+(j)}, \quad \text{and} \quad \boldsymbol{\varphi}_i(j) = \frac{\boldsymbol{\sigma}_j(i)}{\lambda_i^{1/2}}, \tag{5.1}$$

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 5.8. *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 3.10) and that $\boldsymbol{\sigma}_i^+$ is perpendicular to $\mathcal{S}_{\{i\}^c}$ (Lemma 3.5). Hence, computing the inverse simplex would imply that we had computed normal vectors to n hyperplanes. The typical procedure for this 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 (3.8) and (3.9)). Consequently, given a H-description of one of these simplices, the vertices of its inverse are recoverable in quadratic time. This observation will be used several times and is worth encoding.

Observation 5.1. *Given an H-description of $\mathcal{S}$ (resp., $\mathcal{S}^+$) the vertices of $\mathcal{S}^+$ (resp., $\mathcal{S}$) are obtainable in quadratic time.*

Proof. An H-description of $\mathcal{S}$ involves parameters $\mathbf{u}_1, \dots, \mathbf{u}_n$ and $\beta_1, \dots, \beta_n$ such that $\mathcal{S} = \cap_i\{\boldsymbol{x} : \langle \boldsymbol{x}, \mathbf{v}_i\rangle \geq \beta_i\} = \{\boldsymbol{x} : \langle \boldsymbol{x}, -\mathbf{u}_i/(n\beta_i)\rangle \geq -\frac{1}{n}\}$. Using Equation (3.6) (also written above) shows that $\boldsymbol{\sigma}_i^+ = -\mathbf{u}_i/(n\beta_i)$. Computing this for all i requires times $O(n^2)$ (we need to obtain each coordinate). ⊠

This immediately leads to the following bound on computing an H-description from a V-description.

Lemma 5.9. *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 5.8 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 $\mathcal{S}^+$ is that given the V-description of $\mathcal{S}$ or $\mathcal{S}^+$, we have immediate—that is, $O(1)$ time—access to the H-description of its inverse.

A similar result holds for transitioning 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 5.10. *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 lower bounds hold in this case. First, suppose that we obtain a V-description of $\mathcal{S}_G$ from G. Notice that

$$\sum_{i=1}^{n-1} \boldsymbol{\sigma}_i(j)^2 = \lambda_j \sum_{i=1}^{n-1} \boldsymbol{\varphi}_j(i)^2 = \lambda_j\left(1 - \frac{1}{n}\right),$$

so

$$\lambda_j = \frac{\sum_{i=1}^{n-1} \boldsymbol{\sigma}_i(j)^2}{1 - 1/n},$$

which can be computed in $O(n)$ time. Then, as per Equation (5.1), knowledge of the eigenvalues furnishes knowledge of the eigenvectors in $O(n^2)$ time. This implies that obtaining such a V-description requires $\Omega(n^\tau)$ time. Running almost identical arguments for $\mathcal{S}^+$, $\widehat{\mathcal{S}}$, or $\widehat{\mathcal{S}}^+$ gives the following.

Lemma 5.11. *If the* V*-description of the combinatorial simplex, the 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 prospects are equally bleak for generating an H-description from G. The argument is similar.

Lemma 5.12. *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* $O(g(n)+n^2)$ *by Observation 5.1. Consequently, by Lemma 5.11,* $g(n)=\Omega(n^\tau)$.

The problem of generating the graph from various simplices is more complicated. We note first that we can generate G from a V-description of $\mathcal{S}$ in cubic time. Given $\{\boldsymbol{\sigma}_i\}$ we can compute the weight between vertex i and j as $\langle\boldsymbol{\sigma}_i,\boldsymbol{\sigma}_j\rangle=-w(i,j)$ which requires linear time. Performing the computation for all pairs and thus obtaining all the edge information takes $O(n^3)$.

It's less clear whether cubic time is also a lower bound for generating G from the vertices $\{\boldsymbol{\sigma}_i\}$. Using the following observation, any algorithm which does so in sub-cubic time does not compute one of the dot products $\langle\boldsymbol{\sigma}_i,\boldsymbol{\sigma}_j\rangle$.

Observation 5.2. *Any algorithm which determines whether two vertices in* $\mathbb{R}^n$ *are orthogonal requires* $\Omega(n)$ *time.*

The proof is found in Appendix A.4. However, it seems possible (if unlikely) that an algorithm could infer the edge weights of the graph without computing $\Omega(n^2)$ dot products. We leave the question as an open problem.

Between different descriptions of the simplices. Here we investigate the interplay between the various different descriptions of the simplices. The arguments are largely similar to those in the section on transitioning between $\mathcal{S}$ and $\mathcal{S}^+$.

The following is an immediate consequence of Lemma 3.23 and Observation 5.1. It applies to all simplices.

Corollary 5.1. *If* $\mathcal{T}$ *is a centred simplex in* H*-description, we can obtain a* V*-description of* $\mathcal{T}^*$ *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 $\widehat{\mathcal{S}}_G$, it is difficult to see how to obtain a similar result for the normalized simplex.

Lemma 5.13. *Generating a* 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 V-description takes time $t(n)$. Due to the properties of the hyperplane representations, this yields access to both sets of vertices ($\{\boldsymbol{\sigma}_i\}$ and $\{\boldsymbol{\sigma}_i^+\}$) in time $t(n) + O(n^2)$ (Observation 5.1). Using Equation (5.1), 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 $t(n) + O(n^2)$. Hence $t(n) = \Omega(n^\tau)$. ⊠

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.

Finally, 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 two sections, therefore, attempt dimensionality reduction. The first considers the problem of reducing the dimensionality of the simplex itself. The second considers low rank approximations of the Laplacian which are shown to yield polytopes on n vertices in low dimensional spaces. We see that, depending on the rank of the approximation and the eigenvalues of the Laplacian, certain properties of this polytope approximate those of the simplex. As we will see, this provides some theoretical justification for the recent work of Torres *et al.* [TCER19].

