The Graph-Simplex Correspondence and its Algorithmic Foundations

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Abstract

Lay Summary

Acknowledgements

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Nomenclature[2]

Simplex Geometry

$\mathcal{T}$	General simplex
$\mathcal{T}^D$	Dual simplex to $\mathcal{T}$
$\mathbf{\Sigma}(\mathcal{T})$	Vertex matrix of simplex $\mathcal{T}$
$\mathcal{S}_G$ ($\widehat{\mathcal{S}}_G$)	(Normalized) Simplex associated to graph G.
$\mathcal{S}_G^+$ ($\widehat{\mathcal{S}}_G^+$)	Inverse simplex of $\mathcal{S}_G$ ($\widehat{\mathcal{S}}_G$).
$\mathcal{T}\restriction_U, \mathcal{T}_U, \mathcal{T}[U]$	Face of simplex $\mathcal{T}$ restricted to U
$\mathbf{\Sigma}_G$ ($\widehat{\mathbf{\Sigma}}_G$)	Vertex matrix of the simplex $\mathcal{S}_G$ ($\widehat{\mathcal{S}}_G$).
$\mathbf{\Sigma}_G^+$ ($\widehat{\mathbf{\Sigma}}_G^+$)	Vertex matrix of the simplex $\mathcal{S}_G^+$ ($\widehat{\mathcal{S}}_G^+$).
$\{\boldsymbol{\sigma}_i\}$ ($\{\widehat{\boldsymbol{\sigma}}_i\}$)	Vertex vectors of (normalized) simplex
$\boldsymbol{a}(\mathcal{T}_U)$	Altitude vector from $\mathcal{T}_U$ to $\mathcal{T}_{U^c}$
$\boldsymbol{c}(\mathcal{T}_U)$	Centroid of simplex $\mathcal{T}_U$

Graph Theory

$V(G)$, $E(G)$	Vertex set and edge set of graph G
$\boldsymbol{A}_G$	Adjacency matrix of graph G
$\boldsymbol{W}_G$	Weight matrix of graph G
$w_G(i,j)$	Weight of edge (i,j) in G
$\delta_G(i)$	Neighbours of i in G
$w_G(i)$	Weight of vertex $i \in V(G)$, i.e., $\sum_{j\in\delta_G(i)} w(i,j)$
$\mathrm{vol}_G(U)$	Volume of set U, i.e., $\sum_{i\in U} w(i)$.

Spectral Graph Theory

$\boldsymbol{L}_G$ ($\widehat{\boldsymbol{L}}_G$)	Combinatorial (Normalized) Laplacian Matrix of graph G
$\mathcal{L}_G$ ($\widehat{\mathcal{L}}_G$)	Quadratic form associated with $\boldsymbol{L}_G$ ($\widehat{\boldsymbol{L}}_G$)
$\{\lambda_i(G)\}$ ($\{\lambda_i(G)\}$)	Eigenvalues of $\boldsymbol{L}_G$ ($\widehat{\boldsymbol{L}}_G$). Sorted in decreasing order.
$\mathbf{\Lambda}_G$ ($\widehat{\mathbf{\Lambda}}_G$)	Diagonal Eigenvalue matrix of $\boldsymbol{L}_G$ ($\widehat{\boldsymbol{L}}_G$)
$\{\boldsymbol{\varphi}_i(G)\}$ ($\{\widehat{\boldsymbol{\varphi}}_i(G)\}$)	Eigenvectors of $\boldsymbol{L}_G$ ($\widehat{\boldsymbol{L}}_G$)
$\mathbf{\Phi}_G$ ($\widehat{\mathbf{\Phi}}_G$)	Eigenvector matrix of $\boldsymbol{L}_G$ ($\widehat{\boldsymbol{L}}_G$)

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

Miscellaneous

$\mathbb{R}$	Real numbers
$\mathbb{Q}$	Rational numbers
$\mathbb{C}$	Complex numbers
$\mathbb{N}$	Natural numbers
δ_{ij}	Kronecker delta function
χ_U	Indicator for event U
$\boldsymbol{\chi}_U$	Indicator vector for set U

Chapter 1

Introduction

§1.1. Think about

1. Been thinking about using the simplex as a means to sparsify the graph. But this is probably backwards. What about leveraging our knowledge vis-a-vis sparsifying graphs to “sparsify” a hyperacute simplex? Given simplex properties which can be expressed as a quadratic product, graph sparsification techniques could yield simplices with more orthogonality relations which maintain approximately the same properties. I suppose the question is whether a simplex with more orthogonality relationships is somehow easier to deal with? That is, why would it be advantageous to store a sparsified simplex?

2. Can we use the simplex to bound eigenvalues?

3. According to Gharan's notes, can optimize over L_2^2 metrics with SDPs. This should have implications for optimizing over the squared distances between vertices, which corresponds to optimizing over effective resistance.

4. In [Fie98], Fielder gives some sort of correspondence involving “ultrametric matrices”. Look this up and understand it—could be interesting.

5. Looking at the random walk of a graph as a path in the simplex didn't yield anything too interesting. What about the other way around? Beginning at a random point in the simplex, if we take a ”random walk” (this would have to be defined appropriately – we take a weighted step towards each vertex with some probability), we end up at some point that we know as a result of graph theory. We also know what governs how quickly we converge to this point, and when the path will be ”straight”. We know it's the sizes of the eigenvalues which govern the convergence; if we're simply given a hyperacute simplex, what do the eigenvalues represent? Can we translate this into a statement about the dynamics of the random walk in terms of the simplex only, and not the graph?

6. Can we define the ”inverse/dual” graph of G as follows: G yields a simplex $\mathcal{S}_G$ which is hyperacute. It is therefore the inverse simplex of graph G^+. How are G and G^+ related? Tried this in Section **??**. Unclear as of yet whether it's interesting.

7. The projection matrix $Y(e,f) = b_e^t \boldsymbol{L}_G^+ b_f \sqrt{w(e)w(f)}$ is symmetric with real eigenvalues (see [V$^+$13]). It thus yields a simplex. Maybe explore its properties.

8. Can use inequalities obtained in the effective resistance literature to obtain inequalities which pertain to all hyperacute simplices. See e.g.,[AALG17]
9. Do low rank approximations of the gram matrix maintain any of the simplex properties? This yields a smaller representation of the graph ... what properties does this representation have?
10. Embedding approximate distance matrix.
11. Applications of Schur Complement? try next
12. Simplex of the quotient graph? (EEP)
13. Dimensionality reduction. Can we reduce the dimensionality in specific ways to maintain interesting properties? Started thinking about this; JL lemma, sparsification, etc
14. Graph partitioning via the simplex?
15. Similarity measures between graphs. Projection onto different subspaces??
16. We could use the correspondence to develop a theory of random simplices. This could be a useful model. Study the random geometry of simplices via this correspondence. The random model could simply be to consider a random graph $G(n,p)$ and look at its simplex. p would roughl correspond to volume of the simplex — higher p implies higher connectivity implies larger volume. Meeeeeeh. Not sure if interesting.

§1.2. Prior Work

Steinitz's theorem which investigates the relationship between undirected graphs arising from convex polyhedra in $\mathbb{R}^3$ [Ste22].

§1.3. Contribution

Chapter 2

Background and Fundamentals

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

§2.1. General Notation

We use the standard notation for sets of numbers: $\mathbb{R}$ (reals), $\mathbb{N}$ (naturals), $\mathbb{Z}$ (integers), $\mathbb{C}$ (complex). We use the subscript ≥ 0 (resp., > 0) to restrict a relevant set to its non-negative (resp., positive) elements ($\mathbb{R}_{\geq 0}$, for example). We will often introduce new notation or definitions by using the notation $\stackrel{\text{def}}{=}$. The complement of a set U (with respect to what will be clear from context) is denoted U^c. Given a set of scalars K, we let $K^{n\times m}$ denote the set of $n \times m$ matrices (n rows and m columns) with elements in K. Matrices will typically be denoted by uppercase letters in boldface, e.g., $\boldsymbol{Q} \in K^{n\times m}$. Matrices will also often be referred to as linear transformations and written, for example, as $\boldsymbol{Q} : K^m \to K^n$. We let $\boldsymbol{Q}(i, \cdot)$ (resp., $\boldsymbol{Q}(\cdot, i)$) denote the i-th row (resp., column) of the matrix $\boldsymbol{Q}$. For a set U, K^U denotes the set of all functions from U to K. Elements of K^U are also called vectors. For any $n \in \mathbb{N}$, set $[n] \stackrel{\text{def}}{=} \{1, 2, \ldots, n\}$. As usual, we let $K^n = K^{[n]}$. Might have to distinguish between vectors and points; unsure whether this is needed yet. Vectors will typically be denoted by lowercase boldcase letters. Lowercase greek letters will often be used for scalars.

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

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

while the *0-norm* of $\boldsymbol{x}$ is the number of non-zero entries of $\boldsymbol{x}$, and is denoted by $\|\boldsymbol{x}\|_0$. Given a vector or matrix, we use the superscript t to denote it's transpose, i.e.,, given $\boldsymbol{Q}$, $\boldsymbol{Q}^t$ is defined as $\boldsymbol{Q}^t(i,j) = \boldsymbol{Q}(j,i)$. The standard inner product on $\mathbb{R}^d$ is denoted as $\langle \cdot, \cdot \rangle$, that is, $\langle \boldsymbol{x}, \boldsymbol{y} \rangle = \sum_i x(i)y(i)$. Elementary properties of the inner product will often be used without justification, such as its bilinearity: $\langle \boldsymbol{x}, \alpha\boldsymbol{y}_1 + \boldsymbol{y}_2 \rangle = \langle \boldsymbol{x}, \alpha\boldsymbol{y}_1 \rangle + \langle \boldsymbol{x}, \boldsymbol{y}_2 \rangle$ for $\alpha \in \mathbb{R}$.

We will often use the shorthand "iff" to mean "if and only if". We use δ_{ij} to denote the Kronecker delta function, i.e., $\delta_{ij} = 1$ if $i = j$ and 0 otherwise. We may sometimes include a comma and write $\delta_{i,j}$.

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

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

or equivalently, the smallest convex set containing X [GKPS67].

§2.2. Linear Algebra

The results derived in this section can be found in any self-contained reference on spectral graph theory (see e.g., [Spi09, CG97]). What's not graph-theoretic in nature—dimension, kernel, similarity, for example—may be found in a generic reference on linear algebra (e.g., [Axl97]).

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

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

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

Proof. Suppose $\{\mathbf{u}_i\}$ and $\{\boldsymbol{w}_i\}$ are biorthogonal bases. Fix $i \in [n]$. By independence, $\mathrm{span}(\mathbf{v}_1, \ldots, \mathbf{v}_{i-1}, \mathbf{v}_{i+1}, \ldots, \mathbf{v}_n)$ is a hyperplane—that is, $\dim(\mathrm{span}(\mathbf{v}_1, \ldots, \mathbf{v}_{i-1}, \mathbf{v}_{i+1}, \ldots, \mathbf{v}_n))^{\perp} = 1$. Both $\mathbf{u}_i$ and $\boldsymbol{w}_i$ are orthogonal to this hyperplane (since they orthogonal to $\mathbf{v}_j$ for all $j \neq i$), thus are either parallel or anti-parallel. Therefore, there exists some $\alpha \in \mathbb{R}$ such that $\mathbf{v}_i = \alpha\boldsymbol{w}_i$. By definition, $\langle \mathbf{v}_i, \mathbf{u}_i \rangle = \langle \mathbf{v}_i, \boldsymbol{w}_i \rangle = 1$, hence $\langle \mathbf{v}_i, \alpha\boldsymbol{w}_i \rangle = \langle \mathbf{v}_i, \boldsymbol{w}_i \rangle$ implying that $\alpha = 1$. This demonstrates that $\mathbf{u}_i = \boldsymbol{w}_i$ for all i. ⊠

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

$$\boldsymbol{M}\boldsymbol{\Phi} = \boldsymbol{M}(\boldsymbol{\varphi}_1, \ldots, \boldsymbol{\varphi}_n) = (\boldsymbol{M}\boldsymbol{\varphi}_1, \ldots, \boldsymbol{M}\boldsymbol{\varphi}_n) = (\lambda_1\boldsymbol{\varphi}_1, \ldots, \lambda_n\boldsymbol{\varphi}_n) = \boldsymbol{\Phi}\boldsymbol{\Lambda}. \tag{2.1}$$

Moreover, if $\{\boldsymbol{\varphi}_i\}_i$ are assumed to be orthonormal then $\boldsymbol{\Lambda}\boldsymbol{\Lambda}^\intercal = \mathbf{I}$ from which it follows from (2.1) that

$$\boldsymbol{M} = \boldsymbol{\Phi}\boldsymbol{\Lambda}\boldsymbol{\Phi}^t = \sum_{i\in[n]} \lambda_i \boldsymbol{\varphi}_i \boldsymbol{\varphi}_i^t, \tag{2.2}$$

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

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

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

The following basic result will be useful for us.

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

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

2.2.1. Pseudoinverse

Moore-Penrose pseudo-inverse: Nice overview by Barata [BH12]. Introduced by Moore [Moo20], rediscovered by Penrose [Pen55, Pen56]. Pseudoinverse of Laplacian discussed by Van Meighem *et al.* [VMDC17].

TODO introduce properties and defns of pseudo inverse.

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

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

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

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

Lemma 2.3 ([BH12]). *Let* $\boldsymbol{M} \in \mathbb{C}^{n\times m}$. *There exists a unique Pseudoinverse of* $\boldsymbol{M}^+$ *of* $\boldsymbol{M}$. *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* $\mathrm{range}(\boldsymbol{M}^+\boldsymbol{M}) = \mathrm{range}(\boldsymbol{M}^+)$.

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

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

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

$$\boldsymbol{M}^+ = \sum_{i=1}^{k} \frac{1}{\lambda_i} \boldsymbol{\varphi}_i \boldsymbol{\varphi}_i^t. \tag{2.3}$$

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

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

Performing a similar computation then demonstrates that

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

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

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

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

§2.3. Spectral Graph Theory

We begin with basic graph theory. We denote a *graph* by a triple $G = (V, E, w)$ where V is the *vertex set*, $E \subseteq V \times V$ is the *edge set* and $w : V \times V \to \mathbb{R}_{\ge 0}$ (the non-negative reals) a *weight function*. We let the domain of w be $V \times V$ for convenience; for $(i, j) \notin E$ we have $w((i, j)) = 0$. We call G *unweighted* if $w((i, j)) = \chi_{(i,j)\in E}$ for all i, j. In this case, we may omit the weight function and simply write $G = (V, E)$. We will typically take $V = [n]$ for simplicity. For a vertex $i \in V$, we denote the set of its neighbours by

$$\delta(i) \overset{\text{def}}{=} \{j \in V : w(i, j) > 0\},$$

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

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

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. 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.

Unless otherwise stated, we will assume that graphs are *undirected*—that is, there is no orientation on the edges. Consequently, we identify each tuple (i,j) with its sister pair (j,i). This implies, for example, that when summing over all edges $(i,j) \in E$ we are *not* summing over all vertices and their neighbours. Indeed, this latter summation double counts the edges: $\sum_{(i,j)\in E} = \frac{1}{2}\sum_i \sum_{j\in\delta(i)}$. We will often write $i \sim j$ to denote an edge (i,j); so, for example, $\sum_{i\sim j} = \sum_{(i,j)\in E}$.

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

2.3.1. Laplacian Matrices

Survey of Laplacian: [Mer94]. Let $G = (V, E, w)$ be a graph, with $V = [n]$ and $|E| = m$. Let $\boldsymbol{W}$ be the *weight matrix* of G, i.e., $\boldsymbol{W} = \mathrm{diag}(w(1), w(2), \dots, w(n))$. The *degree matrix* of G is $\mathrm{diag}(\deg(1), \deg(2), \dots, \deg(n))$. The *adjacency matrix* of G encodes the edge relations, namely, $\boldsymbol{A}_G(i,j) = w((i,j))$ for all $i \neq j$, and $\boldsymbol{A}_G(i,i) = 0$ for all i. Notice that (for undirected graphs) $\boldsymbol{A}_G$ is symmetric. If G is unweighted, then $\boldsymbol{W}_G$ is also called the *degree matrix of* G. The *combinatorial Laplacian* of G is the matrix

$$\boldsymbol{L}_G = \boldsymbol{W}_G - \boldsymbol{A}_G.$$

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

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

Then

$$\boldsymbol{L}_G = \sum_{i\sim j} \boldsymbol{L}_{i,j}. \tag{2.4}$$

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

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

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

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

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

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

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

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

$$\boldsymbol{L}_G = (\boldsymbol{W}_G^{1/2}\boldsymbol{B}_G)^t(\boldsymbol{W}_G^{1/2}\boldsymbol{B}_G). \tag{2.5}$$

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

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

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

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

we find that

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

Therefore, applying Equation 2.4 yields

$$\mathcal{L}_G(f) = f^t \left(\sum_{i\sim j} \boldsymbol{L}_{i,j} \right) f = \sum_{i \sim j} f^t \boldsymbol{L}_{i,j} f = \sum_{i\sim j} w(i,j)(f(i) - f(j))^2. \tag{2.6}$$

The *symmetric normalized Laplacian* or simply the *normalized Laplacian* of G is given by

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

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 2.4 for the normalized Laplacian:

$$\widehat{\boldsymbol{L}}_G = \sum_{i \sim j} \widehat{\boldsymbol{L}}_{i,j}. \tag{2.7}$$

Likewise,

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

As we've done here, we will typically emphasize the associate of elements associated to the normalized Laplacian with a hat. Using Equation (2.7), we see that the quadratic form $\widehat{\mathcal{L}}_G$ associated with $\widehat{\boldsymbol{L}}_G$ acts as

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

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

$$\boldsymbol{L}_G(\boldsymbol{L}_G)^+ = (\boldsymbol{L}_G)^+\boldsymbol{L}_G = \mathbf{I} - \frac{1}{n}\mathbf{1}\mathbf{1}^t, | \tag{2.8}$$

and

$$\widehat{\boldsymbol{L}}_G(\widehat{\boldsymbol{L}}_G)^+ = (\widehat{\boldsymbol{L}}_G)^+\widehat{\boldsymbol{L}}_G = \mathbf{I} - \frac{1}{n}\boldsymbol{D}_G^{1/2}\mathbf{1}(\boldsymbol{D}_G^{1/2}\mathbf{1})^t.$$

What is the following lemma used for?

