Contents

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 3.6. 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.

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., $\boldsymbol{Q} \in K^{n\times m}$. 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 $\text{diag}(x_1, x_2, \ldots, x_n)$ 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 $\delta_{i,j}$.

We will occasionally make use of asymptotic notation, especially when analyzing various algorithms. Let $f, g : U \subseteq \mathbb{R} \to \mathbb{R}$ be functions. Write $f = O(g)$ as $x \to c$ if $\limsup_{x\to c} |f(x)/g(x)| < \infty$, and $f = \Omega(g)$ as $x \to c$ if $g = O(f)$. Write $f = o(g)$ as $x \to c$ if $\lim_{x\to c} |f(x)/g(x)| = 0$ and $f = \omega(g)$ if $g = o(f)$. If $f = O(g)$ and $f = \Omega(g)$ we write $f = \Theta(g)$. Typically we are interested in the behaviour as $x \to \infty$.

§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, $\operatorname{span}(\mathbf{v}_1, \ldots, \mathbf{v}_{i-1}, \mathbf{v}_{i+1}, \ldots, \mathbf{v}_n)$ is a hyperplane—that is, $\dim(\operatorname{span}(\mathbf{v}_1, \ldots, \mathbf{v}_{i-1}, \mathbf{v}_{i+1}, \ldots, \mathbf{v}_n))^\perp = 1$. 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 φ satisfying $\boldsymbol{M}\varphi = \lambda\varphi$ is an *eigenvector* of $\boldsymbol{M}$, and call λ the associated *eigenvalue.* It's clear that if φ is an eigenvector then so it $c\varphi$ 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 $\{\varphi_1, \varphi_2, \ldots, \varphi_n\}$ of $\boldsymbol{M}$ whose corresponding eigenvalues $\{\lambda_1, \ldots, \lambda_n\}$ are all real. Let $\boldsymbol{\Phi} = (\varphi_1, \varphi_2, \ldots, \varphi_n)$ be the matrix whose i-th column is the i-th eigenvector of $\boldsymbol{M}$, and set $\boldsymbol{\Lambda} = \operatorname{diag}(\lambda_1, \ldots, \lambda_n)$. Observe that

$$\boldsymbol{M}\boldsymbol{\Phi} = \boldsymbol{M}(\varphi_1, \ldots, \varphi_n) = (\boldsymbol{M}\varphi_1, \ldots, \boldsymbol{M}\varphi_n) = (\lambda_1\varphi_1, \ldots, \lambda_n\varphi_n) = \boldsymbol{\Phi}\boldsymbol{\Lambda}. \tag{2.1}$$

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

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

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

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

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 2.2 ([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 2.3. *Suppose $\boldsymbol{M} \in \mathbb{C}^{m\times m}$ admits the eigendecomposition*

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

where λ_i, $1 \leq i \leq k$ are the non-zero eigenvalues of $\boldsymbol{M}$ with corresponding orthornomal eigenvectors $\varphi_1, \ldots, \varphi_k$. Then the pseudoinverse of $\boldsymbol{M}$ is

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

Proof. Put $\mathbf{Q} = \sum_{i=1}^{k} \lambda_i^{-1}\varphi_i\varphi_I^t$. 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, $\varphi_i^t\varphi_j = \delta_{i,j}$ for all i, j. Hence,

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

Performing a similar computation then demonstrates that

$$\boldsymbol{M}\mathbf{Q}\boldsymbol{M} = \sum_{i=1}^{k} \varphi_i\varphi_i^t \sum_{j=1}^{k} \lambda_j\varphi_j\varphi_j^t = \sum_{i,j=1} \lambda_i\varphi_i\varphi_i^t\varphi_j\varphi_j^t = \sum_{i=1}^{k} \lambda_i\varphi_i\varphi_i^t = \boldsymbol{M},$$

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

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

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

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

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

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

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, $\operatorname{range}(\boldsymbol{L}^t) = \operatorname{range}(\boldsymbol{L}) = \mathbb{R}^n \setminus \ker(\boldsymbol{L}) = \mathbb{R}^n \setminus \operatorname{span}(\{\mathbf{1}\})$, and $\operatorname{range}(\widehat{\boldsymbol{L}}^t) = \operatorname{range}(\widehat{\boldsymbol{L}}) = \mathbb{R}^n \setminus \ker(\widehat{\boldsymbol{L}}) = \mathbb{R}^n \setminus \operatorname{span}(\{\boldsymbol{W}^{1/2}\mathbf{1}\})$. It follows 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 2.4. $\ker(\boldsymbol{L}^+) \subseteq \ker(\boldsymbol{L})$ *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., $\boldsymbol{x} \in \operatorname{span}(\{\mathbf{1}\}) = \ker(\boldsymbol{L})$. 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 $\varphi_1, \ldots, \varphi_n$. 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 φ. Then,