5.4.1. Dimensionality Reduction: $\mathcal{S}^+$

Assume we are given one of the simplices of a graph. 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 the new, lower dimensional object (note that it won't be a simplex because there will be n points in $\mathbb{R}^d$) 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 (the same argument could be run with any of the simplices). 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
$$\varepsilon(i,j) \overset{\text{def}}{=} \frac{1}{2}(\epsilon_{i,\boldsymbol{o}} - \epsilon_{i,j})\boldsymbol{L}_G^+(i,i) + (\epsilon_{j,\boldsymbol{o}} - \epsilon_{i,j})\boldsymbol{L}_G^+(i,j),$$

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:

$$\begin{aligned}
|\varepsilon(i,j)| &\leq \frac{1}{2}\bigg(|(\epsilon_{i,\boldsymbol{o}} - \epsilon_{i,j})\boldsymbol{L}_G^+(i,i)| + |(\epsilon_{j,\boldsymbol{o}} - \epsilon_{i,j})\boldsymbol{L}_G^+(i,j|\bigg) \\
&\leq \frac{1}{2}\bigg([|\epsilon_{i,j}| + |\epsilon_{i,\boldsymbol{o}}|]\boldsymbol{L}_G^+(i,i) + [|\epsilon_{i,j}| + |\epsilon_{j,\boldsymbol{o}}|]\boldsymbol{L}_G^+(j,j)\bigg) \\
&\leq \frac{1}{2}(2\epsilon\boldsymbol{L}_G^+(i,i) + 2\epsilon\boldsymbol{L}_G^+(j,j)) \leq 2\epsilon M,
\end{aligned}$$

since $|\epsilon_{i,j}|, |\epsilon_{i,\boldsymbol{o}}|, |\epsilon_{j,\boldsymbol{o}}| \leq |\epsilon|$. Setting $f(\boldsymbol{\Sigma}^+) = (f(\boldsymbol{\sigma}_1^+), \dots, f(\boldsymbol{\sigma}_n^+)) \in \mathbb{R}^{d\times n}$, 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 also 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,

$$\left\|f(\boldsymbol{\sigma}_i^+) - f(\boldsymbol{\sigma}_j^+)\right\|_2^2 \in \frac{1}{w(i,j)}\Big[(1-\epsilon),(1+\epsilon)\Big] \Pr_{T\sim\mu}[(i,j) \in T].$$

5.4.2. Dimensionality Reduction: $\boldsymbol{L}_G$

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 $\boldsymbol{L}_k$. We might then ask several questions:

1. Is $\boldsymbol{L}_k$ still a gram matrix? That is, can $\boldsymbol{L}_k$ 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 $\boldsymbol{L}_k$ has rank k then P spans a subspace of dimension k and $\text{conv}(P)$ forms a polytope in that space. What is the relationship between the geometry of $\text{conv}(P)$ and $\mathcal{S}_G$?

2. Is $\boldsymbol{L}_k$ 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 $\boldsymbol{L}_k$, 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 $\widehat{\mathcal{S}}_G$.

Let us consider the natural rank-k approximation to $\boldsymbol{L}_G$:

$$\boldsymbol{L}_k \stackrel{\text{def}}{=} \sum_{i=1}^{k} \lambda_k \boldsymbol{\varphi}_k \boldsymbol{\varphi}_k^t,$$

where we recall that we've ordered the eigenvalues as $\lambda_1 \geq \lambda_2 \geq \dots \lambda_{n-1} > \lambda_n = 0$. Clearly $\boldsymbol{L}_k$ has rank k. It is, moreover, a symmetric PSD matrix. Section 3.1 thus yields the polytope $\mathcal{P}_k \stackrel{\text{def}}{=} \mathcal{P}_{\boldsymbol{L}_k}$ associated with $\boldsymbol{L}_k$. More explicitly, if $\boldsymbol{\Lambda}_k = \operatorname{diag}(\lambda_1, \dots, \lambda_n)$ is the diagonal matrix containing the first k eigenvalues (meaning those associated with $\lambda_1, \dots, \lambda_k$) and $\boldsymbol{\Phi}_k = (\boldsymbol{\varphi}_1 \ \dots ; \boldsymbol{\varphi}_k)$, then $\boldsymbol{L}_k$ is the Gram matrix of the vertices described be the matrix $\boldsymbol{\Sigma}_k = \boldsymbol{\Lambda}_k^{1/2} \boldsymbol{\Phi}_k^t = (\boldsymbol{\sigma}_1^{(k)}, \dots, \boldsymbol{\sigma}_n^{(k)})$ where $\boldsymbol{\sigma}_i^{(k)} = (\boldsymbol{\varphi}_1(i)\lambda_1^{1/2}, \dots, \boldsymbol{\varphi}_k(i)\lambda_k^{1/2})$. Let us emphasize that we are using the subscript (k) to signify that these vertices are those belonging to $\mathcal{P}_k$.

To summarize, the rank k approximation to $\boldsymbol{L}_G$, $\boldsymbol{L}_k$ yields an n-vertex polytope $\mathcal{P}_k \subseteq \mathbb{R}^k$. Naturally, one would hope that $\mathcal{P}_k$ "approximates" various features of $\mathcal{S}_G$, as it is precisely $\mathcal{S}_G$ projected onto a particular k-dimensional subspace. The next few results demonstrate that this is true under certain assumptions placed on the distribution of the eigenvalues.