Lemma 2.5. $\ker(\boldsymbol{L}^+) \subseteq \ker(\boldsymbol{L})$ *and* $\ker(\widehat{\boldsymbol{L}}^+) \subseteq \ker(\widehat{\boldsymbol{L}})$.

Proof. Let $\boldsymbol{x} \in \ker(\boldsymbol{L}^+)$, so $\boldsymbol{L}^+\boldsymbol{x} = \mathbf{0}$. Multiplying by $\boldsymbol{L}$ and using Equation (2.8) gives $\mathbf{0} = \boldsymbol{L}\boldsymbol{L}^+\boldsymbol{x} = (\mathbf{I} - \mathbf{1}\mathbf{1}^t/n)\boldsymbol{x}$, implying that $\boldsymbol{x} = \mathbf{1}\cdot\|\boldsymbol{x}\|_1/n$, i.e., $\boldsymbol{x} \in \mathrm{span}(\{\mathbf{1}\}) = \ker(\boldsymbol{L})$. The argument for the other inclusion is similar. ⊠

2.3.2. The Laplacian Spectrum

Both the combinatorial and normalized Laplacian of an undirected graph G are real, symmetric matrices. By the spectral theorem therefore, they both admit a basis of orthonormal eigenfunctions corresponding to real eigenvalues. Focus for the moment on the combinatorial Laplacian $\boldsymbol{L}_G$, with eigenvalues $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ and corresponding orthonormal eigenfunctions $\boldsymbol{\varphi}_1, \dots, \boldsymbol{\varphi}_n$. A straightforward consequence of Equation 2.5 is that all eigenvalues of $\boldsymbol{L}_G$ are non-negative. Let λ be an eigenvalue with (unit) eigenvector $\boldsymbol{\varphi}$. Then,

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

§2.4. Electrical Flows

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

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

or, more succinctly,

$$\boldsymbol{B}^t \boldsymbol{f} = \boldsymbol{e}. \tag{2.9}$$

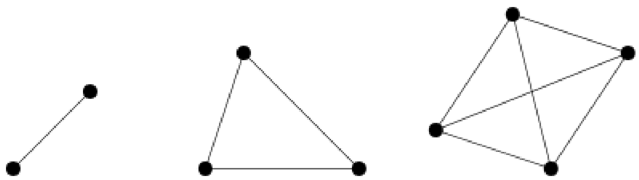


Figure 2.1: Simplices in dimensions one, two, and three.

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

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

so that

$$\boldsymbol{f} = \boldsymbol{W}\boldsymbol{B}\boldsymbol{\rho}. \tag{2.10}$$

Combining (2.9) and (2.10) 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 $\langle \boldsymbol{e}, \mathbf{1}\rangle$ (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

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

Note that here we've relied on the fact that $\boldsymbol{\chi}_i - \boldsymbol{\chi}_j \perp \mathbf{1}$.

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

§2.5. Simplices

Definition 2.3. A set of points $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_k$ 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 2.6. *The set $\{\boldsymbol{x}_1, \ldots, \boldsymbol{x}_k\}$ is affinely independent iff for each j, $\{\boldsymbol{x}_j - \boldsymbol{x}_i\}_{i\neq j}$ is linearly independent.*

Proof. Suppose that $\{\boldsymbol{x}_j - \boldsymbol{x}_i\}_{i\neq j}$ is not linearly independent, and let $\{\beta_i\}$ (not all zero) be such that $\sum_{i\neq j} \beta_i(\boldsymbol{x}_j - \boldsymbol{x}_j) = \mathbf{0}$. 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. ⊠

Lemma 2.7. *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 $\boldsymbol{y} = \sum_{i\in[n]} \alpha_i \boldsymbol{x}_i$.*

Proof. By Lemma 2.6, 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 $\sum_i \alpha_i = 1$. ⊠

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

$$\mathcal{S} = \left\{ \sum_{i=1}^n \boldsymbol{\sigma}_i \alpha_i : \alpha_i \geq 0,\ \sum_{i=1}^n \alpha_i = 1 \right\}.$$

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

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

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 $\mathcal{S}$ corresponding to U* is

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

Trusting the reader's capacity for variation, depending on the situation we may adopt different notation for the faces of a simplex. Often times 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.

The *centroid* of a simplex is the point

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

The centroid of a simplex can be thought of as its centre of mass, assuming that weight is distributed evenly across its surface.

Given a simplex $\mathcal{S}$, an *altitude between faces $\mathcal{S}_U$ and $\mathcal{S}_{U^c}$* is a vector which lies in the orthogonal complement of both $\mathcal{S}_U$ and $\mathcal{S}_{U^c}$ and points from one face to the other. We denote the altitude pointing from $\mathcal{S}_{U^c}$ to $\mathcal{S}_U$ as $\boldsymbol{a}_(\mathcal{S}_U)$. We can write the altitude as $\boldsymbol{a}_U = \boldsymbol{p} - \boldsymbol{q}$ for some $\boldsymbol{p} \in \mathcal{S}_{U^c}$ and $\boldsymbol{q} \in \mathcal{S}_U$, and thus as $\boldsymbol{\Sigma}(\boldsymbol{x}_{U^c} - \boldsymbol{x}_U)$ where $\boldsymbol{x}_{U^c}$ and $\boldsymbol{x}_U$ are the barycentric coordinates of $\boldsymbol{p}$ and $\boldsymbol{q}$.

We will use the symbol $\cong$ to denote isomorphism or congruency between simplices. That is, $\mathcal{S}_1 \cong \mathcal{S}_2$ iff $\mathcal{S}_1$ can be converted to $\mathcal{S}_2$ via translation and rotation.

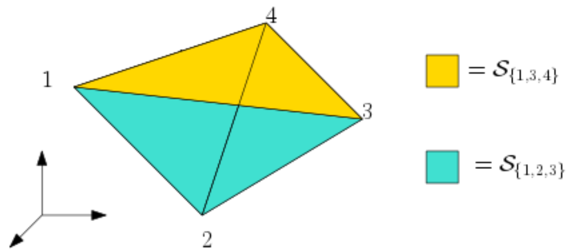


Figure 2.2:

2.5.1. Dual Simplex

Let $\mathbf{\Sigma} = (\boldsymbol{\sigma}_1, \ldots, \boldsymbol{\sigma}_n) \in \mathbb{R}^{n-1\times n}$ be the vertex matrix of a simplex $\mathcal{S} \subseteq \mathbb{R}^{n-1}$. For each $i \in [n-1]$, put $\mathbf{v}_i = \boldsymbol{\sigma}_n - \boldsymbol{\sigma}_i$. Then $\{\mathbf{v}_1, \ldots, \mathbf{v}_{n-1}\}$ is a linearly independent set, and thus admits a sister basis $\{\boldsymbol{\gamma}_1, \ldots, \boldsymbol{\gamma}_{n-1}\}$ 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 $\{\boldsymbol{\gamma}_1, \ldots, \boldsymbol{\gamma}_n\}$ is affinely independent.*

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

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

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

Therefore, the set $\{\boldsymbol{\gamma}_1, \ldots, \boldsymbol{\gamma}_n\}$ determines a simplex, which we call the *dual simplex* of $\mathcal{S}$. Of course, it would highly suboptimal if the notion of a dual simplex depended on the labelling of the vertices of $\mathcal{S}$. More specifically, we defined the vertices of the dual simplex $\boldsymbol{\gamma}_i$ with respect to the vectors $\boldsymbol{\sigma}_n - \boldsymbol{\sigma}_i$. It is not clear a priori whether the vertices of the dual simplex would change were we to relabel the indices of $\{\boldsymbol{\sigma}_i\}$. In fact, they do not—the demonstration of which is the purpose of the following lemma.

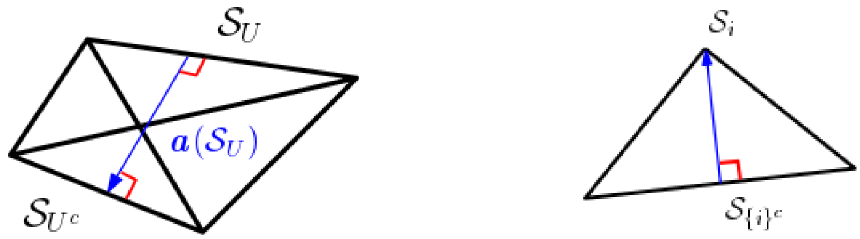
Lemma 2.8. *Let $\{\boldsymbol{\sigma}_1, \ldots, \boldsymbol{\sigma}_n\}$ be a set of affinely independent vectors. Fix $k \in [n-1]$ and define $\mathbf{v}_i = \boldsymbol{\sigma}_n - \boldsymbol{\sigma}_i$ for $i \in [n-1]$ and $\mathbf{u}_i = \boldsymbol{\sigma}_k - \boldsymbol{\sigma}_i$ Should maybe be $\boldsymbol{\sigma}_i - \boldsymbol{\sigma}_n$—run into trouble with negatives later on for $i \in [n] \setminus \{k\}$. If $\{\boldsymbol{\gamma}_1, \ldots, \boldsymbol{\gamma}_n - 1\}$ is the sister basis to $\{\mathbf{v}_1, \ldots, \mathbf{v}_{n-1}\}$ and $\boldsymbol{\gamma}_n = -\sum_{i=1}^{n-1} \boldsymbol{\gamma}_i$, then $\{\boldsymbol{\gamma}_1, \ldots, \boldsymbol{\gamma}_{k-1}, \boldsymbol{\gamma}_{k+1}, \ldots, \boldsymbol{\gamma}_n\}$ is the sister basis to $\{\mathbf{u}_1, \ldots, \mathbf{u}_{k-1}, \mathbf{u}_{k+1}, \ldots, \mathbf{u}_n\}$.*

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

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

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

$$\langle \boldsymbol{\gamma}_i, \boldsymbol{\sigma}_k - \boldsymbol{\sigma}_j \rangle = -\sum_{\ell=1}^{n-1} \langle \boldsymbol{\gamma}_\ell, \boldsymbol{\sigma}_k - \boldsymbol{\sigma}_n + \boldsymbol{\sigma}_n - \boldsymbol{\sigma}_j \rangle$$



$$= \sum_{\ell=1}^{n-1} \langle \boldsymbol{\gamma}_\ell, \boldsymbol{\sigma}_n - \boldsymbol{\sigma}_k \rangle - \sum_{\ell=1}^{n-1} \langle \boldsymbol{\gamma}_\ell, \boldsymbol{\sigma}_n - \boldsymbol{\sigma}_j \rangle = 1 - 1 = 0. \qquad \boxtimes$$

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

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

hence had we set $\mathbf{v}_i = \boldsymbol{\sigma}_k - \boldsymbol{\sigma}_i$ and defined $\boldsymbol{\gamma}_k = -\sum_{i \neq k} \boldsymbol{\gamma}_i$ (as we did for $k = n$), Lemma 2.8 demonstrates that we would produce the same set of vectors for the dual simplex. We honour the fact that the dual simplex is independent of labelling, i.e., well-defined, with the following definition.

Definition 2.5 (Dual Simplex). Given a simplex $\mathcal{S}_1 \subseteq \mathbb{R}^{n-1}$ with vertex set $\boldsymbol{\Sigma}(\mathcal{S}_1) = (\boldsymbol{\sigma}_1, \dots, \boldsymbol{\sigma}_n)$, a simplex $\mathcal{S}_2 \subseteq \mathbb{R}^{n-1}$ with vertex vectors $\boldsymbol{\Sigma}(\mathcal{S}_2) = (\boldsymbol{\gamma}_1, \dots, \boldsymbol{\gamma}_n)$ is called a *dual simplex* of $\mathcal{S}_1$ if for all $k \in [n]$, $\{\boldsymbol{\gamma}_i\}_{i \neq k}$ is the sister basis to $\{\boldsymbol{\sigma}_k - \boldsymbol{\sigma}_i\}_{i \neq k}$.

Theorem 2.1. *Each simplex has a unique dual simplex. Moreover, if $\mathcal{S}_1$ is the dual simplex to $\mathcal{S}_0$, then $\mathcal{S}_0$ is the dual simplex to $\mathcal{S}_1$.*

Proof. Existence follows from Lemma 2.1 using the construction above. Uniqueness follows from Observation 2.1 and Lemma 2.8. The second part of the statement is clear by construction. $\boxtimes$

Definition 2.5 a unwieldy to work with in practice. For this reason we present an alternate characterization of the dual simplex, which lends itself more readily to verification.

Lemma 2.9. *Let $\mathcal{S}_1$ with $\boldsymbol{\Sigma}(\mathcal{S}_1) = (\boldsymbol{\sigma}_1, \dots, \boldsymbol{\sigma}_n)$ and $\mathcal{S}_2$ with $\boldsymbol{\Sigma}(\mathcal{S}_2) = (\boldsymbol{\gamma}_1, \dots, \boldsymbol{\gamma}_n)$ be two simplices in $\mathbb{R}^{n-1}$. A necessary and sufficient condition for $\mathcal{S}_2$ to be the dual of $\mathcal{S}_1$ is that $\boldsymbol{\gamma}_i$ is perpendicular to $\mathcal{S}_1[\{i\}^c]$ for all $i \in [n]$. Not actually sure if this is true anymore. Run into problems with normalization.*

Proof. Suppose first that $\mathcal{S}_1$ and $\mathcal{S}_2$ are dual and consider a fixed $i < n$. Let $\boldsymbol{p}, \boldsymbol{q} \in \mathcal{S}_{\{i\}^c}$ have barycentric coordinates $\boldsymbol{x}$ and $\boldsymbol{y}$ respectively. We need to show that $\langle \boldsymbol{\gamma}_i, \boldsymbol{p} - \boldsymbol{q} \rangle = 0$. Note that $x(i) = y(i) = 0$, and so

$$\begin{aligned} \boldsymbol{p} - \boldsymbol{q} = \boldsymbol{\Sigma}(\boldsymbol{x} - \boldsymbol{y}) &= \sum_{j=1, j\neq i}^{n-1} \boldsymbol{\sigma}_j (x(j) - y(j)) + \boldsymbol{\sigma}_n (x(n) - y(n)) \\ &= \sum_{j=1, j \neq i}^{n-1} \boldsymbol{\sigma}_j (x(j) - y(j)) + \boldsymbol{\sigma}_n \Big(\sum_j y(j) - x(j) \Big) = \sum_{j=1, j\neq i}^{n-1} (\boldsymbol{\sigma}_j - \boldsymbol{\sigma}_n)(x(j) - y(j)). \end{aligned}$$

Now, by definition, $\langle \boldsymbol{\gamma}_i, \boldsymbol{\sigma}_j - \boldsymbol{\sigma}_n \rangle = \delta_{i,j}$ so it follows that

$$\langle \boldsymbol{\gamma}_i, \boldsymbol{p} - \boldsymbol{q} \rangle = \sum_{j=1, j\neq i}^{n-1} \langle \boldsymbol{\gamma}_i, \boldsymbol{\sigma}_j - \boldsymbol{\sigma}_n \rangle (x(j) - y(j)) = 0,$$

as desired. We now consider $i = n$. Recall that $\boldsymbol{\gamma}_n = -\sum_{i<n} \boldsymbol{\gamma}_i$. Moreover, $\langle \boldsymbol{\gamma}_i, \boldsymbol{\sigma}_j \rangle = \delta_{i,j} - \langle \boldsymbol{\gamma}_i, \boldsymbol{\gamma}_n \rangle$. Using similar arithmetic as above,

$$\begin{aligned}
\langle \boldsymbol{\gamma}_n, \boldsymbol{p} - \boldsymbol{q} \rangle &= -\sum_{i<n} \left\langle \boldsymbol{\gamma}_i, -\sum_{j<n} \boldsymbol{\sigma}_j (x(j) - y(j)) \right\rangle \\
&= -\sum_{i<n} \left\langle \boldsymbol{\gamma}_i, -\sum_{j<n} (\delta_{i,j} - \langle \boldsymbol{\sigma}_i, \boldsymbol{\sigma}_n \rangle)(x(j) - y(j)) \right\rangle \\
&= -\sum_{i<n} \left(x(i) - y(i) - \langle \boldsymbol{\gamma}_i, \boldsymbol{\sigma}_n \rangle \sum_{j<n} x(j) - y(j) \right) = 0,
\end{aligned}$$

since $\boldsymbol{x}$ and $\boldsymbol{y}$ are barycentric coordinates. Conversely, suppose that $\langle \boldsymbol{\gamma}_i, \boldsymbol{\Sigma x} - \boldsymbol{\Sigma y} \rangle = 0$ for every $\boldsymbol{\Sigma x}, \boldsymbol{\Sigma y} \in \mathcal{S}_{\{i\}^c}$. For $k \neq i$ and any $j \in [n]$, we need to show that $\langle \boldsymbol{\gamma}_i, \boldsymbol{\sigma}_k - \boldsymbol{\sigma}_j \rangle = \delta_{ij}$. For $j \neq i$, we can take $\boldsymbol{x} = \boldsymbol{\chi}_k$ and $\boldsymbol{y} = \boldsymbol{\chi}_j$ above to obtain $\langle \boldsymbol{\gamma}_i, \boldsymbol{\Sigma x} - \boldsymbol{\Sigma y} \rangle = \langle \boldsymbol{\gamma}_i, \boldsymbol{\sigma}_k - \boldsymbol{\sigma}_j \rangle = 0 = \delta_{ij}$. For $j = i$, ⊠