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

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

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

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

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

On the other hand, consider a non-zero vector φ which is orthogonal to all of the above vectors. Then

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

implying that there exists $\ell \in [k]$ such that $\varphi(i) \neq \varphi(j)$ for some $i, j \in V_\ell$. Hence, $\boldsymbol{L}(\varphi) > 0$ and so $\boldsymbol{L}\varphi \neq 0$. 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

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

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

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 φ of $\boldsymbol{L}$ corresponding to the zero eigenvalue, observe that

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

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

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

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

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

§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,

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

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 $\langle \boldsymbol{e}, \boldsymbol{1}\rangle$ (recall that $\boldsymbol{L}_G^+$ is the inverse of $\boldsymbol{L}_G$ in the space $\mathrm{span}(\boldsymbol{1})^t$).

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 $\boldsymbol{\chi}_i - \boldsymbol{\chi}_j \perp \boldsymbol{1}$.

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

§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 $\sum_{i\in[n]} \alpha_i \boldsymbol{x}_i = \boldsymbol{0}$ with $\sum_{i\in[n]} \alpha_i = 0$ is $\alpha_1 = \cdots = \alpha_n = 0$.

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

Lemma 2.5. *The set* $\{\boldsymbol{x}_1, \ldots, \boldsymbol{x}_k\}$ *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 $\sum_{i\neq j} \beta_i(\boldsymbol{x}_j - \boldsymbol{x}_j) = \boldsymbol{0}$. Putting $\beta = \sum_i \beta_i$, we can write this as

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

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

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

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

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

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

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

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

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

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

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

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.

Bunch of stuff commented out here. Not sure what's needed. Deals with faces as subsets affine spaces, etc.

2.5.1. Dual Simplex

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

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

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

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

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

Therefore, the set $\{\boldsymbol{\gamma}_1, \dots, \boldsymbol{\gamma}_n\}$ determines a simplex, which we call the *dual simplex* of $\mathcal{S}$. 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 2.6. *Let $\{\boldsymbol{\sigma}_1, \dots, \boldsymbol{\sigma}_n\}$ 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 $\{\boldsymbol{\gamma}_1, \dots, \boldsymbol{\gamma}_n - 1\}$ is the sister basis to $\{\mathbf{v}_1, \dots, \mathbf{v}_{n-1}\}$ and $\boldsymbol{\gamma}_n = -\sum_{i=1}^{n-1} \boldsymbol{\gamma}_i$, then $\{\boldsymbol{\gamma}_1, \dots, \boldsymbol{\gamma}_{k-1}, \boldsymbol{\gamma}_{k+1}, \dots, \boldsymbol{\gamma}_n\}$ is the sister basis to $\{\mathbf{u}_1, \dots, \mathbf{u}_{k-1}, \mathbf{u}_{k+1}, \dots, \mathbf{u}_n\}$.*

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,

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

⊠

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

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

hence had we set $\mathbf{v}_i = \boldsymbol{\sigma}_k - \boldsymbol{\sigma}_i$ and defined $\boldsymbol{\gamma}_k = -\sum_{i\neq k} \boldsymbol{\gamma}_i$ (as we did for $k = n$), Lemma 2.6 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 2.6. The second part of the statement is clear by construction. ⊠

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 2.7. *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

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

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 $j = i$, ⊠

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 $\boldsymbol{M} = \sum_{i=1}^{d} \lambda_i \varphi_i \varphi_i^t$ for some $d \leq n$ (i.e., $\boldsymbol{M}$ has eigenvalue zero with multiplicity $n-d$) where the eigenvectors $\{\varphi_i\}_{i=1}^d$ 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 $\boldsymbol{\Phi}_M = (\varphi_1, \dots, \varphi_d)$, $\boldsymbol{\Lambda}_M = \mathrm{diag}(\lambda_1, \dots, \lambda_d)$ (note the respective absences of $\varphi_{d+1}, \dots, \varphi_n$ 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

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

and the polytope

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

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

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

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

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

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 $\boldsymbol{\sigma}_i^+(j) = \varphi_j(i)/\lambda_j^{1/2}$. 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 $\operatorname{rank}(\boldsymbol{L}_G) = \operatorname{rank}(\widehat{\boldsymbol{L}}_G) = n-1$, 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 $\ker(\boldsymbol{\Sigma}) = \ker(\boldsymbol{\Sigma}^t\boldsymbol{\Sigma}) = \ker(\boldsymbol{L}) = \operatorname{span}(\{\mathbf{1}\})$, 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 $\boldsymbol{\alpha} \in \ker(\widehat{\boldsymbol{\Sigma}}) = \ker(\widehat{\boldsymbol{L}}) = \operatorname{span}(\{\sqrt{\boldsymbol{w}}\})$, 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,