The first property worth noticing is that $\mathcal{P}_k$ remains centred at the origin. Indeed, $\boldsymbol{c}(\mathcal{P}_k) = \frac{1}{n}\boldsymbol{\Sigma}_k \boldsymbol{1} = \frac{1}{n}\boldsymbol{\Lambda}_k^{1/2}\boldsymbol{\Phi}_k^t \boldsymbol{1} = \boldsymbol{0}_k$. Next, we might wonder whether the lengths of the centroids to different faces are similar in $\mathcal{S}_G$ and $\mathcal{P}_k$. Fix $U \subseteq [n]$ and compute

$$\begin{aligned}
\Big| \|\boldsymbol{c}(\mathcal{S}_G[U])\|_2^2 - \|\boldsymbol{c}(\mathcal{P}_k[U])\|_2^2 \Big| &= \frac{1}{|U|^2} \Big| \boldsymbol{\chi}_U^t \boldsymbol{\Sigma}^t \boldsymbol{\Sigma} \boldsymbol{\chi}_U - \boldsymbol{\chi}_U^t \boldsymbol{\Sigma}_k^t \boldsymbol{\Sigma}_k \boldsymbol{\chi}_U \Big| \\
&= \frac{1}{|U|^2} \Big| \boldsymbol{\chi}_U^t (\boldsymbol{L}_G - \boldsymbol{L}_k) \boldsymbol{\chi}_U \Big| \\
&= \frac{1}{|U|^2} \Big| \boldsymbol{\chi}_U^t \Big(\sum_{i \in [n-1]} \lambda_i \boldsymbol{\varphi}_i \boldsymbol{\varphi}_i^t - \sum_{i \in [k]} \lambda_i \boldsymbol{\varphi}_i \boldsymbol{\varphi}_i^t \Big) \boldsymbol{\chi}_U \Big| \\
&\leq \frac{1}{|U|^2} \sum_{i=k+1}^{n-1} |\lambda_i \boldsymbol{\chi}_U^t \boldsymbol{\varphi}_i \boldsymbol{\varphi}^t \boldsymbol{\chi}_U| \\
&= \frac{1}{|U|^2} \sum_{i=k+1}^{n-1} \langle \boldsymbol{\chi}_U, \boldsymbol{\varphi}_i \rangle^2,
\end{aligned}$$

where, by Cauchy-Schwarz, $\langle \boldsymbol{\chi}_U, \boldsymbol{\varphi}_i \rangle^2 \leq \|\boldsymbol{\chi}_U\|_2^2 \|\boldsymbol{\varphi}_i\|_2^2 = |U|^2$, hence

$$\Big| \|\boldsymbol{c}(\mathcal{S}_G[U])\|_2^2 - \|\boldsymbol{c}(\mathcal{P}_k[U])\|_2^2 \Big| \leq \sum_{i=k+1}^{n-1} \lambda_i \leq \lambda_{k+1}(n-(k+1)). \tag{5.2}$$

Thus, if λ_k is sufficiently small as a function of n and k, the lengths of the centroids are approximately equal. We summarize with the following Lemma.

LEMMA 5.14. *If* $\lambda_{k+1} = o((n-k)^{-1})$, *then* $\left| \|\boldsymbol{c}(\mathcal{S}_G[U])\|_2^2 - \|\boldsymbol{c}(\mathcal{P}_k[U])\|_2^2 \right| = o(1)$.

Proof. Assume $\lambda_k = o((n-k)^{-1})$ and apply Equation (5.2). ⊠

Remark 5.3. The above result should seem intuitively plausible. How well $\boldsymbol{L}_k$ approximates $\boldsymbol{L}_G$ relies precisely on the size of λ_k. We should thus expect the same to be true of $\mathcal{P}_k$ and $\mathcal{S}_G$.

Next, we investigate the relative distances between the vertex vectors. The difference in distances between the vectors of $\mathcal{S}_G$ and $\mathcal{P}_k$ is

$$\begin{aligned}
\left| \|\boldsymbol{\sigma}_i - \boldsymbol{\sigma}_j\|_2^2 - \left\|\boldsymbol{\sigma}_i^{(k)} - \boldsymbol{\sigma}_j^{(k)}\right\|_2^2 \right| &= \left| \sum_{\ell \in [n-1]} (\boldsymbol{\sigma}_i(\ell) - \boldsymbol{\sigma}_j(\ell))^2 - \sum_{\ell \in [k]} (\boldsymbol{\sigma}_i(\ell) - \boldsymbol{\sigma}_j(\ell))^2 \right| \\
&= \left| \sum_{\ell \in [n-1]} \lambda_\ell (\boldsymbol{\varphi}_\ell(i) - \boldsymbol{\varphi}_\ell(j))^2 - \sum_{\ell \in [k]} \lambda_\ell (\boldsymbol{\varphi}_\ell(i) - \boldsymbol{\varphi}_\ell(j))^2 \right| \\
&= \left| \sum_{\ell=k+1}^{n-1} \lambda_\ell (\boldsymbol{\varphi}_\ell(i) - \boldsymbol{\varphi}_\ell(j))^2 \right| \\
&\le \lambda_{k+1} \sum_{\ell=k+1}^{n-1} |\boldsymbol{\varphi}_\ell(i) - \boldsymbol{\varphi}_\ell(j)|^2 .
\end{aligned}$$

The goal is thus to bound the final summation in terms of some function of n or k, so that we may provide sufficient conditions on λ_{k+1} in order for $\left\|\boldsymbol{\sigma}_i^{(k)} - \boldsymbol{\sigma}_j^{(k)}\right\|_2^2$ to approximate $\|\boldsymbol{\sigma}_i - \boldsymbol{\sigma}_j\|_2^2$. We proceed as follows.

$$\begin{aligned}
\sum_{\ell=k+1}^{n-1} |\boldsymbol{\varphi}_\ell(i) - \boldsymbol{\varphi}_\ell(j)|^2 &= \left| \sum_{\ell=k+1}^{n-1} |\boldsymbol{\varphi}_\ell(i) - \boldsymbol{\varphi}_\ell(j)|^2 \right| \\
&= \left| \sum_{\ell=k+1}^{n-1} \boldsymbol{\varphi}_\ell(i)^2 + \boldsymbol{\varphi}_\ell(j)^2 - 2\boldsymbol{\varphi}_\ell(i)\boldsymbol{\varphi}_\ell(j) \right| \\
&\le \sum_{\ell=k+1}^{n-1} \boldsymbol{\varphi}_\ell(i)^2 + \sum_{\ell=k+1}^{n-1} \boldsymbol{\varphi}_\ell(j)^2 + 2\left| \sum_{\ell=k+1}^{n-1} \boldsymbol{\varphi}_\ell(i)\boldsymbol{\varphi}_\ell(j) \right| \\
&\le \sum_{\ell=k+1}^{n-1} \boldsymbol{\varphi}_\ell(i)^2 + \sum_{\ell=k+1}^{n-1} \boldsymbol{\varphi}_\ell(j)^2 + 2\left(\sum_{\ell=k+1}^{n-1} \boldsymbol{\varphi}_\ell(i)^2 \sum_{m=k+1}^{n-1} \boldsymbol{\varphi}_m(j)^2 \right)^{1/2} \\
&\le \sum_{\ell \in [n]} \boldsymbol{\varphi}_\ell(i)^2 + \sum_{\ell \in [n]}^{n-1} \boldsymbol{\varphi}_\ell(j)^2 + 2\left(\sum_{\ell \in [n]}^{n-1} \boldsymbol{\varphi}_\ell(i)^2 \sum_{m=k+1}^{n-1} \boldsymbol{\varphi}_m(j)^2 \right)^{1/2} . \qquad (5.3)
\end{aligned}$$