2.5.2. Angles in a Simplex

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

$$\cos \phi_{ij}(\mathcal{T}) = \frac{\langle \boldsymbol{\gamma}_i, \boldsymbol{\gamma}_j \rangle}{\|\boldsymbol{\gamma}_i\|_2 \cdot \|\boldsymbol{\gamma}_j\|_2},$$

where $\{\boldsymbol{\gamma}_i\}$ are the vertices of $\mathcal{T}^D$. 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,

$$\cos \theta_{ij}(\mathcal{T}) = -\frac{\langle \boldsymbol{\gamma}_i, \boldsymbol{\gamma}_j \rangle}{\|\boldsymbol{\gamma}_i\|_2 \cdot \|\boldsymbol{\gamma}_j\|_2}, \tag{2.11}$$

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

Definition 2.6. We call the simplex $\mathcal{T} \subseteq \mathbb{R}^{n-1}$ *hyperacute* if $\theta_{ij}(\mathcal{T}) \leq \pi/2$ for all $i, j \in [n]$. If $\mathcal{T}$ is not hyperacute, it is called *obtuse.*

Chapter 3

The Graph-Simplex Correspondence

§3.1. Convex Polyhedra of Matrices

Unclear whether to leave this or just discuss the simplex of a graph immediately. Consider an arbitrary real and symmetric matrix $\boldsymbol{M} \in \mathbb{R}^{n\times n}$ which admits 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 respective absences of $\boldsymbol{\varphi}_{d+1}, \dots, \boldsymbol{\varphi}_n$ and $\lambda_{d+1}, \dots, \lambda_n$), suggests that we might consider $\boldsymbol{\Lambda}_M^{1/2} \boldsymbol{\Phi}_M$ as a vertex matrix, thus $\boldsymbol{M}$ as a gram matrix. Inorexably compelled by this intuition, define the vertices $\boldsymbol{\sigma}_1, \dots, \boldsymbol{\sigma}_n$ given by

$$\boldsymbol{\sigma}_i = (\boldsymbol{\Lambda}_{\boldsymbol{M}}^{1/2} \boldsymbol{\Phi}_{\boldsymbol{M}})^t(\cdot, i) = (\boldsymbol{\varphi}_i(1)\lambda_1^{1/2}, \boldsymbol{\varphi}_i(2)\lambda_2^{1/2}, \dots, \boldsymbol{\varphi}_i(n)\lambda_n^{1/2})^t,$$

and the polytope

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

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

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

Observe that the polytope $\mathcal{S}(\boldsymbol{M})$ is d-dimensional: Introduce dimension of polytope in prelims

$$\operatorname{rank}(\boldsymbol{\Sigma}) = \operatorname{rank}(\boldsymbol{\Sigma}^t\boldsymbol{\Sigma}) = \operatorname{rank}(\boldsymbol{M}) = d.$$

The Inverse Polytope. With $\boldsymbol{M}$ as above, consider the pseudo-inverse of $\boldsymbol{M}$ which we can write as

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

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

3.1.1. The Simplex of a Graph

For an undirected graph G, the previous section yields several polytopes corresponding to G. The most structurally rich among these are the polytopes $\mathcal{S}_G \stackrel{\text{def}}{=} \mathcal{P}_{\boldsymbol{L}_G}$ and $\widehat{\mathcal{S}}_G \stackrel{\text{def}}{=} \mathcal{P}_{\widehat{\boldsymbol{L}}_G}$ corresponding to G's combinatorial and normalized Laplacians. We let $\boldsymbol{\Sigma}_G = (\boldsymbol{\sigma}_1, \dots, \boldsymbol{\sigma}_n)$ and $\widehat{\boldsymbol{\Sigma}}_G = (\widehat{\boldsymbol{\sigma}}_1, \dots, \widehat{\boldsymbol{\sigma}}_n)$ denote the vertices of $\mathcal{S}_G$ and $\widehat{\mathcal{S}}_G$, respectively. 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 in fact simplices. Consequently, we will often refer to $\mathcal{S}_G$ as the *simplex of* G, and to $\widehat{\mathcal{S}}_G$ as the *normalized simplex of* G. If G is clear from context we will often drop it from the subscript.

Why do we need this? We know the simplices are well-defined due to the rank

LEMMA 3.1. *The vertices $\{\boldsymbol{\sigma}_i\}$ and $\{\widehat{\boldsymbol{\sigma}}_i\}$ are affinely independent.*

Proof. Suppose $\boldsymbol{\alpha} = (\alpha_1, \dots, \alpha_n)$ is such that $\sum_{i=1}^n \alpha_i \boldsymbol{\sigma}_i = \mathbf{0}$, i.e., $\boldsymbol{\alpha} \in \ker(\boldsymbol{\Sigma})$. Since $\ker(\boldsymbol{\Sigma}) = \ker(\boldsymbol{\Sigma}^t\boldsymbol{\Sigma}) = \ker(\boldsymbol{L}) = \text{span}(\{\mathbf{1}\})$, there exists some $k \in \mathbb{R}$ such that $\boldsymbol{\alpha} = k\mathbf{1}$. If $\langle \boldsymbol{\alpha}, \mathbf{1}\rangle = \langle k\mathbf{1}, \mathbf{1}\rangle = kn = 0$ 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 $\langle k\sqrt{\boldsymbol{w}}, \mathbf{1}\rangle = k\sum_i w(i) = 0$, so $\boldsymbol{\alpha} = \mathbf{0}$. ⊠

For the inverse simplex and normalized simplex of G we have

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

Let $\widetilde{\boldsymbol{\Phi}}$ be the matrix containing all eigenvectors of $\boldsymbol{L}_G$ (i.e., also containing $\mathbf{1}/\sqrt{n}$). Note that because $\widetilde{\boldsymbol{\Phi}}^t\widetilde{\boldsymbol{\Phi}} = \mathbf{I}$ it follows that $\widetilde{\boldsymbol{\Phi}}\widetilde{\boldsymbol{\Phi}}^t = \mathbf{I}$ as well. Therefore,

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

From this, it follows that

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

hence,

$$\boldsymbol{\Sigma}^t\boldsymbol{\Sigma}^+ = (\boldsymbol{\Sigma}^+)^t\boldsymbol{\Sigma} = \mathbf{I} - \frac{\mathbf{J}}{n}. \tag{3.1}$$

For the inverse normalized simplex on the other hand, one has (Section 2.3.2)

$$\boldsymbol{\varphi}_n \in \text{span}(\boldsymbol{W}_G^{1/2}\mathbf{1}),$$

and since we are working with normalized eigenfunctions ($\|\boldsymbol{\varphi}_n\|_2 = 1$), 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

$$\widehat{\mathbf{\Sigma}}^t\widehat{\mathbf{\Sigma}}^+ = (\widehat{\mathbf{\Sigma}}^+)^t\widehat{\mathbf{\Sigma}} = \mathbf{I} - \frac{\sqrt{\boldsymbol{w}}\sqrt{\boldsymbol{w}}^t}{\mathrm{vol}(G)}. \tag{3.2}$$

Exploring the relationships between the vertex matrices and themselves meanwhile, we find that

$$\begin{aligned}\mathbf{\Sigma}^+(\mathbf{\Sigma}^+)^t &= \begin{pmatrix} \sum_i \boldsymbol{\sigma}_i^+(1)\boldsymbol{\sigma}_i^+(1) & \dots & \sum_i \boldsymbol{\sigma}_i^+(1)\boldsymbol{\sigma}_i^+(n) \\ \vdots & \ddots & \vdots \\ \sum_i \boldsymbol{\sigma}_i^+(n)\boldsymbol{\sigma}_i^+(1) & \dots & \sum_i \boldsymbol{\sigma}_i^+(n)\boldsymbol{\sigma}_i^+(n) \end{pmatrix} \\ &= \begin{pmatrix} \lambda_1^{-1}\langle \boldsymbol{\varphi}_1, \boldsymbol{\varphi}_1\rangle & \dots & \lambda_1^{-1/2}\lambda_n^{-1/2}\langle \boldsymbol{\varphi}_1, \boldsymbol{\varphi}_n\rangle \\ \vdots & \ddots & \dots \\ \lambda_1^{-1/2}\lambda_n^{-1/2}\langle \boldsymbol{\varphi}_n, \boldsymbol{\varphi}_1\rangle & \dots & \lambda_n^{-1}\langle \boldsymbol{\varphi}_n, \boldsymbol{\varphi}_n\rangle \end{pmatrix} = \mathbf{\Lambda}^{-1},\end{aligned} \tag{3.3}$$

and likewise,

$$\widehat{\mathbf{\Sigma}}^+(\widehat{\mathbf{\Sigma}}^+)^t = \widehat{\mathbf{\Lambda}}^{-1}. \tag{3.4}$$

3.1.2. The Graph of a Simplex

In this section we demonstrate that each hyperacute (more precisely, each non-obtuse) simplex is the inverse simplex of a graph G.

Should be able to prove this on our own by appealing to the dual simplex

LEMMA 3.2 ([Fie93]). *Given a simplex $\mathcal{T} \subseteq \mathbb{R}^{n-1}$ centered at the origin, let $\boldsymbol{Q}$ be the Gram matrix of its normalized outernormals. That is, $\boldsymbol{Q}(i,j) = \langle \mathbf{u}_i, \mathbf{u}_j\rangle$ where $\mathbf{u}_i$ is the outer normal to the face $\mathcal{T}_{\{i\}^c}$. If $\boldsymbol{Q}_1, \boldsymbol{Q}_2 \in \mathbb{R}^{n\times n}$ are defined by*

$$\boldsymbol{Q}_1 = diag\Big(\|\boldsymbol{a}(\mathcal{S}_1)\|_2^{-1}, \dots, \|\boldsymbol{a}(\mathcal{S}_n)\|_2^{-1}\Big),$$

and

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

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

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

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

$$\mathbf{\Sigma}^t\mathbf{\Sigma}(i,j) = \begin{cases} \left\|\boldsymbol{a}(\mathcal{S}_i^+)\right\|_2^{-2}, & \text{if } i = j, \\ -\cos\theta_{i,j}^+\left\|\boldsymbol{a}_i^+\right\|_2^{-1}\cdot\left\|\boldsymbol{a}_j^+\right\|_2^{-1}, & \text{if } i \neq j. \end{cases}$$

(Here $\theta^+ i, j$ is the angle between $\mathcal{S}^+_{\{i\}^c}$ and $\mathcal{S}^+_{\{j\}^c}$.) We claim that $\boldsymbol{\Sigma}^t\boldsymbol{\Sigma}$ is the Laplacian matrix of some graph G. First, the matrix is symmetric. Second, for each i, $(\boldsymbol{\Sigma}^t\boldsymbol{\Sigma})(i,i) = \left\|\boldsymbol{a}_i^+\right\|_2^{-2} > 0$, and for $i \neq j$, $(\boldsymbol{\Sigma}^t\boldsymbol{\Sigma})(i,j) \leq 0$ since $\theta^+_{i,j} \leq \pi/2$ by assumption (note therefore the importance that $\mathcal{S}^+$ 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 $i \neq n$,

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

hence $\boldsymbol{\Sigma}^t\boldsymbol{\Sigma}\mathbf{1} = \mathbf{0}$, meaning that

$$(\boldsymbol{\Sigma}^*\boldsymbol{\Sigma})(i,i) = -\sum_{j\neq i}(\boldsymbol{\Sigma}^*\boldsymbol{\Sigma})(i,j).$$

If we construct a weighted graph $G = (V, E, \boldsymbol{w})$ on n vertices with edge weights $\boldsymbol{w}(i,j) = (\boldsymbol{\Sigma}^t\boldsymbol{\Sigma})(i,j)$, it then follows that $\boldsymbol{\Sigma}^t\boldsymbol{\Sigma} = \boldsymbol{L}_G$.

We summarize the material in Sections 3.1.1 and 3.1.2 with the following theorem.

Theorem 3.1. *There exists a bijection between hyperacute Need to define hyperacute as allowing angles of $\pi/2$ simplices in $\mathbb{R}^{n-1}$ centered at the origin and connected, weighted graphs on n vertices.*

in light of the theorem, may want to think about structuring the discussion so that $\mathcal{S}^+$ is actually the main object, while $\mathcal{S}$ is secondary.

§3.2. Simplices of Special Graphs

Simplex of Complement Graph, G^c Suppose G is unweighted. The complement of G, G^c, has adjacency matrix $\boldsymbol{A}_{G^c} = \mathbf{1}\mathbf{1}^t - \mathbf{I} - \boldsymbol{A}_G$ and degree matrix $\boldsymbol{D}^c = \boldsymbol{D}_{G^c} = (n-1)\mathbf{I} - \boldsymbol{D}_G$ since $\deg(i)_{G^c} = n - 1 - \deg(i)_G$. The Laplacian of G^c thus reads as

$$\boldsymbol{L}^c = \boldsymbol{D}^c - \boldsymbol{A}^c = n\mathbf{I} - \boldsymbol{D}_G - \mathbf{1}\mathbf{1}^t + \boldsymbol{A}_G = n\mathbf{I} - \mathbf{1}\mathbf{1}^t - \boldsymbol{L}_G.$$

Of course, $\mathbf{1}$ is still an eigenfunction of $\boldsymbol{L}^c$. For $\boldsymbol{\varphi} \perp \mathbf{1}$, we have

$$\boldsymbol{L}^c\boldsymbol{\varphi} = n\boldsymbol{\varphi} - \mathbf{1}\langle\mathbf{1}, \boldsymbol{\varphi}\rangle - \boldsymbol{L}\boldsymbol{\varphi} = (n - \lambda)\boldsymbol{\varphi},$$

which 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 $w_H(i,j) \le w_G(i,j)$ for all $i,j \in [n]$. Then, for any $f : V \to \mathbb{R}$ we see that

$$\mathcal{L}_G(f) = \sum_{i\sim j} w_G(i,j)(f(i)-f(j))^2 \ge \sum_{i\sim j} w_H(i,j)(f(i)-f(j))^2 = \mathcal{L}_H(f).$$

Therefore,

$$\|\boldsymbol{\Sigma}_H f\|_2^2 \le \|\boldsymbol{\Sigma}_G f\|_2^2.$$

In particular, taking $f = \chi_i$ for any i, this yields $\|\boldsymbol{\sigma}_i(G)\|_2^2 \ge \|\boldsymbol{\sigma}_i(H)\|_2^2$.

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 $\|\sigma_i(G)\|_2^2 = c \cdot \|\boldsymbol{\sigma}_i(H)\|_2^2$. Meanwhile however, the normalized simplex is unaffected by the re-weighting:

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

Product Graphs

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

Suppose G has eigenvalues $\lambda_1 \ge \cdots \ge \lambda_n$ and corresponding eigenvectors $\boldsymbol{\varphi}_1, \ldots, \boldsymbol{\varphi}_n$ as usual. Let H have eigenvalues $\mu_1 \ge \cdots \ge \mu_m$ and corresponding eigenvectors $\boldsymbol{\psi}_1, \ldots, \boldsymbol{\psi}_m$. We claim that $G \times H$ has $m+n$ eigenvalues $\{\lambda_i + \mu_j\}_{i\in[n], j\in[m]}$ with eigenvectors $\{f_{i,j}\}_{(i,j)\in[n]\times[m]}$ given by

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

Indeed:

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

$$
\begin{aligned}
&= \lambda_u \boldsymbol{\varphi}_u(i)\boldsymbol{\psi}_v(j) + \mu_v \boldsymbol{\psi}_v(j)\boldsymbol{\varphi}_u(i) \\
&= (\lambda_u + \mu_v)\boldsymbol{\varphi}_u(i)\boldsymbol{\psi}_v(j) = (\lambda_u + \mu_v) f_{uv}(ij),
\end{aligned}
$$

as desired. Consequently, the product graph yields a simplex with vertices

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

3.2.1. Examples

Explore certain graphs whose eigenvalues and eigenvectors are easy to compute.

The Complete Graph, K_n. First let us consider the combinatorial simplex, $\mathcal{S}^{\mathrm{c}}(K_n)$. The combinatorial 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

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

since $\sum_i \boldsymbol{\varphi}(i) = \langle \boldsymbol{\varphi}, \mathbf{1}\rangle = 0$. finish this

Cycle Graph

Path Graph

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

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

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

$$\cos\theta_{ij}(\mathcal{S}_p) = -\langle \boldsymbol{\chi}_i, \boldsymbol{\chi}_j\rangle = -\delta_{ij},\ i,j \in [n-1], \quad \text{and} \quad \cos\theta_{in}(\mathcal{S}_p) = \frac{\langle \boldsymbol{\chi}_i, \mathbf{1}\rangle}{\|1\|} = 1/\sqrt{n},\ i \in [n].$$

This implies that $\theta_{ij}(\mathcal{S}_p) = 0$ for $i \neq j$, $i,j \neq n$ and $\theta_{in}(\mathcal{S}_p) \in= (0, \pi/2)$. The angles in $\mathcal{S}_p$ and $\widetilde{\mathcal{S}}_p$ don't change, but those it seems like those in the shifted simplex do. What is going on here?

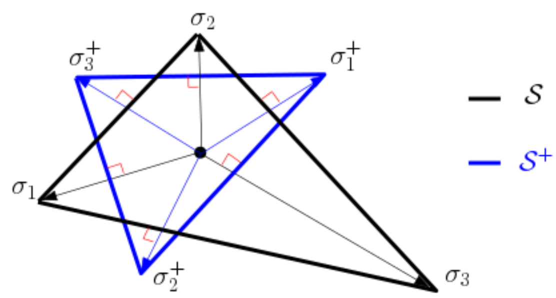


Figure 3.1: A simplex of a graph and its inverse.

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

Fix a graph $G = (V, E, w)$ with $|V| = n$. The first property of $\mathcal{S} = \mathcal{S}_G$ that's worth noting is that it is centred at the origin: $\boldsymbol{c}(\mathcal{S}) = n^{-1}\boldsymbol{\Lambda}^{-1/2}\boldsymbol{\Phi}^t\mathbf{1} = \mathbf{0}$, since $\langle \boldsymbol{\varphi}_i, \mathbf{1}\rangle = 0$ for all $i < n$. Likewise, $\boldsymbol{c}(\mathcal{S}^+) = \mathbf{0}$.