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

From this, it follows that

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

hence,

$$\boldsymbol{\Sigma}^t\boldsymbol{\Sigma}^+ = (\boldsymbol{\Sigma}^+)^t\boldsymbol{\Sigma} = \mathbf{I} - \mathbf{1}\mathbf{1}^t/n. \tag{3.1}$$

For the inverse normalized simplex, on the other hand, one has $\widehat{\varphi}_n(i)\widehat{\varphi}_n(j) = \sqrt{w(i)w(j)}/n$, implying that

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

and so

$$\widehat{\boldsymbol{\Sigma}}^t\widehat{\boldsymbol{\Sigma}}^+ = (\widehat{\boldsymbol{\Sigma}}^+)^t\widehat{\boldsymbol{\Sigma}} = \mathbf{I} - \sqrt{\boldsymbol{w}}\sqrt{\boldsymbol{w}}^t/n, \tag{3.2}$$

where $\boldsymbol{w} = (w(1), \dots, w(n))$ and $\sqrt{\boldsymbol{w}} = (\sqrt{w(1)}, \dots, \sqrt{w(n)})$.

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

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

$$= \begin{pmatrix} \lambda_1^{-1}\langle \varphi_1, \varphi_1\rangle & \dots & \lambda_1^{-1/2}\lambda_n^{-1/2}\langle \varphi_1, \varphi_n\rangle \\ \vdots & \ddots & \dots \\ \lambda_1^{-1/2}\lambda_n^{-1/2}\langle \varphi_n, \varphi_1\rangle & \dots & \lambda_n^{-1}\langle \varphi_n, \varphi_n\rangle \end{pmatrix} = \mathbf{\Lambda}^{-1}, \tag{3.3}$$

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.

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

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

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 $\mathbf{\Sigma}^t\mathbf{\Sigma}$:

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

(Here $\theta^+ i,j$ is the angle between $\mathcal{S}^+_{\{i\}^c}$ and $\mathcal{S}^+_{\{j\}^c}$.) We claim that $\mathbf{\Sigma}^t\mathbf{\Sigma}$ is the Laplacian matrix of some graph G. First, the matrix is symmetric. Second, for each i, $(\mathbf{\Sigma}^t\mathbf{\Sigma})(i,i) = \left\|\boldsymbol{a}_i^+\right\|_2^{-2} > 0$, and for $i \neq j$, $(\mathbf{\Sigma}^t\mathbf{\Sigma})(i,j) \leq 0$ since $\theta_{i,j}^+ \leq \pi/2$ by assumption (note therefore the importance that $\mathcal{S}^+$ is hyperacute). Finally, denote $\mathbf{\Sigma} = (\boldsymbol{\sigma}_1, \dots, \boldsymbol{\sigma}_n)$, 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 $i \neq n$,

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

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

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

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

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 $\varphi \perp \mathbf{1}$, we have

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

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

$$\sigma_i(j) = \varphi_j(i)\sqrt{n - \lambda_j},$$

and the inverse simplex has vertices

$$\sigma_i(j)^+ = \frac{\varphi_j(i)}{\sqrt{n - \lambda_j}}.$$

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 $\lambda_1 \geq \cdots \geq \lambda_n$ and corresponding eigenvectors $\varphi_1, \ldots, \varphi_n$ as usual. Let H have eigenvalues $\mu_1 \geq \cdots \geq \mu_m$ and corresponding eigenvectors $\boldsymbol{\psi}_1, \ldots, \boldsymbol{\psi}_m$. We claim that $G \times H$ has $m + n$ eigenvalues $\{\lambda_i + \mu_j\}_{i\in[n],j\in[m]}$ with eigenvectors $\{f_{i,j}\}_{(i,j)\in[n]\times[m]}$ given by

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

Indeed:

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

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 φ perpendicular to $\mathbf{1}$, we have

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

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

Cycle Graph

Path Graph

§3.3. Properties of $\mathcal{S}_G$

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 $\langle \varphi_i, \mathbf{1}\rangle = 0$ for all $i < n$. Likewise, $\boldsymbol{c}(\mathcal{S}^+) = \mathbf{0}$.

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

Lemma 3.3. *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 3.4. *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 3.5. *Let $\mathcal{S}$ be the simplex of a graph $G = (V, E, w)$, and fix $U \subseteq V$. For any non-empty $E \subseteq U^c$,*

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

Proof. Let $\boldsymbol{x} \in \mathcal{S}_U$ be arbitrary. For any $i \in U^c$ we have $\langle \boldsymbol{p}, \boldsymbol{\sigma}_i^+ \rangle = -1/n$. 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 3.5 gives us an alternate way to prove Lemma 3.4. 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.,

$$\mathcal{S} = \bigcap_i \mathcal{H}_i.$$

Moreover, $\boldsymbol{x} \in \bigcap_i \mathcal{H}_i$ iff $\langle \boldsymbol{x}, \boldsymbol{\sigma}_i^+ \rangle + 1/n \geq 0$ for all i, i.e., $(\langle \boldsymbol{x}, \boldsymbol{\sigma}_1^+ \rangle, \ldots, \langle \boldsymbol{x}, \boldsymbol{\sigma}_n^+ \rangle) + \mathbf{1}/n \geq \mathbf{0}$, meaning $\boldsymbol{x}$ satisfies (3.5).