Now, recall that due to double orthogonality of the eigenvector matrix we have

$$\sum_{\ell=1}^{n} \boldsymbol{\varphi}_\ell(i)\boldsymbol{\varphi}_\ell(j) = \delta_{ij}.$$

The right hand side of (5.3) is therefore equal to 6. Consequently, combining the previous few equations yields

$$\left| \|\boldsymbol{\sigma}_i - \boldsymbol{\sigma}_j\|_2^2 - \left\|\boldsymbol{\sigma}_i^{(k)} - \boldsymbol{\sigma}_j^{(k)}\right\|_2^2 \right| \leq 6\lambda_{k+1} = O(\lambda_{k+1}).$$

LEMMA 5.15. *If $\lambda_{k+1} = o(1)$ then* $\left| \|\boldsymbol{\sigma}_i - \boldsymbol{\sigma}_j\|_2^2 - \left\|\boldsymbol{\sigma}_i^{(k)} - \boldsymbol{\sigma}_j^{(k)}\right\|_2^2 \right| = o(1).$

Summarizing, we see that under assumptions on the sizes of the eigenvalues (which relates directly to how good of an approximation $\boldsymbol{L}_k$ is to $\boldsymbol{L}_G$), the features of the polytope $\mathcal{P}_k$ will approximate those of $\mathcal{S}_G$. As we stated previously, this could help explain in part the success of the experiments run by Torres *et al.* [TCER19] on a new Laplacian eigenmap method. In their work, they assume they are given $\mathcal{P}_k$ and attempt to reconstruct certain graph features, most notably its connectivity. Since the connectivity of a graph is related to the centroids of $\mathcal{S}_G$ (Section 3.4), if k is sufficiently small then the centroids $\mathcal{P}_k$ will approximately recover the edge relations.

5.4.3. Distance Matrix of $\mathcal{S}_G^+$

We end with a brief section which demonstrates that we can leverage several results from the literature on Laplacian optimization to approximate the distance matrix of $\mathcal{S}_G^+$. An elegant result of Spielman and Srivastava [SS11] allows us to build a matrix which approximately represents the effective resistances.

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

$$r = \frac{\max_{i,j} w(i,j)}{\min_{i,j} w(i,j)}.$$

Therefore, 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 $\widetilde{\boldsymbol{R}}$.

Ideally, after computing $\widetilde{\boldsymbol{R}}$, we'd like to compute vertices which (approximately) obey the distances represented by $\widetilde{\boldsymbol{R}}$ (note that $\widetilde{\boldsymbol{R}}$ may not be a valid distance matrix since it is only an approximation). The usual approach to generating points from a (true) distance matrix $\boldsymbol{D}$ is *Multidimensional Scaling (MDS)* [KW78]. Typically, practitioners are interested in generating points which approximately obey the pairwise distance in $\boldsymbol{D}$, but lie in a lower dimensional space. While this sounds promising, MDS relies on the the eigendecomposition of the distance matrix which requires cubic time. Of course, this is too slow for our purposes: If we allow cubic time, then we can simply perform an eigendecomposition of $\boldsymbol{L}_G$ and recover the vertices of $\mathcal{S}_G^+$ exactly. Moreover, it's unclear whether MDS works when the given distances are only approximate. We therefore leave the reader with the following open problem:

Problem: Given an approximate Euclidean distance matrix $\widetilde{\boldsymbol{D}}$ and a parameter $\epsilon > 0$, can a set of vertices be computed which obey the distances given by $\widetilde{\boldsymbol{D}}$ within an additive factor of ϵ in sub-cubic time?

Chapter 6

Conclusion

One must imagine Sisyphus happy.

— Albert Camus, *The Myth of Sisyphus*

This dissertation has expounded and expanded upon the graph-simplex correspondence, a relationship which associates with each connected, weighted graph G four simplices: $\mathcal{S}_G$, $\mathcal{S}_G^+$ (the combinatorial simplices), $\widehat{\mathcal{S}}_G$, and $\widehat{\mathcal{S}}_G^+$ (the normalized simplices). Presenting and building on the previous work of Fiedler [Fie93, Fie11] and Devriendt and Van Mieghem [DVM18], we have seen the synthesis of the geometry of these simplices with properties of the graph. At a high level:

1. The geometry of $\mathcal{S}_G$ is closely related to the connectivity of G, the geometry of $\mathcal{S}_G^+$ is related the effective resistance of G. The squared volume of $\mathcal{S}_G$ is proportional to the number (total weight) of spanning trees in G, to which the squared volume of $\mathcal{S}_G^+$ is inversely proportional;

2. The volume of the faces of $\mathcal{S}_G^+$ are closely related to the entries of the Laplacian matrix and consequently to the length of the vertices of $\mathcal{S}_G$;

3. The Steiner Ellipsoids of $\mathcal{S}_G$ and $\mathcal{S}_G^+$ are determined by the eigenvalues of $\boldsymbol{L}_G$. For any of a graph's simplices, the ratio of the volume of its Steiner Ellipsoid to its own volume is a constant.

More broadly, we have seen that graphs and simplices are related by elegant block matrix equations which can be used to examine the structure of both objects. The correspondence also provided the insight used to give a general formula for both the volume of a simplex and its Steiner Ellipsoid in terms of the dual simplex. Additionally, it helped provide intuition concerning the general behaviour of the dual simplex.