Secondly, let us notice that $\mathcal{S}_G^+$ is intimately related to the effective resistance of the graph G. Indeed,

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

Lemma 3.3. *The combinatorial simplex $\mathcal{S}_G$ of a graph G is hyperacute iff $\boldsymbol{L}_G^+$ is a Laplacian.Is the pseudoinverse Laplacian ever a Laplacian?*

Proof. Using Equation 2.11 and the fact that $\mathcal{S}_G^+ = \mathcal{S}_G^D$, 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 $\boldsymbol{L}_G^+(i,i) \ge 0$). ☒

Should hold between every simplex and its dual. Probably move into prelims section

Lemma 3.4. *Let $\mathcal{S}$ and $\mathcal{S}^+$ be the simplex and inverse simplex of a graph $G = (V, E)$. For any non-empty $U \subseteq V$, the faces $\mathcal{S}_U^+$ and $\mathcal{S}_{U^c}$ are orthogonal. In other words, if $\boldsymbol{p}_1, \boldsymbol{p}_2 \in \mathcal{S}_U^+$ and $\boldsymbol{q}_1, \boldsymbol{q}_2 \in \mathcal{S}_{U^c}$, then $\langle \boldsymbol{p}_1 - \boldsymbol{p}_2, \boldsymbol{q}_1 - \boldsymbol{q}_2\rangle = 0$.*

Proof. Let $\boldsymbol{p} \in \mathcal{S}_U^+$ and $\boldsymbol{q} \in \mathcal{S}_{U^c}$. Letting their barycentric coordinates be $\boldsymbol{x_p}$ and $\boldsymbol{x_q}$ respectively, write

$$\langle \boldsymbol{p}, \boldsymbol{q}\rangle = \boldsymbol{x_p}(\boldsymbol{\Sigma}^+)^t\boldsymbol{\Sigma}\boldsymbol{x_q} = \boldsymbol{x_p}(\mathbf{I} - \mathbf{1}\mathbf{1}^t/n)\boldsymbol{x_q},$$

where we've employed Equation (3.1). Now, $\boldsymbol{x_p}(i) = 0$ for all $i \in U^c$ and $\boldsymbol{x_q}(j) = 0$ for all $j \in U$. Therefore, $\langle \boldsymbol{x_p}, \boldsymbol{x_q} \rangle = 0$. Moreover, $\|\boldsymbol{x_p}\|_1 = \|\boldsymbol{x_q}\|_1 = 1$ and so the above simplifies to $\langle \boldsymbol{p}, \boldsymbol{q} \rangle = -1/n$. Consequently, if $\boldsymbol{p}_1, \boldsymbol{p}_2 \in \mathcal{S}_U^+$ and $\boldsymbol{q}_1, \boldsymbol{q}_2 \in \mathcal{S}_{U^c}$ we have

$$\langle \boldsymbol{p}_1 - \boldsymbol{p}_2, \boldsymbol{q}_1 - \boldsymbol{q}_2 \rangle = 0,$$

completing the proof. ⊠

The following lemma presents an alternate characterization of the simplex.

LEMMA 3.5. *For a simplex $\mathcal{S}$ of a graph G,*

$$\mathcal{S} = \left\{ \boldsymbol{x} \in \mathbb{R}^{n-1} : \boldsymbol{x}^t \boldsymbol{\Sigma}^+ + \frac{\mathbf{1}^t}{n} \geq \mathbf{0}^t \right\}. \tag{3.5}$$

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

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

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

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

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

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

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

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

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

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

LEMMA 3.6. *Let $\mathcal{S}$ be the simplex of a graph $G = (V, E, w)$, and fix $U \subseteq V$. For any non-empty $E \subseteq U^c$,*

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

and

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

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

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

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

Lemma 3.6 gives us an alternate way to prove Lemma 3.5. For any i, taking $U = N \setminus \{i\}$ and $E = \{i\}$, it implies that $\mathcal{S}_{\{i\}^c}$ is a subset of the hyperplane

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

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

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

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

$$\mathcal{S} = \bigcap_i \mathcal{H}_i^{\geq}. \tag{3.6}$$

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 (3.5). We emphasize that a very similar discussion applies to $\mathcal{S}^+$, in which case one has

$$\mathcal{S} = \bigcap_i (\mathcal{H}_i^+)^{\geq}, \tag{3.7}$$

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

Global Connectivity Given $U \subseteq V(G)$ then *cut-set* of U is

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

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

$$w(\delta U) = \sum_{i,j \in E} w(i,j) |\chi_U(i) - \chi_U(j)| = \sum_{i,j \in E} w(i,j)(\chi_U(i) - \chi_U(j))^2 = \mathcal{L}(\chi_U).$$

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

$$\|c(\mathcal{S}_U)\|_2^2 = \frac{w(\delta U)}{|U|^2}. \tag{3.8}$$

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

$$\left\|c(\mathcal{S}_U^+)\right\|_2^2 = \frac{w(\delta^+ U)}{|U|^2}, \tag{3.9}$$

where we define $w(\delta^+ U) \stackrel{\text{def}}{=} \langle \boldsymbol{\Sigma}^+ \chi_U, \boldsymbol{\Sigma}^+ \chi_U \rangle = \langle \chi_U, \boldsymbol{L}^+ \chi_U \rangle$.

Centroid and Altitudes

Recall that the altitude between $\mathcal{S}[U]$ and $\mathcal{S}[U^c]$ of a simplex $\mathcal{S}$ 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 $\mathcal{S}_{U^c}$.

LEMMA 3.7. *Let $U\subseteq V$ be non-empty. Then the vectors $c(\mathcal{S}_U)$ and $c(\mathcal{S}_{U^c})$ are antiparallel. In particular, $(n-|U|)c_{U^c}=|U|c_U$ and*

$$\frac{c_U}{\|c_U\|_2}=-\frac{c_{U^c}}{\|c_{U^c}\|_2}.$$

Proof. This is a straightforward computation: Observing that $\chi_U=n-\chi_{U^c}$ we have

$$c_U=|U|^{-1}\boldsymbol{\Sigma}\chi_U=|U|^{-1}\boldsymbol{\Sigma}(\mathbf{1}-\chi_{U^c})=-|U|^{-1}\boldsymbol{\Sigma}\chi_{U^c}=-|U|^{-1}\frac{|U^c|}{|U^c|}\boldsymbol{\Sigma}\chi_{U^c}=\frac{n-|U|}{|U|}c_{U^c},$$

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

LEMMA 3.8. *For a simplex $\mathcal{S}$ of a graph $G=(V,E)$ and any $U\subseteq V$, $U\neq\emptyset$,*

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

and

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

Proof. We prove the first set of equalities only; the second is obtained similarly. Put $\boldsymbol{a}_U=\boldsymbol{a}(\mathcal{S}_U)$ and $c_U=c(\mathcal{S}_U)$. By definition, $\boldsymbol{a}_U$ is orthogonal to both $\mathcal{S}_U$ and $\mathcal{S}_{U^c}$. need the following claim: Any vector perpendicular to $\mathcal{S}_U$ can be written as $\boldsymbol{\Sigma}^+x_{U^c}$. Why the hell is this true? $\mathcal{S}^+x_{U^c}$ represents the simplex $\mathcal{S}^+_{U^c}$ which we know is perpendicular to $\mathcal{S}_U$. However, does it follow it is the *only* thing perpendicular to $\mathcal{S}_U$?? Since $\boldsymbol{a}_U$ begins at $\mathcal{S}_U$ and ends at $\mathcal{S}_{U^c}$ it follows that

$$\frac{\boldsymbol{a}_U}{\|\boldsymbol{a}_U\|_2}=-\frac{\boldsymbol{\Sigma}^+f_{U^c}}{\|\boldsymbol{\Sigma}^+f_{U^c}\|_2}=\frac{\boldsymbol{\Sigma}^+f_U}{\|\boldsymbol{\Sigma}^+f_U\|_2}.$$

By Lemma 3.7, taking $f_{U^c}=\chi_{U^c}/|U^c|$ and $f_U=\chi_U/|U|$ yields a solution to the above equation. We claim there are no other solutions, up to scaling. Indeed, let g_{U^c} and g_U satisfy the above, and normalize them so that $\|\boldsymbol{\Sigma}^+g_{U^c}\|_2=\|\boldsymbol{\Sigma}^+g_U\|_2=1$. Then we have $\boldsymbol{\Sigma}^+(g_U+g_{U^c})=0$ and so $g_U+g_{U^c}=k\mathbf{1}$ since $\ker(\boldsymbol{\Sigma}^+)=\mathrm{span}(\{\mathbf{1}\})$. Hence g_U and g_{U^c} are scaled versions of f_U and f_{U^c}. ⊠

LEMMA 3.9. *For any non-empty $U\subseteq V$, $\|a_U^+\|_2^2=1/w(\delta U)$ and $\|a_U\|_2^2=1/w(\delta^+U)$.*

Proof. By definition of the altitude there exists barycentric coordinates $\boldsymbol{x}_U$ and $\boldsymbol{x}_{U^c}$ such that $a^+U=\boldsymbol{\Sigma}^+(\boldsymbol{x}_U-\boldsymbol{x}_{U^c})$. Combining this representation of a_U^+ with that given by Lemma 3.8, write

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

where the final equality comes from using the definition of the centroid in the numerator, and Equation 3.8 in the denominator. Recalling the relation between $\mathbf{\Sigma}$ and $\mathbf{\Sigma}^+$ given by Equation 3.1 and that $\boldsymbol{x}_U$ and $\boldsymbol{x}_{U^c}$ are barycentric coordinates, we can rewrite the above as

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

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

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

⊠

Lemma 3.10. *The vectors* $\boldsymbol{\sigma}_i^+$ *and* $\boldsymbol{a}(\mathcal{S}_i)$ *are antiparallel.*

Proof. First, notice that $\boldsymbol{\sigma}_i^+ = \boldsymbol{\chi}_i\mathbf{\Sigma}^+ = \boldsymbol{c}(\mathcal{S}_{\{i\}}^+)$ and so

$$\left\|\boldsymbol{\sigma}_i^+\right\|_2 = \left\|\boldsymbol{c}(\mathcal{S}_{\{i\}}^+)\right\|_2 = \left\|w(\delta^+\{i\})\right\|_2 = \frac{1}{\|\boldsymbol{a}_i\|_2},$$

where the penultimate and final inequalities follow from Equation (3.9) and Lemma 3.9, respectively. Let $\boldsymbol{x} = \boldsymbol{x}_{\{i\}^c}$ be the barycentric coordinate of the face $\S_{\{i\}^c}$ such that $\boldsymbol{a}_i = \mathbf{\Sigma}(\boldsymbol{x} - \boldsymbol{\chi}_i)$. Then,

$$\begin{aligned} \left\langle \frac{\boldsymbol{\sigma}_i^+}{\|\boldsymbol{\sigma}_i\|_2}, \frac{\boldsymbol{a}_i}{\|\boldsymbol{a}_i\|_2}\right\rangle &= \frac{1}{\left\|\boldsymbol{\sigma}_i^+\right\|_2\|\boldsymbol{a}_i\|_2}\Big(\langle\boldsymbol{\sigma}_i^+, \mathbf{\Sigma}\boldsymbol{x}\rangle - \langle\boldsymbol{\sigma}_i^+, \mathbf{\Sigma}\boldsymbol{\chi}_i\rangle\Big) \\ &= \boldsymbol{\chi}_i^t(\mathbf{\Sigma}^+)^t\mathbf{\Sigma}\boldsymbol{x} - \boldsymbol{\chi}_i^t(\mathbf{\Sigma}^+)^t\mathbf{\Sigma}\boldsymbol{\chi} \\ &= \boldsymbol{\chi}_i^t(\mathbf{I} - \mathbf{J}/n)\boldsymbol{x} - \boldsymbol{\chi}_i^t(\mathbf{I} - \mathbf{J}/n)\boldsymbol{\chi}_i \\ &= -\frac{\boldsymbol{\chi}_i^t\mathbf{1}\mathbf{1}^t\boldsymbol{x}}{n} - 1 + \frac{\boldsymbol{\chi}_i^t\mathbf{1}\mathbf{1}^t\boldsymbol{\chi}_i}{n} = -1, \end{aligned}$$

since $\mathbf{1}^t\boldsymbol{x} = \mathbf{1}^t\boldsymbol{\chi}_i = 1$. ⊠

Lemma 3.11. *For any non-empty* $U \subseteq V$*,*

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

Proof. This is a consequence of identities (3.8) and (3.9) and Lemmas 3.8 and 3.9. Applying the latter and then the former, observe that

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

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

LEMMA 3.12. *Let $G = (V, E, w)$ be a weighted, undirected graph. Then*

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

Proof. For $i, j \in V$, observe that $\chi^t_{U_1} \boldsymbol{L}_e \chi_{U_2} = -w(i, j)$. Therefore,

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

which proves the first equality. The second is shown similarly by employing Lemma 3.11 and the previous identity:

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

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

Here we study the normalized simplex $\widehat{\mathcal{S}}_G$ of the graph G, a somewhat less accessible object than its unnormalized counterpart. The normalized simplex is, roughly speaking, distorted by the weights of the vertices. Consequently, many of the relationships between $\mathcal{S}_G$ and $\mathcal{S}^+_G$ are lost between $\widehat{\mathcal{S}}_G$ and $\widehat{\mathcal{S}}^+_G$. The first issue is that, in general, $\widehat{\mathcal{S}}_G$ and its inverse are not centred at the origin. Indeed, recall that the zero eigenvector $\widehat{\boldsymbol{\varphi}}_n$ of $\widehat{\boldsymbol{L}}_G$ sits in the space $\text{span}(\boldsymbol{W}_G^{1/2}\mathbf{1})$, which is distinct from $\text{span}(\mathbf{1})$ unless $\boldsymbol{W}_G^{1/2} = d\mathbf{I}$ for some d, in which case G is regular. If G is not regular, we thus have that $\boldsymbol{\varphi}_i \in \text{span}(\boldsymbol{W}_G^{1/2}\mathbf{1}) \subseteq \text{span}(\mathbf{1})^\perp$ for all $i < n$ implying that $\langle \boldsymbol{\varphi}_i, \mathbf{1}\rangle \neq 0$. In this case then,

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

The above argument proves the following.

LEMMA 3.13. *The centroid of $\widehat{\mathcal{S}}_G$ coincides with the origin of $\mathbb{R}^{n-1}$ iff G is regular.*

Given this, one might wonder whether the origin is even a point in the simplex $\widehat{\mathcal{S}}$. It is easily seen that it is, however. Consider the barycentric coordinate $\mathbf{u} = \sqrt{\boldsymbol{w}}/\left\|\sqrt{\boldsymbol{w}}\right\|_1$, where $\sqrt{\boldsymbol{w}} = (w(1)^{1/2}, \dots, w(n)^{1/2})$. 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. That is, in general $\widehat{\mathcal{S}}^+_G$ is the not the dual of $\widehat{\mathcal{S}}_G$.

LEMMA 3.14. *The inverse simplex $\widehat{\mathcal{S}}^+_G$ is the dual of $\widehat{\mathcal{S}}_G$ iff G is regular.*

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

$$\langle \widehat{\boldsymbol{\sigma}}_i^+, \widehat{\boldsymbol{\sigma}}_j - \widehat{\boldsymbol{\sigma}}_k \rangle = \delta_{ij} - \delta_{ik} + \frac{\sqrt{w(i)w(k)}}{n} - \frac{\sqrt{w(i)w(j)}}{n}. \tag{3.10}$$

First suppose that G is k-regular. Then for $i \neq k$, Equation (3.10) becomes $\langle \widehat{\boldsymbol{\sigma}}_i^+, \widehat{\boldsymbol{\sigma}}_j - \widehat{\boldsymbol{\sigma}}_k \rangle = \delta ij$. Since k was arbitrary, we see that $\{\widehat{\boldsymbol{\sigma}}_i^+\}$ is the sister pair of $\{\widehat{\boldsymbol{\sigma}}_j - \widehat{\boldsymbol{\sigma}}_k\}$. Conversely, suppose G is not regular and let i, k obey $0 \neq w(i) \neq w(k)$. Taking $i = j \neq k$ in (3.10) we see

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

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

Recall from Section 2.3 that a subset of vertices is degree homogenous if each vertex in the set has the same weight.

LEMMA 3.15. *Let $U_1, U_2 \subseteq V(G)$ be two non-empty, degree 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 perpendicular.*

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

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

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

COROLLARY 3.1. *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 3.15 $\widehat{\mathcal{S}}[\{i\}] = \widehat{\boldsymbol{\sigma}}_i$ (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 3.16 $\widehat{\boldsymbol{\sigma}}_i$ (resp., $\widehat{\boldsymbol{\sigma}}_i^+$) is not orthogonal to $\widehat{\mathcal{S}}[\{i\}^c]$ (resp., $\widehat{\mathcal{S}}^+[\{i\}^c]$). ⊠

Centroids and Altitudes. For the normalized Laplacian we have

$$\begin{aligned}
\widehat{\mathcal{L}}(\boldsymbol{\chi}_U) &= \sum_{i\sim j} w(i,j)\left(\frac{\boldsymbol{\chi}_U(i)}{\sqrt{w(i)}} - \frac{\boldsymbol{\chi}_U(j)}{\sqrt{w(j)}}\right)^2 \\
&= \sum_{i\in U, j\in U^c} w(i,j)\left(\frac{\boldsymbol{\chi}_U(i)}{\sqrt{w(i)}} - \frac{\boldsymbol{\chi}_U(j)}{\sqrt{w(j)}}\right)^2 \\
&= \sum_{i\in U, j\in U^c} w(i,j)\frac{\boldsymbol{\chi}_U(i)}{w(i)} \\
&= \sum_{i\in U} \frac{1}{w(i)} \sum_{j\in\delta(i)\cap U^c} w(i,j) \\
&= \sum_{i\in U} \frac{w_{G[i+U^c]}(i)}{w(i)}, \qquad (3.11)
\end{aligned}$$

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

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

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

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

we have

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

and so

$$\left\| c(\widehat{\mathcal{S}}_U) \right\|_2^2 = \frac{1}{|U|^2}\langle \widehat{\boldsymbol{\Sigma}}\chi_U, \widehat{\boldsymbol{\Sigma}}\chi_U\rangle = \frac{1}{|U|^2}\widehat{\mathcal{L}}(\chi_U) = \frac{1}{|U|}\gamma(U,U^c). \qquad (3.12)$$

That is, the length of the centroid $c(\widehat{\mathcal{S}}_U)$ captures the total fraction of weight between U and U^c.