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

$$\|c(\mathcal{S}_U)\|_2^2 = \frac{w(\delta U)}{|U|^2}. \tag{3.6}$$

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

$$\left\| c(\mathcal{S}_U^+) \right\|_2^2 = \frac{w(\delta^+ U)}{|U|^2}, \tag{3.7}$$

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 3.6. *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 3.7. *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

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

By Lemma 3.6, 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 $\left\|\boldsymbol{\Sigma}^+g_{U^c}\right\|_2=\left\|\boldsymbol{\Sigma}^+g_U\right\|_2=1$. Then we have $\boldsymbol{\Sigma}^+(g_U+g_{U^c})=0$ and so $g_U+g_{U^c}=k\mathbf{1}$ since $\ker(\boldsymbol{\Sigma}^+)=\operatorname{span}(\{\mathbf{1}\})$. Hence g_U and g_{U^c} are scaled versions of f_U and f_{U^c}. ⊠

Lemma 3.8. *For any non-empty $U\subseteq V$, $\left\|a_U^+\right\|_2^2=1/w(\delta U)$ 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 3.7, write

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

where the final equality comes from using the definition of the centroid in the numerator, and Equation 3.6 in the denominator. Recalling the relation between $\boldsymbol{\Sigma}$ and $\boldsymbol{\Sigma}^+$ 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 3.9. *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 (3.7) and Lemma 3.8, 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 3.10. *For any non-empty $U \subseteq V$,*

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

Proof. This is a consequence of identities (3.6) and (3.7) and Lemmas 3.7 and 3.8. Applying the latter and then the former, observe that

$$a_U = \frac{\|a_U\|_2}{\left\|c^+_{U^c}\right\|_2} c^+_{U^c} = \frac{\sqrt{w(\delta^+ U)}}{\sqrt{w(\delta^+ U)/|U^c|}} c^+_{U^c} = \frac{n - |U|}{w(\delta^+ U)} c^+_{U^c}.$$

A similar computation holds for a_U^+. ⊠

Lemma 3.11. *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,

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

which proves the first equality. The second is shown similarly by employing Lemma 3.10 and the previous identity:

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

⊠

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

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 $\widehat{\varphi}_n$ 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 $\varphi_i \in \text{span}(\boldsymbol{W}_G^{1/2}\mathbf{1}) \subseteq \text{span}(\mathbf{1})^\perp$ for all $i < n$ implying that $\langle \varphi_i, \mathbf{1}\rangle \neq 0$. In this case then,

$$\boldsymbol{c}(\widehat{\mathcal{S}}_G) = \frac{1}{n}\widehat{\boldsymbol{\Lambda}}^{1/2}\widehat{\boldsymbol{\Phi}}^t\mathbf{1} = \frac{1}{n}\begin{pmatrix} \sqrt{\lambda_1}\langle \varphi_1, \mathbf{1}\rangle \\ \vdots \\ \sqrt{\lambda_{n-1}}\langle \varphi_{n-1}, \mathbf{1}\rangle \end{pmatrix} \neq \mathbf{0}.$$

The above argument proves the following.

Lemma 3.12. *The centroid of $\widehat{\mathcal{S}}_G$ coincides with the origin of $\mathbb{R}^{n-1}$ iff G is regular.*

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

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

Lemma 3.13. *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

$$\langle \widehat{\boldsymbol{\sigma}}_i^+, \widehat{\boldsymbol{\sigma}}_j - \widehat{\boldsymbol{\sigma}}_k\rangle = \delta_{ij} - \delta_{ik} + \frac{\sqrt{w(i)w(k)}}{n} - \frac{\sqrt{w(i)w(j)}}{n}. \tag{3.8}$$