On the more applied side, we explored the algorithmic underpinnings of the correspondence and established that

3. transitioning between various objects in the correspondence (exactly) is lower bounded by the complexity of computing an eigendecompositon;

4. the correspondence can be used to help classify the computational complexity of geometric problems; and

5. there exist low dimensional embeddings of the simplices which approximately maintain their Gram matrix relations, and low rank approximations to the Laplacian yielding low dimensional polytopes approximating the geometry of $\mathcal{S}_G$ and $\mathcal{S}_G^+$.

The main goal, however, was not to achieve any particular result but rather to demonstrate the utility of the graph-simplex correspondence as a tool with which to analyze graphs and simplices. We hope to have succeeded in our role as evangelist and convinced the reader to include the correspondence in their mathematical toolkit. We end by listing several possible directions for future work.

§6.1. Open Problems and Future Directions

We believe there are several exciting avenues for further research.

- In Section 5.2 we gave several examples of how various graph theoretic problems translate to the simplex and vice versa, and examined what implications this had for computational complexity. Due to time and space constraints we were unable to fully explore this area; it seems likely that we have left many results untapped. For example, we mostly explored how specific NP-complete graph problems translated to NP-complete polyhedral problems. It could be fruitful to explore the converse. More importantly for possible applications, problems which are "easy" (polynomial time solvable) in one domain may have analogues in the other, which could result in new efficient algorithms.
- While we gave implicit conditions on the dual of $\widehat{\mathcal{S}}_G$ and $\widehat{\mathcal{S}}_G^+$, we were unable to give their explicit equations. It would be desirable to discover what these are.
- In Section 5.4.3 we presented the problem of embedding an (approximate) distance matrix in sub-cubic time. This question seems like an interesting one in general, even without considering our specific motivation. Related to this is the connection between $\mathcal{S}_G^+$ and the resistive polytope, $\mathcal{R}_G$, given in Section 4.5. Given that $\boldsymbol{L}_G^+$ is a more widely studied object than $\mathcal{S}_G^+$, it's possible that knowledge concerning the pseudoinverse can be leveraged to uncover properties of, or to optimize over, $\mathcal{R}_G$. This could translate to similar results for $\mathcal{S}_G^+$.
- One application of the correspondence that we explored only briefly was that of proving the existence of certain features in simplices and graphs. It seems possible that there are many results along these lines. For example, Alev *et al.* recently demonstrated that any graph can be partitioned into subgraphs such that each subgraph has a low maximum effective resistance and only a fraction of the total edges lie between the subgraphs [AALG17]. This demonstrates that the vertices of any hyperacute simplex can be partitioned into sets such that the maximum pairwise distance between the vertices in any set is "small" and many vertices in distinct sets are orthogonal, or approximately so.
- In a similar vein, it would be interesting to explore under what conditions such results generalize to all simplices. Are there, for instance, necessary and sufficient conditions

on when structural properties of hyperacute simplices generalize to all simplices? If so, then when studying such properties it would be sufficient to restrict one's attention to inverse simplices of graphs.

- Our study of random walks in simplices was severely limited in scope and insight. The natural use of probability distributions over the nodes as barycentric coordinates, however, remains intriguing. Additionally, the connection between the normalized Laplacian and random walks suggests this may be a promising approach for generating new insights into the dynamics of random walks, and stochastic processes on graphs more generally.

Finally, there are two possible abstractions of the graph-simplex correspondence which suggest themselves.

The first comes from considering the natural generalization of simplices to simplicial complexes. A *simplicial complex* is a collection of simplices $\mathfrak{S}$ such that (i) for every $\mathcal{T} \in \mathfrak{S}$, each face of $\mathcal{T}$ is also in $\mathfrak{S}$ and (ii) for all $\mathcal{T}_1, \mathcal{T}_2 \in \mathfrak{S}$, $\mathcal{T}_1 \cap \mathcal{T}_2$ is a face of both $\mathcal{T}_1$ and $\mathcal{T}_2$. It would be interesting to explore whether one can associate with each simplicial complex a graph or set of graphs.

The second involves exploring more fully the mapping we introduced in Section 3.1 which associates a polytope of rank d with each PSD matrix of rank d. Is such geometry a useful way of thinking about these matrices?

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Omitted Proofs

§A.1. Chapter 2

Proof of Observation 2.1. We begin by proving uniqueness. Suppose $\{\mathbf{u}_i\}$ and $\{\boldsymbol{w}_i\}$ are both biorthogonal bases of $\{\mathbf{v}_i\}$. We will show that $\mathbf{u}_i = \boldsymbol{w}_i$ for all i. Fix $i \in [n]$. By independence, $\operatorname{span}(\mathbf{v}_1, \dots, \mathbf{v}_{i-1}, \mathbf{v}_{i+1}, \dots, \mathbf{v}_n)$ is a hyperplane—that is,

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

(Recall that we are working in $\mathbb{R}^n$ and with bases thereof.) 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.

Next we demonstrate that $\boldsymbol{Q}^t = \boldsymbol{M}^{-1}$ where $\boldsymbol{Q} = (\mathbf{u}_1, \dots, \mathbf{u}_n)$ and $\boldsymbol{M} = (\mathbf{v}_1, \dots, \mathbf{v}_n)$. By the orthogonality relationships of dual bases, we have

$$\boldsymbol{Q}^t \boldsymbol{M} = \begin{pmatrix} \mathbf{u}_1^t \\ \vdots \\ \mathbf{u}_n^t \end{pmatrix} \begin{pmatrix} \mathbf{v}_1 & \dots & \mathbf{v}_n \end{pmatrix} = \begin{pmatrix} \langle \mathbf{u}_1, \mathbf{v}_1 \rangle & \dots & \langle \mathbf{u}_1, \mathbf{v}_n \\ \vdots & \ddots & \vdots \\ \langle \mathbf{u}_n, \mathbf{v}_1 \rangle & \dots & \langle \mathbf{u}_n, \mathbf{v}_n \rangle \end{pmatrix} = \mathbf{I}_n.$$