The lemma equivalent to 3.6 for the normalized simplex is as follows.

Lemma 3.17. *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

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

Similarly,

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

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

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

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

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

hence

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

Consequently, $\sum_{i\in F}(\langle \boldsymbol{x}, \widehat{\boldsymbol{\sigma}}_i^+\rangle + \beta_i^{F_c}) \ge \sum_{i\in F^c}(-\beta_i^{F^c} + \beta_i^{F^c}) = 0$, 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 3.17 yields a hyperplane representation of the normalized simplex, as did 3.6 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 3.3, $\widehat{\mathcal{S}}_{\{i\}^c}$ is not contained in the hyperplane $\widehat{\mathcal{H}}_i = \{\boldsymbol{x} : \langle \boldsymbol{x}, \widehat{\boldsymbol{\sigma}}_i^+\rangle + \beta_i = 0\}$, where we take $\beta_i = \beta_i^{\{i\}^c} = \sqrt{w(i)}\max_{j\neq i}\sqrt{w(j)}/\mathrm{vol}(G)$. To see this, take any $k \notin \mathrm{argmax}_{j\neq i}\sqrt{w(j)}$ (such a k exists iff the graph is not regular) and note that while $\boldsymbol{\sigma}_k \in \widehat{\mathcal{S}}_U$ it is not in $\widehat{\mathcal{H}}_i$:

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

by assumption. The other way to see this is to note that $\widehat{\boldsymbol{\sigma}}_i^+$ is not perpendicular to $\mathcal{S}_{\{i\}^c}$ in general by Corollary 3.1.

Centred Simplex Unclear whether this notion is actually useful yet. Unclear whether the centred version is easier to study than the unormalized counterpart.

When discussing general graphs, it will be useful to study a translated copy of $\widehat{\mathcal{S}}_G$ 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 $\{\boldsymbol{\sigma}_i - \boldsymbol{c}(\mathcal{T})\}$. 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 3.2. 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 remark that a simplex and its centred version have the same dual.

OBSERVATION 3.1. *A simplex $\mathcal{T}$ and corresponding centred simplex $\mathcal{T}_0$ share the same dual, i.e., $\mathcal{S}^D = \mathcal{T}_0^D$.*

Proof. Let $\boldsymbol{\Sigma}(\mathcal{T}) = (\boldsymbol{\sigma}_i)$ and $\boldsymbol{\Sigma}(\mathcal{T}^D) = (\gamma_i)$. The vertices of the centred simplex $\mathcal{T}_0$ are $\{\boldsymbol{\sigma}_i - \boldsymbol{c}\}$ where $\boldsymbol{c} = \boldsymbol{c}(\mathcal{T})$. We have $\delta_{ij} = \langle \gamma_i, \boldsymbol{\sigma}_j - \boldsymbol{\sigma}_n\rangle = \langle \gamma_i, (\boldsymbol{\sigma}_j - \boldsymbol{c}) - (\boldsymbol{\sigma}_n - \boldsymbol{c})\rangle$, hence $\mathcal{T}^D$ is dual to $\mathcal{T}_0$. ⊠

Noting that

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

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

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

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

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

In light of Lemma 3.6, one might imagine that if given a simplex in H-description, say $\mathcal{T} = \bigcap_i\{\boldsymbol{x} : \langle \boldsymbol{z}_i, \boldsymbol{x}\rangle \geq b_i\}$ then the vectors $\boldsymbol{z}_i$ are parallel to the dual vertices of $\mathcal{T}$. Lemma 3.17, however, disconfirms this hypothesis. As is illustrated by some ugly arithmetic in Section 3.4, the dual vertices of $\widehat{\mathcal{S}}_G$ are not $\{\widehat{\boldsymbol{\sigma}}_i^+\}$, but $\widehat{\mathcal{S}}_G = \bigcap_i\{\boldsymbol{x} : \langle \boldsymbol{x}, \widehat{\boldsymbol{\sigma}}_i^+\rangle \geq \beta_i/n\}$ by Equation (**??**). It turns out the key difference is that $\mathcal{S}_G$ is centred whereas $\widehat{\mathcal{S}}_G$ is not.

LEMMA 3.18. *Let $\mathcal{T} \subseteq \mathbb{R}^{n-1}$ be a centred simplex with $\mathcal{T} = \bigcap_{i=1}^n\{\boldsymbol{x} \in \mathbb{R}^{n-1} : \langle \boldsymbol{x}, \boldsymbol{z}_i\rangle \geq \alpha_i\}$. Then $\{-\boldsymbol{z}_i/(\alpha_i n)\}$ are the vertices of $\mathcal{T}^D$.*

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

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

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

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

as was to be shown. ⊠

Lemma 3.19. *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 $\mathcal{H}_{i0}^{\geq} = \{\boldsymbol{x} : \langle \boldsymbol{x}, \boldsymbol{z}_i\rangle \geq \alpha_i - \langle \boldsymbol{c}(\mathcal{T}), \boldsymbol{z}_i\rangle\}$. ⊠

Corollary 3.2. *The dual simplex to $\widehat{\mathcal{S}}_G^+$ has vertices*

$$\left\{\frac{\widehat{\boldsymbol{\sigma}}_i^+}{\beta_i + n\langle \boldsymbol{c}(\mathcal{T}), \widehat{\boldsymbol{\sigma}}_i^+\rangle}\right\},$$

where

$$\beta_i = \left(w(i)\sum_{j\neq i} w(j)\right)^{1/2}.$$

Proof. Lemma 3.17 and Equation (**??**) tells us that $\widehat{\mathcal{S}} = \bigcap_i \mathcal{H}_i^{\geq}$ where $\mathcal{H}_i = \{\boldsymbol{x} : \langle \boldsymbol{x}, \widehat{\boldsymbol{\sigma}}_i^+\rangle \geq -\beta_i/n\}$. Lemma 3.19 then implies that

$$\widehat{\mathcal{S}}_0 = \bigcap_i \left\{\boldsymbol{x} : \langle \boldsymbol{x}, \widehat{\boldsymbol{\sigma}}_i^+\rangle \geq -\frac{\beta_i}{n} - \langle \boldsymbol{c}(\mathcal{T}), \widehat{\boldsymbol{\sigma}}_i^+\rangle\right\}.$$

Put $\kappa_i = -\beta_i/n - \langle \boldsymbol{c}(\mathcal{T}), \widehat{\boldsymbol{\sigma}}_i^+\rangle$. Lemma 3.18 then dictates that the dual vertices of $\mathcal{S}_0^D$ obey

$$\left\{\frac{\widehat{\boldsymbol{\sigma}}_i^+}{-n\cdot\kappa_i}\right\} = \left\{\frac{\widehat{\boldsymbol{\sigma}}_i^+}{\beta_i + n\langle \boldsymbol{c}(\mathcal{T}), \widehat{\boldsymbol{\sigma}}_i^+\rangle}\right\}.$$

Finally, since a centred simplex and its uncentred counterpart share the same dual simplex by Observation 3.1, the result follows. ⊠

§3.5. Construction via Extended Menger and Gramian

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

Let a centred, hyperacute simplex $\mathcal{S}^+$ be given. By Theorem 3.1 it is the inverse simplex of a graph G, whose corresponding simplex $\mathcal{S} = \mathcal{S}_G$ is dual to $\mathcal{S}^+$. Therefore, $\boldsymbol{L}_G = \boldsymbol{\Sigma}^t\boldsymbol{\Sigma}$ and $\boldsymbol{L}_G^+ = (\boldsymbol{\Sigma}^+)^t\boldsymbol{\Sigma}$ and the vertices $\boldsymbol{\sigma}_i^+$ of $\mathcal{S}^+$ can be written as $\boldsymbol{\sigma}_i^+ = (\boldsymbol{\varphi}_1(i)\lambda_1^{1/2}, \dots, \boldsymbol{\varphi}_{n-1}(i)\lambda_{n-1}^{1/2})^t$. Hence,

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

That is, the distance between the vertices of $\mathcal{S}^+$ encodes the effective resistance between nodes i and j in G. Let $\boldsymbol{D}^+$ be the distance matrix of $\mathcal{S}^+$ (thus the effective resistance matrix $\boldsymbol{R}_G$ of G).

Detour into electrical networks, not sure where this goes exactly. Observe that starting with the equation $\boldsymbol{R} = \mathbf{1}\text{diag}(\boldsymbol{L}_G^+(i,i))^t + \text{diag}(\boldsymbol{L}_G^+(i,i))\mathbf{1}^t - 2\boldsymbol{L}_G^+$, should explain where this equation comes from it follows that $\boldsymbol{x}^t\boldsymbol{R}\boldsymbol{x} = -2\boldsymbol{x}^t\boldsymbol{L}_G^+\boldsymbol{x}$ for any $\boldsymbol{x} \in \text{span}(\mathbf{1})^\perp$. Therefore,

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

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

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

Let $\overline{d}$ be the average squared distance between all the vertices of $\mathcal{S}^+$, that is

$$\overline{d} \stackrel{\text{def}}{=} \frac{1}{n^2}\sum_{i\leq j}\left\|\boldsymbol{\sigma}_i^+ - \boldsymbol{\sigma}_j^+\right\|_2^2.$$

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

$$\xi(i) \stackrel{\text{def}}{=} \frac{1}{n}\sum_j\left\|\boldsymbol{\sigma}_i^+ - \boldsymbol{\sigma}_j^+\right\|_2^2 - \overline{d},$$

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

Lemma 3.20. *Let $\mathcal{S} \subseteq \mathbb{R}^{n-1}$ be a centred hyperacute simplex with squared distance matrix $\boldsymbol{D}$, and average squared distance vector $\boldsymbol{\xi}$. Denote by $\boldsymbol{\Gamma}$ the vertex matrix of the dual simplex to $\mathcal{S}$. Then,*

$$-\frac{1}{2}\begin{pmatrix} 0 & \mathbf{1}_n^t \\ \mathbf{1}_n & \boldsymbol{D}\end{pmatrix}\begin{pmatrix} \boldsymbol{\xi}^t\boldsymbol{\Gamma}^t\boldsymbol{\Gamma}\boldsymbol{\xi} + 4\overline{d} & -(\boldsymbol{\Gamma}^t\boldsymbol{\Gamma}\boldsymbol{\xi} + 2\mathbf{1}/n)^t \\ -(\boldsymbol{\Gamma}^t\boldsymbol{\Gamma}\boldsymbol{\xi} + 2\mathbf{1}/n) & \boldsymbol{\Gamma}^t\boldsymbol{\Gamma}\end{pmatrix} = \mathbf{I}_{n+1}. \tag{3.13}$$

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

$$\mathbf{\Gamma}^t\mathbf{\Gamma}\boldsymbol{D}\mathbf{\Gamma}^t\mathbf{\Gamma} = -2\mathbf{\Gamma}^t\mathbf{\Gamma}, \tag{3.14}$$

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

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

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

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

and $\boldsymbol{\xi}$ as

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

Meanwhile, the dual simplex to $\mathcal{S}$ is the simplex of the graph G, and hence obeys $\mathbf{\Gamma}^t\mathbf{\Gamma} = \boldsymbol{L}_G$. Consequently, letting $\mathbf{u} = \frac{1}{n}\boldsymbol{R}\mathbf{1} - \frac{1}{n^2}\mathbf{J}\boldsymbol{R}\mathbf{1}$, we can rewrite Equation 3.13 as the purely graph theoretic statement

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

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

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

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

$$-\frac{1}{2}\bigg(\mathbf{1}\boldsymbol{\xi}^t\boldsymbol{L}_G\boldsymbol{\xi} + \frac{4}{n^2}R\mathbf{1} - \boldsymbol{R}\boldsymbol{L}_G\boldsymbol{\xi} - \frac{2}{n}\boldsymbol{R}\mathbf{1}\bigg), \tag{3.15}$$

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

$$\boldsymbol{R}\boldsymbol{L}_G = \mathbf{1}\boldsymbol{\xi}^t\boldsymbol{L}_G - 2\bigg(\mathbf{I} - \frac{1}{n}\mathbf{J}\bigg). \tag{3.16}$$

Equation (3.15) thus becomes

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

using that $\mathbf{J}^2 = n\mathbf{J}$, $R = \frac{1}{2}\mathbf{1}^t\boldsymbol{R}\mathbf{1}$, and $\mathbf{J}\boldsymbol{R}\mathbf{1} = \mathbf{1}(\mathbf{1}^t\boldsymbol{R}\mathbf{1}) = \mathbf{1}R$. Finally, again using (3.16), the bottom right-hand side is

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

This demonstrates that (3.15) holds. We now show that $\boldsymbol{L}_G\boldsymbol{R}\boldsymbol{L}_G = -2\boldsymbol{L}_G$ and that $\boldsymbol{R}\boldsymbol{L}_G\boldsymbol{R}\boldsymbol{x} = -2\boldsymbol{R}\boldsymbol{x}$ for all $\boldsymbol{x} \in \operatorname{span}(\mathbf{1})^\perp$, which will complete the proof. Applying Equation (3.16) we have

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

In the same way as (3.16) was derived, we see that

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

and so

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

as desired. ⊠

Putting aside simplex geometry for the moment, it is worth meditating on the significance of Equation (3.13) as applied to electrical networks. As demonstrated in [VMDC17], the result translates into the matrix equation

$$-\frac{1}{2}\begin{pmatrix} 0 & \mathbf{1}^t \\ \mathbf{1} & \boldsymbol{R} \end{pmatrix} = \begin{pmatrix} \operatorname{diag}(\boldsymbol{L}_G^+(i,i))^t\boldsymbol{L}_G\operatorname{diag}(\boldsymbol{L}_G^+(i,i)) + 4R_G/n^2 & -(\boldsymbol{L}_G\operatorname{diag}(\boldsymbol{L}_G^+(i,i)) + \frac{2}{n}\mathbf{1})^t \\ -(\boldsymbol{L}_G\operatorname{diag}(\boldsymbol{L}_G^+(i,i)) + \frac{2}{n}\mathbf{1}) & \boldsymbol{L}_G \end{pmatrix}^{-1}. \tag{3.17}$$

Let $\boldsymbol{D}$ be the distance matrix of a set X of d points. The matrix

$$\begin{pmatrix} 0 & \mathbf{1}^t \\ \mathbf{1} & \boldsymbol{D} \end{pmatrix} \in \mathbb{R}^{(d+1)\times(d+1)}, \tag{3.18}$$

is called the *Menger matrix of X*.

A variant of the following result was proved by Fiedler [Fie11].

Lemma 3.21. *For a weighted and connected tree $T = (V, E, w)$ on n vertices let the matrix $\boldsymbol{S}_T$ describe the inverse distances between vertices, i.e., for $(i,j) \in E$, $\boldsymbol{S}_T(i,j) = 1/w(i,j)$ and for $(i,j) \notin E$, $\boldsymbol{S}_T(i,j) = \sum_{\ell=1}^{k-1} 1/w(v_\ell, v_{\ell+1})$ where $i = v_1, v_2, \ldots, v_k = j$ is the unique path between i and j. Then,*

$$-\frac{1}{2}\begin{pmatrix} 0 & \mathbf{1}^t \\ \mathbf{1} & \boldsymbol{S}_T \end{pmatrix}\begin{pmatrix} \sum_{i\sim j} 1/w(i,j) & (\boldsymbol{d} - 2\mathbf{1})^t \\ \boldsymbol{d} - 2\mathbf{1} & \boldsymbol{L}_T \end{pmatrix} = \mathbf{I}. \tag{3.19}$$

Proof. We begin by computing the left hand side of the matrix equation. Note that for connected trees on n nodes, there are precisely $n-1$ edges. Therefore, $\mathbf{1}^t\boldsymbol{d} - 2n = \sum_i \deg(i) -$

$2n = 2|E| - 2n = -2$, by the handshaking lemma. Since $\mathbf{1}^t \boldsymbol{L}_T = \mathbf{0}$, it follows that the top row of the resulting matrix is as desired. Next, let us consider the term

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

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

$$\sum_{i\sim j} \frac{1}{w(i,j)} + \sum_{\ell\in[n]} \boldsymbol{S}_T(k,\ell)(\deg(\ell) - 2). \tag{3.20}$$

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 (3.20) is indeed 0. Finally, we consider the term $\mathbf{1}^t\boldsymbol{d} - 2\mathbf{1}\mathbf{1}^t + \boldsymbol{S}_T\boldsymbol{L}_T$, which we need to show is $-2I$. Let us expand the (k,ℓ)-th component of this matrix:

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

For $k = \ell$, we have $\boldsymbol{S}_T(k,\ell) = 0$ and $\boldsymbol{S}_T(k,i) = \boldsymbol{S}_T(\ell,i) = 1/w(i,\ell)$. It follows that the above sum is -2, as desired. Now consider $k \neq \ell$. Fix $i \in \delta(\ell)$ and let $P = (k = v_1, \dots, v_r = \ell)$ be the unique path between k and ℓ. First, suppose that $i \in P$ so that $i = v_{r-1}$. Then $\boldsymbol{S}_T(k, ell) - \boldsymbol{S}_T(k,i) = \sum_{s=1}^{r-1} 1/w(v_s, v_{s+1}) - \sum_{s=1}^{r-2} 1/w(v_s, v_{s+1}) = 1/w(v_{r-1}, v_r) = 1/w(i,\ell)$. Otherwise, if $i \in P$ then the unique path between i and k in T is $P \cup \{\ell\} = (v_1, \ldots, v_r, i)$. 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. ⊠

Corollary 3.3. *Let T be a weighted and connected tree. Then*

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

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

Proof. Let $\boldsymbol{S}_T$ be as it was in Lemma 3.21. 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 $i = v_1, \ldots, v_r = j$ 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 (3.19) and (3.17) yields

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

from which the claim follows. ⊠

Lemma 3.22 ([Men31]). *Let $\boldsymbol{D}$ be the distance matrix of a set X of d points. The $d-1$ dimensional volume of the convex hull of X is proportional to the root of the determinant of the Menger matrix:*

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

Sharpe [Sha67] said something about something which should probably be cited, but not exactly sure what it is yet.