First suppose that G is k-regular. Then for $i \neq k$, Equation (3.8) 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 (3.8) 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 3.14. *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 $\boldsymbol{x}_{U_i}$ be the barycentric coordinate of any point in $\widehat{\mathcal{S}}[U_i]$, $i = 1, 2$, and compute

$$\langle \widehat{\boldsymbol{\Sigma}}\boldsymbol{x}_{U_1}, \widehat{\boldsymbol{\Sigma}}\boldsymbol{x}_{U_2}\rangle = \boldsymbol{x}_{U_1}^t\left(\mathbf{I} - \frac{\sqrt{\boldsymbol{w}}\sqrt{\boldsymbol{w}}^t}{n}\right)\boldsymbol{x}_{U_2}$$

$$= \boldsymbol{x}_{U_1}^t \boldsymbol{x}_{U_2} - \frac{1}{n} \sum_{i \in U_1} \boldsymbol{x}_{U_1}(i)\sqrt{w(i)} \sum_{j \in U_2} \boldsymbol{x}_{U_2}(j)\sqrt{w(j)}$$
$$= -\frac{1}{n}\sqrt{w_1 w_2} \sum_{i \in U_1} \boldsymbol{x}_{U_1}(i) \sum_{j \in U_2} \boldsymbol{x}_{U_2}(j) = -\frac{\sqrt{w_1 w_2}}{n},$$

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. ⊠

Centroids and Altitudes. For the normalized Laplacian we have

$$\begin{aligned}
\widehat{\mathcal{L}}(\chi_U) &= \sum_{i \sim j} w(i,j) \left(\frac{\chi_U(i)}{\sqrt{w(i)}} - \frac{\chi_U(j)}{\sqrt{w(j)}} \right)^2 \\
&= \sum_{i \in U, j \in U^c} w(i,j) \left(\frac{\chi_U(i)}{\sqrt{w(i)}} - \frac{\chi_U(j)}{\sqrt{w(j)}} \right)^2 \\
&= \sum_{i \in U, j \in U^c} w(i,j) \frac{\chi_U(i)}{w(i)} \\
&= \sum_{i \in U} \frac{W(\delta(i) \cap U^c)}{w(i)}.
\end{aligned} \tag{3.9}$$

Let $\gamma(i, B)$ denote the *fractional weight of i in B*; that is,

$$\gamma(i, B) = \frac{1}{w(i)} \sum_{j \in \delta(i) \cap B} w(i,j) = \frac{1}{w(i)} W(\delta(i) \cap U^c),$$

and $\gamma(A, B)$ the *average fractional weight from A to B*:

$$\gamma(A, B) = \frac{1}{|A|} \sum_{i \in A} \gamma(i, B).$$

Then,

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

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

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:

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

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 $\boldsymbol{\Sigma}(\mathcal{T}) - (\boldsymbol{c}(\mathcal{T}) \ \ldots \ \boldsymbol{c}(\mathcal{T}))$ centred at the origin is called the *canonical (or centred) simplex corresponding to* $\mathcal{T}$ and is denoted $\mathcal{T}^0$.

Noting that

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

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

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

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

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

One might imagine (and could be forgiven for doing so) that once centred, the normalized simplex and its inverse would indeed be duals. However, this is not the case. Observe that

$$\begin{aligned}
\langle \boldsymbol{c}(\mathcal{S}^+), \widehat{\boldsymbol{\sigma}}_j - \widehat{\boldsymbol{\sigma}}_k\rangle &= \frac{1}{n}\sum_{\ell=1}^{n-1}\sum_{r=1}^{n}\widehat{\boldsymbol{\sigma}}_r^+(\ell)(\widehat{\boldsymbol{\sigma}}_j(\ell) - \widehat{\boldsymbol{\sigma}}_k(\ell)) \\
&= \frac{1}{n}\sum_{r=1}^{n}\sum_{\ell=1}^{n-1}(\varphi_\ell(r)\varphi_\ell(j) - \varphi_\ell(r)\varphi_\ell(k)) \\
&= \frac{1}{n}\sum_{r=1}^{n}\bigg(\delta_{r,k} - \delta_{r,j} + \frac{\sqrt{w(r)w(k)}}{n} - \frac{\sqrt{w(r)w(j)}}{n}\bigg) \\
&= \frac{\sqrt{w(k)} - \sqrt{w(j)}}{n^2}\sum_{r\in[n]}\sqrt{w(r)},
\end{aligned}$$

so, by Equation (3.8),

$$\begin{aligned}
\langle \widehat{\boldsymbol{\sigma}}_i^+ - \boldsymbol{c}(\widehat{\mathcal{S}}^+), (\widehat{\boldsymbol{\sigma}}_j - \boldsymbol{c}(\mathcal{S})) - (\widehat{\boldsymbol{\sigma}}_k - \boldsymbol{c}(\mathcal{S}))\rangle &= \langle \widehat{\boldsymbol{\sigma}}_i^+, \widehat{\boldsymbol{\sigma}}_j - \widehat{\boldsymbol{\sigma}}_k\rangle - \langle \boldsymbol{c}(\widehat{\mathcal{S}}^+), \widehat{\boldsymbol{\sigma}}_j - \widehat{\boldsymbol{\sigma}}_k\rangle \\
&= \delta_{ij} - \delta_{ik} + \frac{\sqrt{w(i)}}{n}(\sqrt{w(k)} - \sqrt{w(j)}) \\
&\quad - \frac{\sqrt{w(k)} - \sqrt{w(j)}}{n^2}\sum_{r\in[n]}\sqrt{w(r)} \\
&= \delta_{ij} + (\sqrt{w(k)} - \sqrt{w(j)})\bigg(\frac{\sqrt{w(i)}}{n} - \frac{1}{n^2}\sum_{r\in[n]}\sqrt{w(r)}\bigg),
\end{aligned}$$