Observing that $\boldsymbol{M}^{-1}$ exists by independence of $\{\mathbf{v}_1, \dots, \mathbf{v}_n\}$ we apply it to both sides of the above to obtain $\boldsymbol{Q}^t = \boldsymbol{M}^{-1}$. ⊠

Proof of Lemma 2.2. It suffices to show that $\dim \ker \boldsymbol{M} = \dim \ker \boldsymbol{M}^t \boldsymbol{M}$, by rank-nullity. Clearly $\ker \boldsymbol{M} \subseteq \ker \boldsymbol{M}^t \boldsymbol{M}$ since $\boldsymbol{M}\boldsymbol{f} = \mathbf{0}$ implies $\boldsymbol{M}^t \boldsymbol{M} \boldsymbol{f} = \mathbf{0}$. Conversely, if $\boldsymbol{M}^t \boldsymbol{M} \boldsymbol{f} = \mathbf{0}$ then $0 = \boldsymbol{f}^t \boldsymbol{M}^t \boldsymbol{M} \boldsymbol{f} = \|\boldsymbol{M}\boldsymbol{f}\|_2^2$, implying that $\boldsymbol{M}\boldsymbol{f} = \mathbf{0}$. ⊠

Proof of Lemma 2.5. 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

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

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 $\mathbf{Q} = \boldsymbol{M}^+$. ⊠

Proof of Lemma 2.7. By definition

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

whence

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

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

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

Proof of Lemma 2.6. 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 $\boldsymbol{\varphi}_1, \ldots, \boldsymbol{\varphi}_n$. To see the non-negativity of the eigenvalues, we appeal to the *incidence matrix* of G, $\boldsymbol{B}_G$. This is defined in Appendix B. It is easily verified that $\boldsymbol{L}_G = \boldsymbol{B}_G^t \boldsymbol{B}_G$. Therefore, for λ an eigenvalue with (unit) eigenvector $\boldsymbol{\varphi}$,

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

Now, 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 that any vector in span(1) satisfies this condition. On the other hand, consider a non-zero vector $\boldsymbol{\varphi}$ which is orthogonal to $\boldsymbol{1}$. 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 one, and $\ker(\boldsymbol{L}) = \text{span}(\boldsymbol{1})$.

A similar analysis holds for the normalized Laplacian. Using the same argument but replacing $\boldsymbol{B}$ with $\widehat{\boldsymbol{B}} = \boldsymbol{W}^{-1/2}\boldsymbol{B}\boldsymbol{W}^{-1/2}$ 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

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

so $\boldsymbol{W}^{1/2}\boldsymbol{1}$ lies in the kernel of $\widehat{\boldsymbol{L}}$. Conversely, if $\boldsymbol{\varphi} \in \ker(\widehat{\boldsymbol{L}})$, define $\boldsymbol{\varphi}'$ 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

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

so $\boldsymbol{L}\boldsymbol{\varphi} = \boldsymbol{0}$ (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 $\ker(\widehat{\boldsymbol{L}}) = \text{span}(\sqrt{\boldsymbol{w}}$. ⊠

Proof of Lemma 2.8. Throughout the proof let $R = R_G^{\text{tot}}$. We need to show that

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

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

$$-\frac{1}{2}\left(\mathbf{1}\boldsymbol{\Delta}^t\boldsymbol{L}_G\boldsymbol{\Delta} + \frac{4}{n^2}R\mathbf{1} - \boldsymbol{R}\boldsymbol{L}_G\boldsymbol{\Delta} - \frac{2}{n}\boldsymbol{R}\mathbf{1}\right), \tag{A.1}$$

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

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

Observing that $\boldsymbol{\Delta}(i) = \boldsymbol{L}_G^+(i,i) = \frac{1}{n}(\boldsymbol{R}\mathbf{1})(i) - R/n^2$ due to Lemma 2.7, write

$$\boldsymbol{\Delta} = \frac{1}{n}\boldsymbol{R}\mathbf{1} - \frac{R}{n^2}\mathbf{1} = \frac{1}{n}\boldsymbol{R}\mathbf{1} - \frac{1}{2n^2}\mathbf{J}\boldsymbol{R}\mathbf{1},$$

(where we've used that $R = \frac{1}{2}\mathbf{1}^t\boldsymbol{R}\mathbf{1}$). After some re-arranging, Equation (A.1) thus becomes

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

using that $\mathbf{J}^2 = n\mathbf{J}$. Finally, again using (A.2), the bottom right-hand side is

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

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

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

In the same way as (A.2) was derived, we see that

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

and so

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

as desired. ⊠

Proof of Lemma 2.9. 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 $\sum_{i\neq j} \beta_i(\boldsymbol{x}_j - \boldsymbol{x}_j) = \mathbf{0}$. Putting $\beta = \sum_i \beta_i$, we can write this as

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

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 $\sum_i \alpha_i \boldsymbol{x}_i = \mathbf{0}$ where $\sum_i \alpha_i = 0$ and $\alpha_k \neq 0$ for some k. Then,

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

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

Proof of Lemma 2.10. By Lemma 2.9, 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 $\sum_i \alpha_i = 1$. ⊠

Proof of Claim 2.1. 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. ⊠

Proof of Observation 2.2. 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. ⊠

Proof of Lemma 2.11. 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,

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

Proof of Lemma 2.14. Let $\boldsymbol{\Sigma} = \boldsymbol{\Sigma}(\mathcal{S}) = (\boldsymbol{\gamma}_1, \ldots, \boldsymbol{\gamma}_n)$ and $\boldsymbol{\Sigma}^* = \boldsymbol{\Sigma}(\mathcal{S}^*) = (\boldsymbol{\gamma}_1^*, \ldots, \boldsymbol{\gamma}_n^*)$. Let $\boldsymbol{\Sigma}\boldsymbol{x} \in \mathcal{S}_U$ and $\boldsymbol{\Sigma}^*\boldsymbol{y}_1, \boldsymbol{\Sigma}^*\boldsymbol{y}_2 \in \mathcal{S}^*_{U^c}$, where $\boldsymbol{y}_1$ and $\boldsymbol{y}_2$ are barycentric coordinates. Fix $k \in U^c$. We need to show that $\langle \boldsymbol{\Sigma}\boldsymbol{x}, \boldsymbol{\Sigma}^*\boldsymbol{y}_1 - \boldsymbol{\Sigma}^*\boldsymbol{y}_2\rangle = 0$. First, using $\|\boldsymbol{y}_i\| = 1$, $i = 1, 2$, write