Using this and a previous calculated formula for the entries of the pseudoinverse yields

$$\begin{aligned}
\boldsymbol{L}_H^+(i,j) &= \frac{1}{2}\left(\sum_k r_H^{\text{eff}}(i,k) + \sum_k r_H^{\text{eff}}(j,k)\right) - \frac{1}{2} r_H^{\text{eff}}(i,j) - \frac{R_H}{n^2}, \\
&= \frac{1}{2}\sum_k (w_G(i) + w_G(j) + 2w_G(k) + 2w_G(i,k) + 2w_G(j,k)) - \frac{1}{2} w_G(i,j) - \frac{R_H}{n^2} \\
&= \left(\frac{n}{2} + 1\right)(w_G(i) + w_G(j)) - \frac{1}{2} w_G(i,j) + \left(2 - \frac{2}{n} - \frac{2}{n^2}\right) W_G.
\end{aligned}$$

§3.6. Inequalities

The conductance of a graph G is

$$\theta(S) \stackrel{\text{def}}{=} \frac{|\delta(S)|}{|S|}.$$

We have the following inequality:

$$\theta(S) \geq \lambda_2\left(1 - \frac{|S|}{|V|}\right) \geq \frac{\lambda_2}{2},$$

which yields

$$\|\mathbf{\Sigma}\chi S\|_2^2 \geq \frac{|S|}{2}\lambda_{n-1}.$$

We can relate the eigenvalues of G to the geometry of $\mathcal{S}$ via the relation $\mathbf{\Sigma}\mathbf{\Sigma}^t = \mathbf{\Lambda}$. Hence

$$\|\mathbf{\Sigma}\chi_S\|_2^2 \geq \frac{|S|}{2}\mathbf{\Sigma}\mathbf{\Sigma}^t(n-1, n-1) \geq \frac{|S|}{2}\min_i\{(\mathbf{\Sigma}\mathbf{\Sigma}^t)(i,i) : (\mathbf{\Sigma}\mathbf{\Sigma}^t)(i,i) \neq 0\} = \frac{|S|}{2}\min_{i=1}^{n-1}\|\Pi_i(\mathbf{\Sigma})\|_2^2.$$

Lemma 3.23. *If $\boldsymbol{p}$ is any vector pointing from $\mathcal{S}_U$ to $\mathcal{S}_{U^c}$ which has a non-empty intersection with both faces, then $\|\boldsymbol{p}\|_2 \geq \|\boldsymbol{a}(\mathcal{S}_U)\|_2$.*

Proof. Geometry. Work this out. ☒

The following lemma is due to Devriendt and Van Mieghem [DVM18].

Lemma 3.24. *For any f with $\langle f, \mathbf{1}\rangle = 0$,*

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

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

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

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

where the last inequality follows since f is orthogonal to $\mathbf{1}$ by assumption. Using the pseudoinverse relation (3.1), we can continue as

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

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

We obtain several inequalities for the simplex via immediate application of inequalities from the literature on electrical networks.

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

Lemma 3.25. *Let $G = (V, E, w)$ be a weighted graph and let $U \subseteq V$ obey* $\mathrm{vol}(U) < \mathrm{vol}(V)/2$ *and*

$$\theta(U) \geq \frac{\alpha}{\mathrm{vol}(U)^{1/2-\epsilon}}.$$

TODO finish this/decide whether this is worth including.

§3.7. Quadrics

Circumscribed ellipsoid for normalized Laplacian is not necessarily the sphere – could be deformed. **TODO** Read more about quadrics in general but filling this out. Might be more we can say. Also look into any algorithmic work done on quadrics. Does this relationship help us answer anything interesting? Fiedler derivation: [Fie05]. More Fiedler geometry: [Fie93]. A *quadric* in $\mathbb{C}^d$ is a hypersurface of dimension $d-1$ of the form

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

Definition 3.3. The *Steiner Circumscribed Ellipsoid*, or simply the *Steiner Ellipsoid* of a simplex $\mathcal{S}$ with vertices $\{\boldsymbol{\sigma}_i\}$ is a quadric which contains the vertices and whose tangent plane at $\boldsymbol{\sigma}_i$ is parallel to the affine plane spanned by $\{\boldsymbol{\sigma}_j\}_{j\neq i}$.

Theorem 3.2. *The Steiner ellipsoid of a simplex $\mathcal{S}$ is unique and moreover, is the ellipsoid with minimum volume which contains $\mathcal{S}$.*

Owing to its uniqueness, we denote the Steiner ellipsoid of the simplex $\mathcal{S}$ by $\mathcal{E}(\mathcal{S})$. The following lemma gives an explicit representation of $\mathcal{E}(\mathcal{S})$.

Lemma 3.26 ([Fie05]). *The Steiner circumscribed Ellipsoid of $\mathcal{S} = \mathcal{S}(G)$ satisfies*

$$\mathcal{E}(\mathcal{S}) = \left\{\boldsymbol{x} : \boldsymbol{x}^t \boldsymbol{\Sigma}^+ (\boldsymbol{\Sigma}^+)^t \boldsymbol{x} - \frac{n-1}{n} = 0\right\}. \tag{3.21}$$

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

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

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

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

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

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

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

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

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

Perhaps a more insightful representation of $\mathcal{E}(\mathcal{S})$ comes from appealing to Equation (3.3), i.e., $\boldsymbol{\Sigma}\boldsymbol{\Sigma}^t = \boldsymbol{\Lambda}^{-1/2}$. Hence, by (3.21),

$$\mathcal{E}(\mathcal{S}) = \left\{\boldsymbol{x} : \boldsymbol{x}^t\boldsymbol{\Lambda}^{-1}\boldsymbol{x} = \frac{n-1}{n}\right\}. \tag{3.22}$$

On the other hand, it's easy to see that the Steiner ellipsoid of the normalized simplex, $\mathcal{E}(\widehat{\mathcal{S}})$ is simply the unit sphere, i.e., $\mathcal{E}(\widehat{\mathcal{S}}) = \{\boldsymbol{x} : \boldsymbol{x}^t\boldsymbol{x} = 1\}$, since $\|\widehat{\boldsymbol{\sigma}}_i\|_2^2 = 1$. Is this enough to justify it? Therefore, we see that the circumscribed sphere and the circumscribed ellipsoid of the normalized simplex are one and the same.

For the combinatorial simplex, however, it's not even clear whether the circumscribed sphere exists Unless it exists for all simplices?. Demonstrating that it does in fact exist is the purpose of the following lemma.

I think this should hold for more than simply hyperacute simplices, but need to generalize the Menger matrix stuff in order for the result to go through.

LEMMA 3.27. *Let $\mathcal{S}^+ \subseteq \mathbb{R}^{n-1}$ be a hyperacute simplex. The circumscribed sphere of $\mathcal{S}^+$ exists and is given by the set of points $\{\boldsymbol{x} : \boldsymbol{x} = \boldsymbol{\Sigma}\boldsymbol{\alpha},\ \langle\boldsymbol{\alpha}, \mathbf{1}\rangle = 1,\ \langle\boldsymbol{\alpha}, \boldsymbol{D}\boldsymbol{\alpha}\rangle = 0\}$, which is a sphere centred at the point $\frac{1}{2}\boldsymbol{\Sigma}(\boldsymbol{L}_G\boldsymbol{\xi} + \mathbf{1}/n)$ with radius $\frac{1}{2}\sqrt{\boldsymbol{\xi}^t\boldsymbol{L}_G\boldsymbol{\xi} + 4R_G/n^2}$.*

Proof. Set $\boldsymbol{\zeta} = \frac{1}{2}(\boldsymbol{L}_G\boldsymbol{\xi} + \mathbf{1}/n)$ and $r = \boldsymbol{\xi}^t\boldsymbol{L}_G\boldsymbol{\xi} + 4R_G/n^2$. Let us expand $\boldsymbol{x}$ in barycentric coordinates in accordance with Lemma 2.7. 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

$$\|\boldsymbol{x} - \boldsymbol{\Sigma}\boldsymbol{\zeta}\|_2^2 = \frac{1}{4}r, \tag{3.23}$$

and that this equation is equivalent to $\boldsymbol{\alpha}^t\boldsymbol{D}\boldsymbol{\alpha} = 0$. Note first that due to Equation 3.17, $\langle\mathbf{1}, -2\boldsymbol{\zeta}\rangle = \langle\mathbf{1}, -\boldsymbol{L}_G\boldsymbol{\xi} - \frac{2}{n}\mathbf{1}\rangle = -2$, so $\boldsymbol{\zeta} = (\zeta_1, \dots, \zeta_{n-1})$ obeys $\sum_i \zeta_i = 1$. The left hand side of (3.23) 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

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

$$= -\frac{1}{2}\sum_{i,j}(\alpha_i - \zeta_i)(\alpha_j - \zeta_j)\|\boldsymbol{\sigma}_i - \boldsymbol{\sigma}_j\|_2^2. \tag{3.24}$$

Recalling the block matrix equation (3.17) for hyperacute simplices, for all i we have $\mathbf{1}(\boldsymbol{\xi}^t \boldsymbol{L}_G\boldsymbol{\xi} + 4R_G/n^2) - \boldsymbol{D}(\boldsymbol{L}_G\boldsymbol{\xi} + 2\mathbf{1}/n) = \mathbf{0}$, i.e., $r\mathbf{1} - 2\boldsymbol{D} = \mathbf{0}$. Hence

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

Using this, we rewrite the summation in on the right hand side of (3.24) as

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

The equation of the sphere in (3.23) 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 $\boldsymbol{\chi}_\ell^t\boldsymbol{D}\boldsymbol{\chi}_\ell = \sum_{i,j}\boldsymbol{\chi}_\ell(i)\boldsymbol{D}(i,j)\boldsymbol{\chi}_\ell(j) = \boldsymbol{D}(\ell,\ell) = 0$. ⊠

§3.8. Random Walks

Very unclear if there's anything interesting here. Mostly just contains Karel's thought on rws at the moment. Think about:

(1) can we generate a theory/answer questions regarding random walks in simplices using our knowledge of rws in graphs.

(2)Straight lines are geodesics. If in the simplex the path created by a random walk is a straight line, is this telling us the random walk is as "efficient" as possible? Whereas those with curved lines are inefficient? Unclear how to formalized this /where to take it. After thinking about this a bit, probably not: It just says that the eigenvalues corresponding to the vertices which contribute to the starting position are equal.

3.8.1. Discrete Time Random Walks

In a *discrete time random walk (DSRW)* we envision a walker who jumps from vertex i to vertex j with probability proportional to $w(i,j)$. To this end, one defines the transition matrix

$$\boldsymbol{T}(i,j) = \frac{w(i,j)}{w(i)} = \frac{\boldsymbol{A}_G(i,j)}{\sum_{k\in\delta(i)}\boldsymbol{A}_G(i,k)}.$$

It's clear that $\sum_i \boldsymbol{T}(i,j) = 1$. The probability that the walker is at node i at time t is the probability that that she was at node j at time $t-1$ and transitioned to node i. Thus,

$$\pi_i(t) = \sum_j \pi_j(t-1)\boldsymbol{T}(i,j),$$

or, more succinctly,

$$\boldsymbol{\pi}(t) = \boldsymbol{T}\boldsymbol{\pi}(t-1).$$

The stationary distribution $\boldsymbol{\pi}(\infty) \stackrel{\text{def}}{=} \lim_t \boldsymbol{\pi}(t)$ satisfies $\boldsymbol{\pi}(\infty) = \boldsymbol{T}\boldsymbol{\pi}(\infty)$, which yields that The stationary distribution of such a walk is given by

$$\pi_i = \frac{\sum_{j\in\delta(i)} w(i,j)}{\sum_{j,k\in V} w(i,j)},$$

which, for an undirected and unweighted graph simplifies to $\pi_i = \deg(i)/2|E|$.

3.8.2. Continuous Time Random Walks

A *Continuous Time Random Walk* [MPL17] satisfies the equation

$$\frac{d\boldsymbol{\pi}(t)}{dt} = -\boldsymbol{\pi}(t)^t \boldsymbol{W}^{-1}\boldsymbol{L}, \tag{3.25}$$

hence

$$\boldsymbol{\pi}(t)^t = \boldsymbol{\pi}(0)^t \exp\bigl(-\boldsymbol{W}^{-1}\boldsymbol{L}t\bigr).$$

After converging to the stationary distribution there is, by definition, no change in the distribution. Therefore, $d\boldsymbol{\pi}(t)/dt = 0$ and Equation (3.25) reduces to $-\boldsymbol{\pi}(t)\boldsymbol{W}^{-1}\boldsymbol{L} = \boldsymbol{0}$. Therefore, $\boldsymbol{\pi}(t)\boldsymbol{W}^{-1}$ is a left eigenfunction of $\boldsymbol{L}$ or equivalently, $\boldsymbol{W}^{-1}\boldsymbol{\pi}$ is a right eigenfunction with corresponding eigenvalue zero. Hence, $\boldsymbol{W}^{-1}\boldsymbol{\pi} \in \operatorname{span}\{\boldsymbol{1}\}$, i.e., $\boldsymbol{\pi} \in \operatorname{span}\{\boldsymbol{w}\}$. Since $\|\boldsymbol{\pi}(\infty)\|_1 = 1$, we see that

$$\boldsymbol{\pi}(\infty) = \frac{\boldsymbol{w}}{\|\boldsymbol{w}\|_1}.$$

In particular, the CTRW shares the same stationary distribution as the DTRW.

3.8.3. mixing time

The distribution $\boldsymbol{\pi} = (\pi_1, \ldots, \pi_n)$ corresponds to a point in the simplex, namely $\boldsymbol{p}_\pi = \S\boldsymbol{\pi}$. It is thus natural to wonder whether this point tells us anything interesting about the dynamics of the walk.

The *variation distance* between two distributions p_1 and p_2 with finite state space S is given by

$$\|p_1 - p_2\|_V = \frac{1}{2}\sum_{s\in S} |p_1(s) - p_2(s)|.$$

Mixing Time. Let $\boldsymbol{p}_i^t$ be the distribution over the set of vertices V at time t obtained by beginning the random walk at vertex i. Define

$$\Delta(t) = \max_{i \in V} \left\| \boldsymbol{p}_i^t - \boldsymbol{\pi} \right\|_V,$$

where $\|\cdot\|_V$ is the variation distance. Given $\epsilon > 0$ set

$$\tau(\epsilon) = \min\{t : \Delta(t) \leq \epsilon\}.$$

We have

Chapter 4

Algorithmics

This final 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, 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[1] to $\mathcal{S}_G$.) With respect to algorithmic consequences on the other hand, we will attempt to leverage knowledge we have in the hitherto relatively unrelated areas of computational graph theory and high-dimensional computational geometry to draw new conclusions about the complexity of several problems in these areas. For instance, if a graph theoretic problem has an analogue in the simplex, any fact regarding the problems difficulty—whether it's NP-complete, say—translates to an immediate result about its geometric counterpart. In particular, since the simplex of a graph can be generate in polynomial time given the graph (due to the fact that an eigendecomposition can be computed in polynomial time) and vice versa, problems which are solvable in polynomial in either the simplex or graph domain translate to polynomial (yet perhaps not optimal!) problems in the other domain and likewise, problems which are NP-hard in one domain have analogues which are NP-hard in the other.

For the benefit 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.

§4.1. Preliminaries

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

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

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

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.

Some background on computational models and reductions will also be useful. **TODO**

§4.2. Computational Complexity

In this section we investigate the relationships between problems in one domain—either the graph-theoretic or geometric domain—and their analogues in the other. The following result exemplifies the power of the graph-simplex correspondence in yielding results which seem otherwise to be difficult to obtain (certainly more difficult than the following proof, at any rate). First we generalize the no The following result was first stated by Devriendt and Van Mieghem [DVM18], although it was stated only for inverse simplices of graphs. We observe that it can be generalized as follows.

Lemma 4.1. *Computing the altitude of minimum length in a convex polytope is NP-hard.*

Proof. The relationship $\left\|\boldsymbol{a}(\mathcal{S}_U^+)\right\|_2^2 = w(\delta U)^{-1}$ (Lemma 3.11) for the inverse simplex of a graph G demonstrates that the problem of computing a minimum length altitude in any hyperacute simplex is NP-hard, because computing the maximum weight cut in any weighted graph is NP-hard [Kar72]. Since the class of convex polytopes contains the class of hyperacute simplices, the result follows. ⊠

Remark 4.1. In the above statement and its proof, the description of the polytope and simplex was not specified. This is due to the fact that—as discussed above—for simplices there is a polynomial time algorithm to translate betweent the various descriptions. With regard to NP-completeness therefore, the description makes no difference.

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

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

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

and so

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

where the second and fourth inequalities follows from the fact that I is an independent set. Now, suppose we assign each vertex i a weight $f(i) \geq 0$. The Max-Weight Independent-Set problem consists of maximizing $f(I) \overset{\text{def}}{=} \sum_{i\in I} f(i)$ 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 problems tractability.