which is not equal to δ_{ij} unless $w(k) = w(j)$ or $\sqrt{w(i)} = \frac{1}{n}\sum_r\sqrt{w(r)}$. Since this would have to hold for all i, j, k, $i, j \neq k$, both of these conditions imply that the graph would have to be regular. So what IS the dual of these simplices?? Ughgggghghgh wtf is happening

§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 $\boldsymbol{\sigma}_i^+ = (\varphi_1(i)\lambda_1^{1/2}, \ldots, \varphi_{n-1}(i)\lambda_{n-1}^{1/2})^t$. 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 $\boldsymbol{\xi} = (\xi(1), \ldots, \xi(n))$. Then we have the following result.

Lemma 3.15. *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,*

$$-\frac{1}{2}\begin{pmatrix} 0 & \mathbf{1}_n^t \\ \mathbf{1}_n & \boldsymbol{D}\end{pmatrix}\begin{pmatrix} \boldsymbol{\xi}^t\boldsymbol{\Gamma}^t\boldsymbol{\Gamma}\boldsymbol{\xi} + 4\overline{d} & -(\boldsymbol{\Gamma}^t\boldsymbol{\Gamma}\boldsymbol{\xi} + 2\mathbf{1}/n)^t \\ -(\boldsymbol{\Gamma}^t\boldsymbol{\Gamma}\boldsymbol{\xi} + 2\mathbf{1}/n) & \boldsymbol{\Gamma}^t\boldsymbol{\Gamma}\end{pmatrix} = \mathbf{I}_{n+1}. \tag{3.10}$$

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

$$\mathbf{\Gamma}^t\mathbf{\Gamma}\boldsymbol{D}\mathbf{\Gamma}^t\mathbf{\Gamma} = -2\mathbf{\Gamma}^t\mathbf{\Gamma}, \tag{3.11}$$

and in the space $\operatorname{span}(\mathbf{1})^\perp$ *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 3.10 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

$$-\frac{1}{2}\bigg(\mathbf{1}\boldsymbol{\xi}^t\boldsymbol{L}_G\boldsymbol{\xi} + \frac{4}{n^2}R\mathbf{1} - \boldsymbol{R}\boldsymbol{L}_G\boldsymbol{\xi} - \frac{2}{n}\boldsymbol{R}\mathbf{1}\bigg), \tag{3.12}$$

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

$$\boldsymbol{R}\boldsymbol{L}_G = \mathbf{1}\boldsymbol{\xi}^t\boldsymbol{L}_G - 2\bigg(\mathbf{I} - \frac{1}{n}\mathbf{J}\bigg). \tag{3.13}$$

Equation (3.12) 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 $\boldsymbol{J}\boldsymbol{R}\mathbf{1} = \mathbf{1}(\mathbf{1}^t\boldsymbol{R}\mathbf{1}) = \mathbf{1}R$. Finally, again using (3.13), 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 (3.12) 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 (3.13) 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 (3.13) 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 (3.10) as applied to electrical networks. As demonstrated in [VMDC17], the result translates into the matrix equation

$$-\frac{1}{2}\begin{pmatrix} 0 & \mathbf{1}^t \\ \mathbf{1} & \boldsymbol{R} \end{pmatrix} = \begin{pmatrix} \operatorname{diag}(\boldsymbol{L}_G^+(i,i))^t\boldsymbol{L}_G\operatorname{diag}(\boldsymbol{L}_G^+(i,i)) + 4R_G/n^2 & -(\boldsymbol{L}_G\operatorname{diag}(\boldsymbol{L}_G^+(i,i)) + \frac{2}{n}\mathbf{1})^t \\ -(\boldsymbol{L}_G\operatorname{diag}(\boldsymbol{L}_G^+(i,i)) + \frac{2}{n}\mathbf{1}) & \boldsymbol{L}_G \end{pmatrix}^{-1}. \tag{3.14}$$

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

$$\begin{pmatrix} 0 & \mathbf{1}^t \\ \mathbf{1} & \boldsymbol{D} \end{pmatrix} \in \mathbb{R}^{(d+1)\times(d+1)}, \tag{3.15}$$

is called the *Menger matrix of* X.