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

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

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

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

§A.2. Chapter 3

Proof of Lemma 3.4. Let us simply perform the calculation:

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

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

as desired. ⊠

Proof of Lemma 3.9. 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. ⊠

§A.3. Chapter 4

Proof of Lemma 4.5. Before proceeding to the main part of the proof, we recall 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 proceed with the argument. 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 (since $\mathcal{T}$ is hyperacute by assumption). Set

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

Combining Lemma 4.4 and Equation (2.18), write

$$\begin{aligned}
\mathrm{vol}(\mathcal{T})^2 &= \frac{(-1)^n}{((n-1)!)^2 2^{n-1}} \det\left(-2\begin{pmatrix} \alpha & \boldsymbol{r} \\ \boldsymbol{r} & \boldsymbol{L}_G \end{pmatrix}^{-1}\right) \\
&= \frac{-4}{((n-1)!)^2} \left[\det\begin{pmatrix} \alpha & \boldsymbol{r} \\ \boldsymbol{r} & \boldsymbol{L}_G \end{pmatrix}\right]^{-1},
\end{aligned}$$

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,

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

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

Proof of Lemma 4.13. 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,

$$\sum_{i\sim j} \frac{1}{w(i,j)} + \sum_{\ell\in[n]} \boldsymbol{S}_T(k,\ell)(\deg(\ell) - 2). \tag{A.3}$$

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 (A.3) 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 $P = (k = v_1,\ldots,v_r = \ell)$ 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 $P\cup\{\ell\} = (v_1,\ldots,v_r,i)$. 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. ⊠

Proof of Lemma 4.14. 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

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

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

Proof of Lemma 4.16. We prove Equation (4.18) only; Equation (4.19) 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 $\mathbf{J}^2 = n\mathbf{J}$, compute

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

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

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

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]

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

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

Proof of Lemma 4.18. Set $\boldsymbol{\zeta} = \frac{1}{2}(\boldsymbol{L}_G\boldsymbol{\Delta} + \mathbf{1}/n)$ and $r = \boldsymbol{\Delta}^t\boldsymbol{L}_G\boldsymbol{\Delta}4R_G^{\text{tot}}/n^2$. Let us expand $\boldsymbol{x}$ in barycentric coordinates in accordance with Lemma 2.10. Put $\boldsymbol{x} = \sum_i \alpha_i\boldsymbol{\sigma}_i$ where $\sum_i \alpha_i = \sum_i \beta_i = 1$. Let $\boldsymbol{\alpha} = (\alpha_1, \dots, \alpha_n)$. The claim is that the circumscribed sphere of $\mathcal{S}^+$ is given by the equation

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

and that this equation is equivalent to $\boldsymbol{\alpha}^t\boldsymbol{D}\boldsymbol{\alpha} = 0$. Note first that due to Equation 2.18, $\langle \mathbf{1}, -2\boldsymbol{\zeta}\rangle = \langle \mathbf{1}, -\boldsymbol{L}_G\boldsymbol{\Delta} - \frac{2}{n}\mathbf{1}\rangle = -2$, so $\boldsymbol{\zeta} = (\zeta_1, \dots, \zeta_{n-1})$ obeys $\sum_i \zeta_i = 1$. The left hand side of (A.4) then becomes

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

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

$$\begin{aligned}\langle \boldsymbol{x} - \boldsymbol{\Sigma\zeta}, \boldsymbol{x} - \boldsymbol{\Sigma\zeta}\rangle &= \frac{1}{2}\Bigg(\sum_j(\alpha_j - \zeta_j)\sum_i(\alpha_i - \zeta_i)\|\boldsymbol{\sigma}_i - \boldsymbol{\sigma}_n\|_2^2 \\ &\qquad + \sum_i(\alpha_i - \zeta_i)\sum_j(\alpha_j - \zeta_j)\|\boldsymbol{\sigma}_j - \boldsymbol{\sigma}_n\|_2^2 \\ &\qquad - \sum_{i,j}(\alpha_i - \zeta_i)(\alpha_j - \zeta_j)\|\boldsymbol{\sigma}_i - \boldsymbol{\sigma}_j\|_2^2\Bigg) \\ &= -\frac{1}{2}\sum_{i,j}(\alpha_i - \zeta_i)(\alpha_j - \zeta_j)\|\boldsymbol{\sigma}_i - \boldsymbol{\sigma}_j\|_2^2. \end{aligned} \tag{A.5}$$

Recalling the block matrix equation (2.18) for hyperacute simplices, for all i we have

$$\mathbf{1}(\boldsymbol{\Delta}^t \boldsymbol{L}_G \boldsymbol{\Delta} + 4R_G^{\text{tot}}/n^2) - \boldsymbol{D}(\boldsymbol{L}_G\boldsymbol{\Delta} + 2\mathbf{1}/n) = \mathbf{0},$$

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 (A.5) as

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

The equation of the sphere in (A.4) 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 $\boldsymbol{\chi}_\ell^t\boldsymbol{D}\boldsymbol{\chi}_\ell = \sum_{i,j}\boldsymbol{\chi}_\ell(i)\boldsymbol{D}(i,j)\boldsymbol{\chi}_\ell(j) = \boldsymbol{D}(\ell,\ell) = 0$. ⊠