Lemma 4.2. Vertex-Weighted Independent-Set *is NP-Complete.*

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

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

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

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

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

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

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

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

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

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

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

Lemma 4.3. *Let $\mathcal{P}$ be a convex polytope with vertex set V. The optimization problem*

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

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

Proof. Let $\mathcal{P}$ be the combinatorial simplex of a graph G. Using that $\langle \boldsymbol{\sigma}_i, \boldsymbol{\sigma}_j\rangle = w(i,j)$, the condition that $\langle \boldsymbol{\sigma}_i, \boldsymbol{\sigma}_j\rangle = 0$ for all $i, j \in I$ translates to $(i,j) \in E(G)$ for all $i, j \in I$. Moreover, Equation (3.8) in Section 3.3 gives us

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

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

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

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

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

Lemma 4.4. *Let $\mathcal{P}$ be a convex polytope with vertex set V. The optimization problem*

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

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

Proof. The proof is similar to the previous lemma. For $\mathcal{P}$ the normalized simplex of a graph G, the condition $\langle \boldsymbol{\sigma}_i, \boldsymbol{\sigma}_j \rangle = 0$ once again implies that I must be an independent set. Notice that for such an I, if $i \in I$ then $\delta(i) \cap I^c = \delta(i)$ (none of i's neighbours are in I). Therefore, Equation (3.11) yields

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

Equation (3.12) then implies that

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

so the optimization problem can be formulated as

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

which is the Independent-Set problem. ⊠

Need to say more about this

Theorem 4.1. *Deciding whether two polytopes are isomorphic is Graph-Isomorphism-Hard. Moreover, subpolytope isomorphism is NP-hard.*

Proof. Let two graphs G_1 and G_2 be given. Compute their corresponding inverse simplices $\mathcal{S}_1^+$ and $\mathcal{S}_2^+$. If $\mathcal{S}_1^+ \cong \mathcal{S}_2+$, then there exists a (linear) mapping $\boldsymbol{T}$ between the vertices such that $\boldsymbol{T}\boldsymbol{\sigma}_1^+ = \boldsymbol{\sigma}_2^+$ for all $\boldsymbol{\sigma}_1^+ \in \boldsymbol{\Sigma}(\mathcal{S}_1^+)$ and $\boldsymbol{\sigma}_2^+ \in \boldsymbol{\Sigma}(\mathcal{S}_2^+)$. In this case, the matrix obtained by the dot products of the vectors $\boldsymbol{T}\boldsymbol{\Sigma}(\mathcal{S}_1^+)$ yields $\boldsymbol{L}_{G_1}$, implying that $G_1 \cong G_2$. ⊠

The first result was also proved in [KS08].

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

In this section we investigate the computational aspects of transitioning between various simplices and between the graph and its simplices. We are interested in obtaining computational results which are strictly sub-cubic in time, i.e., $o(n^3)$ because in cubic time one can solve linear systems and compute eigendecompositions.

We 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[2] of $2^{-\epsilon}$, while there exists algorithms

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

Figure 4.1: Summary of results for precise mappings. A slash refers to a difference in runtimes when the graph is available versus when it isn't. The quantity before the slash indicates the runtime *without* the graph, after the slash the runtime *with* the graph. A question mark indicates that the runtime isn't known.

which run in time $O(n^3 + n \log^2 \log \epsilon)$ [PC99]. We let $L(n)$ denote the runtime of Laplacian Eigendecomposion, and we assume that $L(n) = \omega(n^2)$. This must be the case.

fix this section Thus, for instance, given G it is trivial to compute all of $\mathcal{S}_G, \mathcal{S}_G^+, \widehat{\mathcal{S}}_G$, and $\widehat{\mathcal{S}}_G^+$ by finding the eigendecomposition of $\boldsymbol{L}_G$ from which we can construct the relevant vertex set. Moreover, starting with a simplex with vertex set $\boldsymbol{\Sigma}$, one can compute $\boldsymbol{\Sigma}^t\boldsymbol{\Sigma}$ in cubic time. If the simplex is the simplex if a graph then this yields the Laplacian (or the pseudoinverse of the Laplacian) of the graph, which as above allows us to compute any of the simplices. In what follows therefore, we attempt to beat the barrier of $O(n^3)$.

A question which is raised by the above discussion is one of certifying whether a given simplex $\mathcal{T}$ is the combinatorial, normalized, or one of their duals of some graph G. Again, in cubic time we can compute $\boldsymbol{\Sigma}^t\boldsymbol{\Sigma}$ and thus decide whether $\boldsymbol{\Sigma}^t\boldsymbol{\Sigma}$ is equal to $\boldsymbol{L}_G$ for some graph G. In quadratic 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. Beyond computing $\boldsymbol{\Sigma}(\mathcal{T})^t\boldsymbol{\Sigma}(\mathcal{T})$ however, it's not clear how to obtain the original graph or the combinatorial simplex.

4.3.1. Precise Mappings

We begin by exploring the complexity of transitioning between the different objects *precisely*—e.g., given G compute its precise combinatorial simplex. The subsequent section will explore various approximations.

The results obtained in this section are summarized in Figure

Between $\mathcal{S}$ and $\widehat{\mathcal{S}}$. Let us consider the computational complexity of transitioning between $\mathcal{S}$ and $\widehat{\mathcal{S}}$ and vice versa. Let ϕ_{ij} (resp., $\widehat{\phi}_{ij}$) be the angle between $\boldsymbol{\sigma}_i$ and $\boldsymbol{\sigma}_j$ (resp., $\widehat{\boldsymbol{\sigma}}_i$ and $\widehat{\boldsymbol{\sigma}}_j$). Using the typical formula for the dot product in Euclidean space we have

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

using that $\|\widehat{\boldsymbol{\sigma}}_i\|_2 = 1$ for all i. That is, the angles between vertices in $\mathcal{S}$ in $\widehat{\mathcal{S}}$ are the same. Suppose we are given the simplex $\mathcal{S}$ and told it is the combinatorial simplex of a graph. For each $\boldsymbol{\sigma}_i = \boldsymbol{\Sigma}(\mathcal{S})$, define a new vertex

$$\boldsymbol{\gamma}_i = \frac{\boldsymbol{\sigma}_i}{\|\boldsymbol{\sigma}_i\|_2}.$$

Is it evident that the angle between $\boldsymbol{\gamma}_i$ and $\boldsymbol{\gamma}_j$ is identical to that between $\boldsymbol{\sigma}_i$ and $\boldsymbol{\sigma}_j$:

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

Therefore, it follows that the simplex with vertices is congruent to $\widehat{\mathcal{S}}$. This yields the following result.

Lemma 4.5. *Given a combinatorial simplex $\mathcal{S}$, a simplex congruent to $\widehat{\mathcal{S}}$ can be computed in time $O(n^2)$.*

Proof. Given $\mathcal{S}$, define the vertices $\boldsymbol{\gamma}_i$ as above. Computing $\|\boldsymbol{\sigma}_i\|_2$ takes time $O(n)$ and must be done for each vertex. ⊠

Given the relative ease with which we can transition from $\mathcal{S}$ to $\widehat{\mathcal{S}}$, it is somewhat surprising that it is much more difficult to transition from $\widehat{\mathcal{S}}$ to $\mathcal{S}$, especially if the underlying graph G is not given. The obvious tactic is, given the vertices $\{\widehat{\boldsymbol{\sigma}}_i\}$, to define vertices $\widehat{\boldsymbol{\sigma}}_i\sqrt{w(i)}$, which, since $\sqrt{w(i)} = \|\boldsymbol{\sigma}_i\|_2$, have the same magnitude as $\boldsymbol{\sigma}_i$. As above, the scaling does not affect the angle between the vertices, and thus the simplex with these vertices is congruent to $\mathcal{S}$. However, it's not clear how to obtain the value $\sqrt{w(i)}$ from $\widehat{\mathcal{S}}$. Using that $\langle \widehat{\boldsymbol{\sigma}}_i, \widehat{\boldsymbol{\sigma}}_j\rangle = (w(i)w(j))^{-1/2}$ we can write

$$w(i)^{1/2} = -\sum_{j\neq i} w(j)^{-1/2} \Big/ \sum_{j\neq i}\langle \widehat{\boldsymbol{\sigma}}_i, \widehat{\boldsymbol{\sigma}}_j\rangle,$$

which yields a non-linear system of equations.

Of course, if we are given the graph then we have access to $\sqrt{w(i)}$ and can compute $\widehat{\boldsymbol{\sigma}}_i w(i)^{1/2}$ in time $O(n)$. The following result is then immediate.

Lemma 4.6. *Given a graph $G = (V, E, w)$ and its normalized simplex $\widehat{\mathcal{S}}_G$, a simplex congruent to the combinatorial simplex $\mathcal{S}_G$ can be computed in $O(n^2)$ time.*

Think about possible lower bounds on computing $\mathcal{S}$ from $\widehat{\mathcal{S}}$ when no graph is given. Doing so would imply knowledge of $\sqrt{\boldsymbol{w}}$ (taking ratio of lengths of vertices). What does this imply? Does knowledge of $\boldsymbol{w}$ give us some knowledge of the graph structure from which we can extract a lower bound?

$\mathcal{S}$ and $\mathcal{S}^+$. Let us suppose that we can generate $\mathcal{S}^+$ from $\mathcal{S}$ (or vice versa) in time $O(g(n))$. Note that for $i < n$,

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

hence knowledge of $\{\boldsymbol{\sigma}_i\}$ and $\{\boldsymbol{\sigma}_i^+\}$ yields knowledge of the eigendecomposition of the underlying graph G in $O(n^2)$ time ($O(n)$ to determine all the eigenvalues and $O(n^2)$ to determine the eigenvectors). The same argument holds *mutatis mutandis* for the normalized Laplacian.

Lemma 4.7. *If a* V*-description of* $\mathcal{S}^+$ *(resp.,* $\widehat{\mathcal{S}}^+$*) can be generated from a* V*-description of* $\mathcal{S}$ *(resp.,* $\widehat{\mathcal{S}}$*) or vice versa in time* $O(g(n))$*, then* Laplacian Eigendecomposion *can be solved in time* $O(g(n)+n^2)$ *for arbitrary weighted graphs. Consequently* $g(n) = \Omega(n^\omega)$*.*

An alternate way of seeing that constructing the inverse simplex from its dual is computationally challenging is to recall from Section 3.3 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 3.6) and that that $\boldsymbol{\sigma}_i^+$ is perpendicular to $\mathcal{S}_{\{i\}^c}$ (Lemma 3.4). Hence, computing the inverse simplex would imply that we had computed normal vectors to n hyperplanes, the typical procedure for which typically involves computing an $n \times n$ determinant and requires $O(n^3)$ time.

We now consider transitioning between different descriptions of $\mathcal{S}$ and $\mathcal{S}^+$. Let us recall that the H-description of $\mathcal{S}$ and $\mathcal{S}^+$ yield immediate insight into the vertices of its inverse as $\mathcal{S} = \cap_i\{\boldsymbol{x} : \langle \boldsymbol{x}, \boldsymbol{\sigma}_i^+\rangle \geq -1/n\}$ and $\mathcal{S}^+ = \cap_i\{\boldsymbol{x} : \langle \boldsymbol{x}, \boldsymbol{\sigma}_i\rangle \geq -1/n\}$ (Equations (3.6) and (3.7)). Consequently, given given a H-description of one of these simplices, the vertices of its inverse are recoverable in quadratic time. This yields the following result.

Lemma 4.8. *Suppose we can compute an* H*-description of* $\mathcal{S}$ *(resp.,* $\mathcal{S}^+$*))given its* V*-description in time* $t(n)$*. Then a* V*-description of* $\mathcal{S}^+$ *(resp.,* $\mathcal{S}$*) is recoverable in time* $t(n) + O(n^2)$*, implying by Lemma 4.7 that* $t(n) = \Omega(n^\omega)$*.*

We also note that a consequence of the relationship between the vertices of $\mathcal{S}$ and the H-description of $\mathcal{S}^+$ that given V-description of $\mathcal{S}$ or $\mathcal{S}^+$, we have immediate access to the H-description of its inverse.

Between G and $\mathcal{S}$ or $\widehat{\mathcal{S}}$. Similar kinds of results hold in these cases. Assume that we obtain the simplex $\mathcal{S}_G$ from G. Notice that

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

so

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

which can be computed in $O(n)$ time. Then, as above, knowledge of the eigenvalues furnishes knowledge of the eigenvectors in $O(n^2)$ time. Running almost identical arguments for $\mathcal{S}^+$, $\widehat{\mathcal{S}}$, or $\widehat{\mathcal{S}}^+$ yields an almost equivalent result as in the previous section.

Lemma 4.9. *If either the combinatorial or normalized simplex or their inverses can be generated from a graph G in $O(g(n))$ time, then* Laplacian Eigendecomposion *can be solved in time $O(g(n)+n^2)$ for arbitrary weighted graphs. Consequently $g(n)=\Omega(n^\omega)$.*

The information encoded in the dot products between vertices allow us to make queries regarding the edge weights, but each query takes $O(n)$ time since we must compute a dot product between two vectors of length $n-1$. Hence, re-constructing the graph or its Laplacian takes $O(n^3)$ if we wish do it precisely.

Let us now consider transitioning between G and the H-description of a simplex. The following lemma summarizes the consequences of this relationship.

Lemma 4.10. *Given a graph G suppose an H-description of $\mathcal{S}$ (resp., $\mathcal{S}^+$) can be generated in time $g(n)$. Then a V-description of $\mathcal{S}^+$ (resp., $\mathcal{S}$ can be obtained in time $O(g(n)+n^2)$ starting from G. Consequently, by Lemma 4.9, $g(n)=\Omega(n^\omega)$.*

Between different descriptions of the simplices. Here we investigate the interplay between the various different descriptions of the simplices.

The following is an immediate consequence of Lemma 3.18.

Corollary 4.1. *If $\mathcal{T}$ is a centred simplex in H-description, we can obtain a V-description of $\mathcal{T}^D$ in quadratic time. In particular, given an H-description of the combinatorial simplex $\mathcal{S}_G$ (resp., inverse combinatorial simplex $\mathcal{S}_G^+$) of a graph G, a V-description of $\mathcal{S}_G^+$ (resp., $\mathcal{S}_G$) is obtainable in quadratic time.*

Due to the fact that $\widehat{\mathcal{S}}_G^+$ is not the dual of $\widehat{\mathcal{S}}_G$ Lemma 3.18 is less useful here.

Lemma 4.11. *Generating an V-description of the simplex $\mathcal{S}$ given its H-description requires time $\Omega(n^\tau)$ for any $\mathcal{S}\in\{\mathcal{S}_G,\mathcal{S}_G^+\}$.*

Proof. Consider $\mathcal{S}_G$; the argument is similar for $\mathcal{S}_G^+$. Suppose obtaining the H-description takes time $t(n)$. Due to the properties of the hyperplane representations, this yields access to both sets of vertices in time $t(n)+O(n^2)$. Using the arithmetic in the previous section, this implies that we can obtain the eigenvalues and eigenvectors of G in time $O(n^2)$, i.e., we can solve Laplacian Eigendecomposion in time $t(n)+O(n^2)$ implying that $t(n)=\Omega(n^\tau)$. ⊠

4.3.2. Approximations

Low Rank Approximation Define low rank approximation Let us suppose the we have obtained a low rank—k, say—approximation of $\boldsymbol{L}_G$, written $\widetilde{\boldsymbol{L}}$. We might then ask several questions:

1. Is $\widetilde{\boldsymbol{L}}$ still a gram matrix? That is, can $\widetilde{\boldsymbol{L}}$ be written $\widetilde{\boldsymbol{\Sigma}}^t\widetilde{\boldsymbol{\Sigma}}$ where $\widetilde{\boldsymbol{\Sigma}}$ is the vertex matrix of some set of points, $P=\{\boldsymbol{p}_1,\dots,\boldsymbol{p}_\ell\}$? If so, what is the relationship between $\boldsymbol{\Sigma}$ and $\widetilde{\boldsymbol{\Sigma}}$, where $\boldsymbol{\Sigma}=\boldsymbol{\Sigma}(\mathcal{S}_G)$ is the usual vertex matrix of the combinatorial simplex of G? If $\widetilde{\boldsymbol{L}}$ has rank k then P spans a subspace of dimension k and $\operatorname{conv}(P)$ forms a polytope in that space. What is the relationship between the geometry of $\operatorname{conv}(P)$ and $\mathcal{S}_G$?

2. Is $\widetilde{\boldsymbol{L}}$ useful in helping estimate properties of the simplex $\mathcal{S}_G$? For example, if one could bound the difference in the quadratic products of $\boldsymbol{L}_G$ and $\widetilde{\boldsymbol{L}}$, this would imply (via the results in Section 3.3) 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 examine a specific low rank approximation proposed by Drineas and Mahoney [DM05], which finds low rank approximations to Gram matrices. We will give a brief overview of their method in general, and then elaborate on how it applies to our case in particular. Let $\boldsymbol{M} \in \mathbb{R}^{n\times m}$ be a gram matrix. Using the probability distribution $F(i) = \boldsymbol{M}(i,i)^2/\operatorname{tr}(\boldsymbol{M}^2)$ sample $a \leq m$ columns of $\boldsymbol{M}$ independently at random and with replacement, where a is some given parameter. Let $I \subseteq [n]$, $|I| \leq a$, be the indices of sampled columns. Let $\boldsymbol{C} \in \mathbb{R}^{n\times a}$ be the matrix formed by these columns (that is, $\boldsymbol{C} = \boldsymbol{M}(\cdot, I)$). Let $\boldsymbol{Q}$ be the matrix $\boldsymbol{M}(I,I) \in \mathbb{R}^{a\times a}$, i.e., the submatrix of M with entries corresponding to indices in I, and $\boldsymbol{Q}_k^+$ the optimal rank k-approximation to $\boldsymbol{Q}^+$, the pseudoinverse of $\boldsymbol{Q}$ (section 2.2.1). The low rank approximation to $\boldsymbol{M}$ is then

$$\widetilde{\boldsymbol{M}} \stackrel{\text{def}}{=} \boldsymbol{C}\boldsymbol{M}(I,I)_k^+\boldsymbol{C}^t.$$

THEOREM 4.2 ([DM05]). *Let $\boldsymbol{M}$ be a gram matrix and let $\widetilde{\boldsymbol{M}}$ be as above. Let $\epsilon > 0$, $k \leq c \in \mathbb{N}$. If $c = \Omega(k/\epsilon^4)$, then*

$$\left\|\boldsymbol{M} - \widetilde{\boldsymbol{M}}\right\|_\kappa \leq \|\boldsymbol{M} - \boldsymbol{M}_k\|_\kappa + \epsilon\operatorname{tr}(\boldsymbol{M}^2),$$

for $\kappa = 2, F$.