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

Lemma 3.16. *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,*

$$-\frac{1}{2}\begin{pmatrix} 0 & \mathbf{1}^t \\ \mathbf{1} & \boldsymbol{S}_T \end{pmatrix}\begin{pmatrix} \sum_{i\sim j} 1/w(i,j) & (\boldsymbol{d} - 2\mathbf{1})^t \\ \boldsymbol{d} - 2\mathbf{1} & \boldsymbol{L}_T \end{pmatrix} = \mathbf{I}. \tag{3.16}$$

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,

$$\sum_{i\sim j}\frac{1}{w(i,j)}+\sum_{\ell\in[n]}\boldsymbol{S}_T(k,\ell)(\deg(\ell)-2). \tag{3.17}$$

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

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

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

Corollary 3.1. *Let T be a weighted and connected tree. Then*

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

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

Proof. Let $\boldsymbol{S}_T$ be as it was in Lemma 3.16. 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 (3.16) and (3.14) yields

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

from which the claim follows. ⊠

Lemma 3.17 ([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:*

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

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

§3.6. The Inverse Graph

Let G be a connected and weighted graph. G admits the hyperacute combinatorial simplex $\mathcal{S}_G$ which, by Theorem 3.1, is the inverse simplex of a graph H. It thus obeys

$$\|\boldsymbol{\sigma}_i - \boldsymbol{\sigma}_j\|_2^2 = r_H^{\mathrm{eff}}(i,j).$$

Expanding both sides for $i \neq j$ and using the definition of the effective resistance yields

$$w_G(i) + w_G(j) + 2w_G(i,j) = \boldsymbol{L}_H^+(i,i) + \boldsymbol{L}_H^+(j,j) - 2\boldsymbol{L}_H^+(i,j).$$

Here we using the subscript G to reinforce the fact that the weights are those of the original graph, G. We can calculate the entries of the pseudoinverse $\boldsymbol{L}_H^+$ more explicitly. Put

$$W_G \overset{\mathrm{def}}{=} \sum_{i<j} w(i,j) = \frac{1}{2}\sum_i \sum_j w(i,j) = \frac{1}{2}\sum_i w(i).$$

That is, W_G is the total weight of the graph G. Recall that R_H is the total effective resistance of H and compute

$$\begin{aligned} R_H &= \sum_{i<j} r^{\mathrm{eff}}(i,j) \\ &= \sum_{i<j} (w_G(i) + w_G(j) + 2w_G(i,j)) \\ &= \frac{1}{2}\sum_{i,j} (w_G(i) + w_G(j)) + 2W_G \\ &= (2n+2)W_G \end{aligned}$$

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

$$\boldsymbol{L}_H^+(i,j) = \frac{1}{2}\left(\sum_k r_H^{\mathrm{eff}}(i,k) + \sum_k r_H^{\mathrm{eff}}(j,k)\right) - \frac{1}{2} r_H^{\mathrm{eff}}(i,j) - \frac{R_H}{n^2},$$

$$= \frac{1}{2}\sum_k (w_G(i) + w_G(j) + 2w_G(k) + 2w_G(i,k) + 2w_G(j,k)) - \frac{1}{2}w_G(i,j) - \frac{R_H}{n^2}$$
$$= \left(\frac{n}{2}+1\right)(w_G(i) + w_G(j)) - \frac{1}{2}w_G(i,j) + \left(2 - \frac{2}{n} - \frac{2}{n^2}\right)W_G.$$

§3.7. Inequalities

The conductance of a graph G is

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

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 3.18. *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 3.19. *For any f with $\langle f, \mathbf{1}\rangle = 0$,*

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

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

Proof. Let F^+ be as above and let $F^- \overset{\text{def}}{=} [n] \setminus F^+ = \{i : f(i) < 0\}$. 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 $\boldsymbol{R}_G = n\sum_i \lambda_i^{-1} = n\,\mathrm{tr}(\boldsymbol{\Sigma}\boldsymbol{\Sigma}^t)$, facts/inequalities pertaining to the effective resistance can be translated to the simplex.

Lemma 3.20. *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.

§3.8. Steiner Circumscribed Ellipsoid

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

$$\mathcal{E}(\mathcal{S}) = \left\{\boldsymbol{x} : \boldsymbol{x}^t\boldsymbol{\Sigma}^+(\boldsymbol{\Sigma}^+)^t\boldsymbol{x} - \frac{n-1}{n} = 0\right\}. \tag{3.18}$$

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 $\mathcal{E}(\mathcal{S})$. 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

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

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., $\mathbf{\Sigma}\mathbf{\Sigma}^t = \mathbf{\Lambda}^{-1/2}$. Hence, by (3.18),

$$\mathcal{E}(\mathcal{S}) = \left\{ \boldsymbol{x} : \boldsymbol{x}^t \mathbf{\Lambda}^{-1} \boldsymbol{x} = \frac{n-1}{n} \right\}. \tag{3.19}$$

§3.9. 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.