§A.4. Chapter 5

Proof of Observation 5.2. Let $\mathcal{A}$ be a purported sublinear time algorithm which performs this task. Let $\boldsymbol{x}, \boldsymbol{y} \in \mathbb{R}^n$ be two inputs to $\mathcal{A}$. Assume they both contain no zero entries ($\mathcal{A}$ claims to work for all vectors). Since $\mathcal{A}$ is sublinear, there exists some $i \in [n]$ such that $\mathcal{A}$ does not examine $x(i)$. Therefore, we may vary $x(i)$ without changing $\mathcal{A}$'s output. If $\mathcal{A}$ output "yes", meaning that it believes $\boldsymbol{x}$ and $\boldsymbol{y}$ to be orthogonal, put

$$x(i) = \frac{1 - \sum_{j \neq i} x(j)y(j)}{y(i)}.$$

Then $\langle \boldsymbol{x}, \boldsymbol{y} \rangle = 1$, so they are are not orthogonal. Similarly, if $\mathcal{A}$ output "no", then put

$$x(i) = -\frac{\sum_{j \neq i} x(j)y(j)}{y(j)},$$

so that $\langle \boldsymbol{x}, \boldsymbol{y} \rangle = 0$. Therefore, $\mathcal{A}$ cannot be correct on all inputs. ⊠

Intuition Behind Effective Resistance

Here we provide a derivation of effective resistance using the analogy of a graph as an electrical network.

Given an undirected, weighted graph $G = (V, E, w)$, place an arbitrary orientation the edges (say, for example, (i, j) is directed from i to j iff $i < j$) and for each edge e, let $e^- \in V$ denote the vertex at which e ends, and e^+ the vertex at which it begins. Set

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

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

$$\boldsymbol{B}^t \boldsymbol{f} = \boldsymbol{e}. \tag{B.2}$$

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

$$\boldsymbol{f} = \boldsymbol{W}\boldsymbol{B}\boldsymbol{\rho}. \tag{B.3}$$

Combining (B.2) and (B.3) 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 $\boldsymbol{\chi}_i - \boldsymbol{\chi}_j \perp \mathbf{1}$. This gives rise to Definition 2.2.

Figures

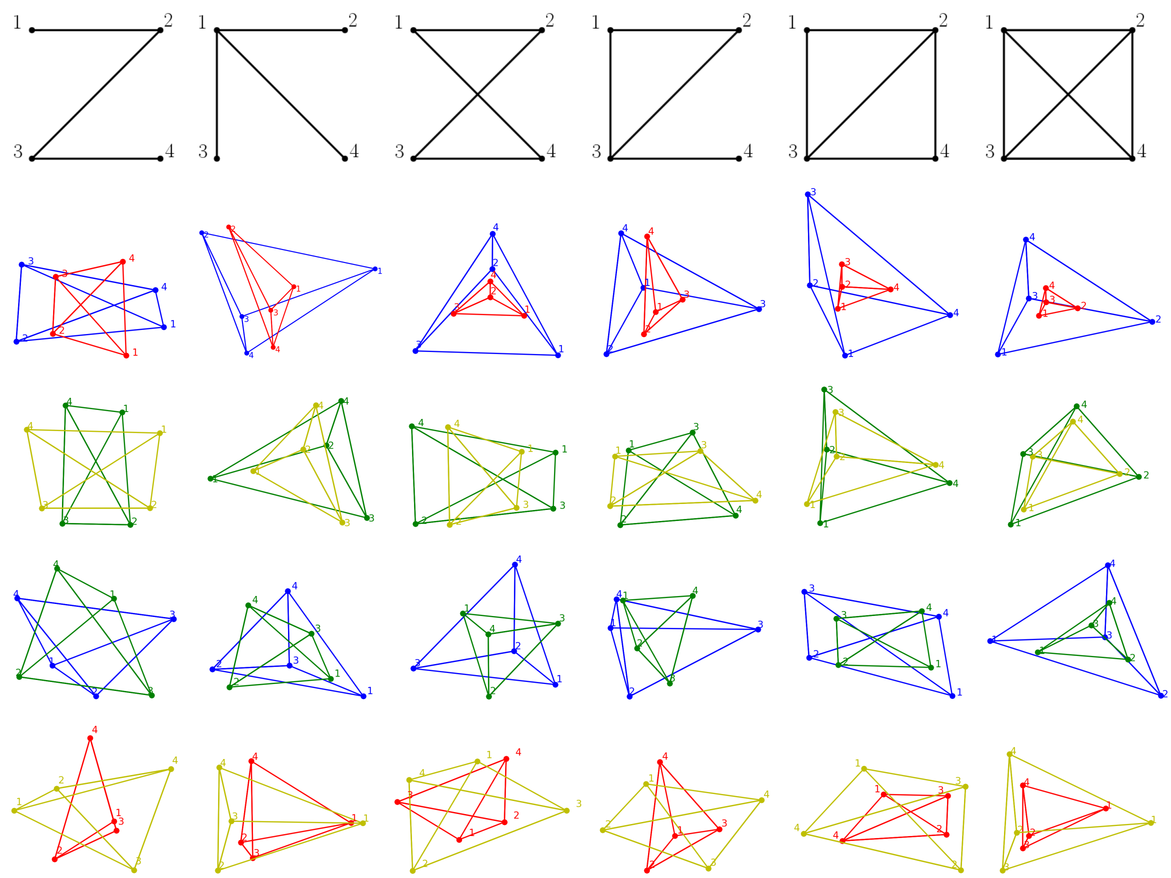

Figure C.1: The six unique unweighted graphs on four vertices, up to isomorphism, and a comparison of all of their simplices. Below each graph in the first row are its two combinatorial simplices ($\mathcal{S}_G$ and $\mathcal{S}_G^+$), then its two normalized simplices ($\widehat{\mathcal{S}}_G$ and $\widehat{\mathcal{S}}_G^+$), then its combinatorial and normalized simplex ($\mathcal{S}_G$ and $\widehat{\mathcal{S}}_G$), followed in the final row by the two inverse simplices ($\mathcal{S}_G^+$ and $\widehat{\mathcal{S}}_G^+$). The combinatorial simplex and its inverse are coloured blue and red respectively, and the normalized simplex and its inverse are in green and yellow respectively. The relative size of the the simplices in each subfigure are to scale but the same scale is not maintained across figures.