Let us analyze how this result translates to the case when $\boldsymbol{M} = \boldsymbol{L}_G$. Let I and $\boldsymbol{C}$ be as above. First we observe that $\boldsymbol{L}_G(I,I)$ is simply the Laplacian on the subgraph $G[I]$. Put $\widetilde{G} = G[I]$. Performing an eigendecomposition, write

$$\boldsymbol{L}_{\widetilde{G}} = \sum_{r=1}^{|I|} \mu_r \boldsymbol{\nu}_r \boldsymbol{\nu}_r^t,$$

for where $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_{|I|} = 0$ and $\{\boldsymbol{\nu}_r\}$ are the eigenvalues and eigenvectors of $\boldsymbol{L}_{\widetilde{G}}$, respectively. The results of Section 2.2.1 then dictate that

$$\boldsymbol{L}_{\widetilde{G}}^+ = \sum_{r=1}^{|I|} \frac{1}{\mu_r} \boldsymbol{\nu}_r \boldsymbol{\nu}_r^t,$$

and so the best rank k approximation to $\boldsymbol{L}_{\widetilde{G}}$ is given by

$$\boldsymbol{L}_k \stackrel{\text{def}}{=} (\boldsymbol{L}_{\widetilde{G}}^+)_k = \sum_{r=1}^{k} \frac{1}{\mu_r} \boldsymbol{\nu}_r \boldsymbol{\nu}_r^t.$$

The approximation for $\boldsymbol{L}_G$ is thus given by $\widetilde{\boldsymbol{L}} = \boldsymbol{C}\boldsymbol{L}_k\boldsymbol{C}^t = \boldsymbol{C}\boldsymbol{L}_k^{1/2}\boldsymbol{L}_k^{t/2}\boldsymbol{C}^t = (\boldsymbol{L}_k^{t/2}\boldsymbol{C}^t)^t\boldsymbol{L}_k^{t/2}\boldsymbol{C}^t$. That is, we can view $\widetilde{\boldsymbol{L}}$ as the gram matrix of the vectors given by the columns of $\widetilde{\boldsymbol{\Sigma}} = (\boldsymbol{L}_k^{t/2}\boldsymbol{C}^t)$.

Let us examine $\widetilde{\mathbf{\Sigma}}^t = \mathbb{C}\boldsymbol{L}_k^{t/2}$. First consider $\operatorname{rank}(\boldsymbol{C})$, which we claim is $|I|$. Suppose $\boldsymbol{C}\boldsymbol{f} = \mathbf{0}$, where $\boldsymbol{f} : I \to \mathbb{R}$. Extend $\boldsymbol{f}$ to $\widehat{\boldsymbol{f}} : [n] \to \mathbb{R}$ by setting $\widehat{\boldsymbol{f}}(u) = 0$ for all $u \in [n] \setminus I$. Then

$$(\boldsymbol{L}_G\widehat{\boldsymbol{f}})(k) = \sum_{i\in[n]} \boldsymbol{L}_G(k,i)\widehat{\boldsymbol{f}}(i) = \sum_{i\in I} \boldsymbol{L}_G(k,i)\boldsymbol{f}(i) + \sum_{i\in[n]\setminus I} \boldsymbol{L}_G(k,i)\widehat{\boldsymbol{f}}(i) = \sum_{i\in I} \boldsymbol{C}(k,i)\boldsymbol{f}(i) = 0,$$

implying that $\boldsymbol{L}_G\widehat{\boldsymbol{f}} = \mathbf{0}$, so $\widehat{\boldsymbol{f}} \in \operatorname{span}(\mathbf{1}))$. However, as long as $|I| \neq [n]$, this is impossible since $\widehat{\boldsymbol{f}}([n] \setminus I) = \mathbf{0}$. Therefore, so long as $c < n$, we have $\operatorname{rank}(\boldsymbol{C}) = c$. We now claim that $\operatorname{rank}(\boldsymbol{C}\boldsymbol{L}_k^{t/2}) = \operatorname{rank}(\boldsymbol{L}_k^{t/2})$, which is easier to prove in the abstract.

Lemma 4.12. *Let $\boldsymbol{S} : \mathbb{R}^n \to \mathbb{R}^\ell$, $T \in \mathbb{R}^m \to \mathbb{R}^n$ be linear maps with* $\operatorname{rank}(\boldsymbol{S}) = \ell$. *Then* $\operatorname{rank}(\boldsymbol{S}\boldsymbol{T}) = \operatorname{rank}(\boldsymbol{T})$.

Proof. If $\boldsymbol{T}\boldsymbol{f} = \mathbf{0}$ then clearly $\boldsymbol{S}\boldsymbol{T}\boldsymbol{f} = \mathbf{0}$ so $\dim\ker(\boldsymbol{T}) \leq \dim\ker(\boldsymbol{S}\boldsymbol{T})$. On the other hand, if $\boldsymbol{S}\boldsymbol{T}\boldsymbol{f} = \mathbf{0}$ then because $\boldsymbol{S}$ is full rank, $\boldsymbol{T}\boldsymbol{f} = \mathbf{0}$ implying that $\dim\ker\boldsymbol{T} \geq \ker\boldsymbol{S}\boldsymbol{T}$. By the rank nullity Theorem (e.g., [Axl97]) $\operatorname{rank}(\boldsymbol{S}\boldsymbol{T}) + \dim\ker\boldsymbol{S}\boldsymbol{T} = n = \operatorname{rank}(\boldsymbol{T}) + \dim\ker\boldsymbol{T}$ from which the result follows immediately. ⊠

Taking $\boldsymbol{C} = \boldsymbol{S}$ and $\boldsymbol{T} = \boldsymbol{L}_k^{t/2}$ in the above lemma gives that $\operatorname{rank}(\boldsymbol{C}\boldsymbol{L}_k^{t/2}) = k$. Consequently, the vertex matrix $\widetilde{\mathbf{\Sigma}} \in \mathbb{R}^{|I|\times n}$ contains n vectors in $\mathbb{R}^{|I|}$. Moreover,

$$\operatorname{rank}(\widetilde{\boldsymbol{L}}) = \operatorname{rank}(\widetilde{\mathbf{\Sigma}}^t\widetilde{\mathbf{\Sigma}}) = \operatorname{rank}(\widetilde{\mathbf{\Sigma}}) = k,$$

meaning the n vectors span a k-dimensional space.

One might hope that the approximation matrix $\widetilde{\boldsymbol{L}}$ was a Laplacian, but this does not seem to be the case in general. While it is true that $\widetilde{\boldsymbol{L}}(i,i) \geq 0$ (by virtue of being a gram matrix) and that $\widetilde{\boldsymbol{L}}\mathbf{1} = \mathbf{0}$ (this follows since $\boldsymbol{C}^t\mathbf{1} = \mathbf{0}$ because the rows of $\boldsymbol{C}^t$ are columns and hence rows of $\boldsymbol{L}_G$). However,

$$\widetilde{\boldsymbol{L}}(i,j) = \sum_{r,s=1}^{c} \boldsymbol{C}(i,r)\boldsymbol{C}(j,s)\boldsymbol{L}_k(r,s),$$

which does not look to be necessarily non-positive.

Embedding $\mathcal{S}$ in lower dimensions Johnson-Lindenstrauss Lemma [JL84, DG03]:

Theorem 4.3 (Johnson-Lindenstrauss Lemma). *Let $E \subseteq \mathbb{R}^k$ 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 $\mathbf{u}, \mathbf{v} \in E$.

Theorem 4.4 ([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*

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

Consider inverse simplex for which we have $\left\|\boldsymbol{\sigma}_i^+ - \boldsymbol{\sigma}_j^+\right\|_2^2 = r(i,j)$ where $r(i,j)$ is the effective resistance between vertices i and j. Add a point $\boldsymbol{o}$ which is the centroid of these points. Thus $\left\|\boldsymbol{\sigma}_i^+ - \boldsymbol{o}\right\|_2^2 = \boldsymbol{L}_G^+(i,i)$ for all i. Note that we can compute this in linear time since

$$\left\|\boldsymbol{\sigma}_i^+ - \boldsymbol{o}\right\|_2^2 = \left\|\boldsymbol{\sigma}_i^+\right\|_2^2 = \frac{1}{W(\delta(\{i\}))} = \frac{1}{w(i)}.$$

Applying JL transform to obtain $n+1$ points in $\mathbb{R}^d$, for $d = O(\log(n)/\epsilon^2)$. Let f be the mapping, e.g., $\boldsymbol{\sigma}_i^+$ mapped 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 $\boldsymbol{x}, \boldsymbol{y} \in \{\boldsymbol{\sigma}_1^+, \ldots, \boldsymbol{\sigma}_n^+, \boldsymbol{o}\}$. Apply a linear transformation to the points so that $f(\boldsymbol{o})$ coincides with the origin $\boldsymbol{0} \in \mathbb{R}^d$. Note that this does not affect the distances between the points themselves, and does not damage the approximation. Update f to reflect this transformation. Then,

$$\left\|f(\boldsymbol{\sigma}_i^+)\right\|_2^2 = \left\|f(\boldsymbol{\sigma}_i^+) - f(\boldsymbol{o})\right\|_2^2 = (1+\epsilon_{i,\boldsymbol{o}})\left\|\boldsymbol{\sigma}_i^+ - \boldsymbol{o}\right\|_2^2 = (1+\epsilon_{i,\boldsymbol{o}})\boldsymbol{L}_G^+(i,i).$$

Hence,

$$\begin{aligned}
\left\|f(\boldsymbol{\sigma}_i^+) - f(\boldsymbol{\sigma}_j +)\right\|_2^2 &= \langle f(\boldsymbol{\sigma}_i^+) - f(\boldsymbol{\sigma}_j^+), f(\boldsymbol{\sigma}_i^+) - f(\boldsymbol{\sigma}_j +)\rangle \\
&= \left\|f(\boldsymbol{\sigma}_i^+)\right\|_2^2 + \left\|f(\boldsymbol{\sigma}_j^+)\right\|_2^2 - 2\langle f(\boldsymbol{\sigma}_i^+), f(\boldsymbol{\sigma}_j^+)\rangle,
\end{aligned}$$

implying that

$$\begin{aligned}
\langle f(\boldsymbol{\sigma}_i^+), f(\boldsymbol{\sigma}_j^+)\rangle &= -\frac{1}{2}\left((1+\epsilon_{i,j})\left\|\boldsymbol{\sigma}_i^+ - \boldsymbol{\sigma}_j^+\right\|_2^2 - (1+\epsilon_{i,\boldsymbol{o}})\boldsymbol{L}_G^+(i,i) - (1+\epsilon_{j,\boldsymbol{o}})\boldsymbol{L}_G^+(j,j)\right) \\
&= -\frac{1}{2}((1+\epsilon_{i,j})r(i,j) - (1+\epsilon_{i,\boldsymbol{o}})\boldsymbol{L}_G^+(i,i) - (1+\epsilon_{j,\boldsymbol{o}})\boldsymbol{L}_G^+(j,j)) \\
&= -\frac{1}{2}((1+\epsilon_{i,j})(\boldsymbol{L}_G^+(i,i) - \boldsymbol{L}_G^+(j,j) - 2\boldsymbol{L}_G^+(i,j)) \\
&\qquad - (1+\epsilon_{i,\boldsymbol{o}})\boldsymbol{L}_G^+(i,i) - (1+\epsilon_{j,\boldsymbol{o}})\boldsymbol{L}_G^+(j,j)) \\
&= (1+\epsilon_{i,j})\boldsymbol{L}_G^+(i,j) + \varepsilon(i,j),
\end{aligned}$$

where

$$\varepsilon(i,j) \stackrel{\text{def}}{=} \frac{1}{2}(\epsilon_{i,\boldsymbol{o}} - \epsilon_{i,j})\boldsymbol{L}_G^+(i,i) + (\epsilon_{j,\boldsymbol{o}} - \epsilon_{i,j})\boldsymbol{L}_G^+(i,j),$$

is an error term dictated by $\epsilon_{i,j}, \epsilon_{i,\boldsymbol{o}}$ and $\epsilon_{j,\boldsymbol{o}}$. Setting

$$M \stackrel{\text{def}}{=} \max_i \boldsymbol{L}_G^+(i,i),$$

we can bound the error term via repeated applications of the triangle inequality:

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

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

$$
\boldsymbol{L}_G^+ - O(\epsilon M)\mathbf{I} \leq f(\boldsymbol{\Sigma}^+)^t f(\boldsymbol{\Sigma}^+) \leq \boldsymbol{L}_G^+ + O(\epsilon M)\mathbf{I}.
$$

In other words, we can approximately recover the Gram matrix $\boldsymbol{L}_G^+ = \boldsymbol{\Sigma}^+\boldsymbol{\Sigma}^+$ using the lower dimensional matrix $f(\boldsymbol{\Sigma}^+)$.

Given a graph $G = (V, E, w)$, we can compute all the approximate distances $\left\|\boldsymbol{\sigma}_i^+ - \boldsymbol{\sigma}_j^+\right\|_2^2 = r(i,j)$ 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 $\widetilde{\boldsymbol{R}}$. Question: Does JL Lemma work with approximate distances??

Possible reduction techniques: (1) Projection of simplex onto subspace $\mathbb{R}^k \subseteq \mathbb{R}^n$, probably either the subspace corresponding to largest or smallest eigenvalues. (2) Graph Sparsification: Keeps the same dimension, but removes many edges, i.e., many vertices becomes orthogonal. (3) JL Lemma approach.

Obviously the JL embedding approach does not maintain the fact that the dot product between non-neighbours is zero. But does it approximate this information? I.e., is the dot product smaller for non-neighbours than it is for neighbours?

For example, it maintains approximate information about random spanning trees. We know that

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

where μ is the uniform distribution over all spanning trees. Hence the new JL body approximately maintains this information.

Another thought, about how to do the embedding quickly: Karel says that replacing λ_j with $\lambda_j^{1/2}$ still yields a Laplacian, i.e., $f(\boldsymbol{L}_G) = \boldsymbol{\Phi} f(\boldsymbol{\Lambda})\boldsymbol{\Phi}^t = \sum_i f(\lambda_i)\boldsymbol{\varphi}_i\boldsymbol{\varphi}_i^t$ with $f(x) = \sqrt{x}$ is still a Laplacian. What's the graph which corresponds to this Laplacian? Can we get to that graph from the original graph, without calculating eigendecomposition? Let this graph be G'. Then $\boldsymbol{L}_{G'}^+ = \boldsymbol{L}_G^{+/2}$, implying that by Spielman Teng we can get a good approximation of $\boldsymbol{L}_G^{+/2}$ (if we can compute G' quickly). Thus, we can get an approximate resistive embedding. Perhaps we can then get an approximate simplex from the resistive embedding by projection onto appropriate subspace (really need to figure out what this subspace is).

Resistive Embedding Notice that the effective resistance is encoded naturally by the simplex $\mathcal{S}(G)$:

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

That is, the distance between the vertices of the inverse simplex are precisely the effective resistances.

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:

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

Claim 4.1. *Sort this out. Seems true but should make sure. The polytope defined by the vertices $\{\boldsymbol{\mu}_i\}$ sits in an $n-1$ dimensional subspace. That is, there exists a linear map $\boldsymbol{T} : \mathbb{R}^n \to \mathbb{R}^{n-1}$ such that $\boldsymbol{T}\boldsymbol{\mu} \subseteq \mathbb{R}^{n-1}$ is a simplex.*

Based on above, should have that $\boldsymbol{T}\boldsymbol{\mu}$ is a shifted/rotated/reflected copy of $\mathcal{S}$. So there exists a map $\boldsymbol{M} : \mathbb{R}^{n-1} \to \mathbb{R}^{n-1}$ such that $\boldsymbol{M}\boldsymbol{T}\boldsymbol{\mu} = \boldsymbol{\Sigma}$.

We have

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

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

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

Moreover,

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

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 $\|\boldsymbol{\mu}_i\|_2^2 = \boldsymbol{L}_G^+(i,i)$.

If we can figure out the map which projects the polyhedron onto the correct subspace, the relationships of the simplex will hold and we can maybe use this to discover interesting eigenvector/eigenvalue properties.

Let $\mathcal{R} = \text{conv}(\boldsymbol{\mu}_1, \ldots, \boldsymbol{\mu}_n)$ be the convex polygon defined by the vertices $\{\boldsymbol{\mu}_i\}$. Note that $\boldsymbol{L}_G^{+/2}$ is $\mathcal{R}$'s associated vertex matrix.

The centroid of $\mathcal{R}$ coincides with the origin of $\mathbb{R}^n$:

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

Lemma 4.13. *The all ones vector is orthogonal to $\mathcal{R}$.*

Proof. We need to show that for all $\boldsymbol{p}, \boldsymbol{q} \in \mathcal{R}$, $\langle \mathbf{1}, \boldsymbol{p} - \boldsymbol{q} \rangle = 0$. 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 $\boldsymbol{\varphi}_i \in \operatorname{span}(\mathbf{1})^\perp$ 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 (3.8). Indeed, there exists an isometry between $\mathcal{R}$ and $\mathcal{S}$; therefore,

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

What is the "inverse" of $\mathcal{R}$?? This inverse will relate to a lot of graph properties. If we can obtain a closed form analytical expression this could yield new relationships.

Answer: Inverse simply has vertices $\boldsymbol{L}_G^{1/2} \boldsymbol{\chi}_i$.

Chapter 5

Conclusion

§5.1. Open Problems and Future Directions

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