3.9.1. 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 $\boldsymbol{\pi}(\infty) \overset{\text{def}}{=} \lim_t \boldsymbol{\pi}(t)$ 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 $\pi_i = \deg(i)/2|E|$.

3.9.2. Continuous Time Random Walks

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

$$\frac{d\boldsymbol{\pi}(t)}{dt} = -\boldsymbol{\pi}(t)^t \boldsymbol{W}^{-1}\boldsymbol{L}, \tag{3.20}$$

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 (3.20) 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.

3.9.3. mixing time

The distribution $\boldsymbol{\pi} = (\pi_1, \dots, \pi_n)$ 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

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

We have

Chapter 4

Algorithmic Implications

§4.1. Computational Complexity

Corollary 4.1. *Computing the minimum altitude in the inverse simplex of a graph is an NP-hard optimization problem.*

Proof. Follows from the fact that computing the maximum weighted cut is NP-hard. ⊠

Independent Set Let $I \subseteq V$ be an independent set in G, i.e., if $i,j \in I$ then $(i,j) \notin E$. Consider

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

where the second and fourth inequalities follows from the fact that I is an independent set.

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, seeing as it reduces to the usual independent set maximization problem by taking $f(i) = 1$ for all i.

Suppose $f(i) = \alpha w(i)$ for all i, i.e., we assign the vertex weights as a linear function of their total edge weight. For an independent set I we have

$$f(I) = \alpha w(I) = \alpha W(\delta I) = \alpha \frac{|I|}{\|c(\mathcal{S}_I)\|_2^2}.$$

In the simplex, the criteria that I is an independent set translates to the property that $\langle \boldsymbol{\sigma}_i, \boldsymbol{\sigma}_j\rangle = 0$ for all $i,j \in I$. We can thus say something **TODO**What? Need to decide whether problem is easy or hard about the constrained optimization problem

$$\begin{aligned} \min_I \quad & \frac{\|c(\mathcal{S}_I)\|_2^2}{|I|} \\ \text{s.t.} \quad & \langle \boldsymbol{\sigma}_i, \boldsymbol{\sigma}_j\rangle = 0,\ i,j \in I. \end{aligned}$$

The normalized Laplacian, meanwhile, removes the weights from consideration. For an independent set I and a vertex $i \in I$ note that $W(\delta(i) \cap I^c) = w(i)$ since $\delta(i) \cap I^c = \delta(i)$ by definition of an independent set. Therefore, Equation (3.9) yields

$$\widehat{\mathcal{L}}(\chi_I) = \sum_{i\in I} \frac{W(\delta(i)\cap I^c)}{w(i)} = |I|,$$

implying that

$$\left\| c(\widehat{\mathcal{S}}_I) \right\|_2^2 = \frac{1}{|I|^2}\widehat{\mathcal{L}}(\chi_I) = \frac{1}{|I|}.$$

Since maximizing the cardinality of an independent set is an NP-hard problem, we have that

$$\begin{aligned} \max_I \quad & \left\| c(\widehat{\mathcal{S}}_I) \right\|_2^2 \\ \text{s.t.} \quad & \langle \boldsymbol{\sigma}_i, \boldsymbol{\sigma}_j \rangle = 0, \ i, j \in I, \end{aligned}$$

is an NP-hard problem.

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

The first result was also proved in [KS08].

Formulate MST in terms of hyperacute simplices. Seems somewhat surprising that this high-dimensional geometric problem is solvable in poly time. On the other hand, what seems like a related problem in "geometric" space, Hamiltonian cycle/path, is hard. Probably worth mentioning but not thinking too much about.

§4.2. Transitioning between simplices

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 4.1. *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.

§4.3. Embeddings

Johnson-Lindenstrauss Lemma [JL84, DG03]:

Theorem 4.2 (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 4.3 ([SS11]). *For any $\epsilon > 0$ and graph $G = (V, E, w)$, there exists an algorithm which computes a matrix $\widetilde{\boldsymbol{R}} \in \mathbb{R}^{O(\log(n)\epsilon^{-2})\times n}$ such that*

$$(1-\epsilon)r(i,j) \leq \left\|\widetilde{\boldsymbol{R}}(\boldsymbol{\chi}_i - \boldsymbol{\chi}_j)\right\|_2^2 \leq (1+\epsilon)r(i,j).$$

The algorithm runs in time $\widetilde{O}(|E|\log(r)/\epsilon^2)$, where

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

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 $\boldsymbol{x}, \boldsymbol{y} \in \{\boldsymbol{\sigma}_1^+, \dots, \boldsymbol{\sigma}_n^+, \boldsymbol{o}\}$. Apply a linear transformation to the points so that $f(\boldsymbol{o})$ coincides with the origin $\mathbf{0} \in \mathbb{R}^d$. Note that this does not affect the distances between the points themselves, and does not damage the approximation. Update f to reflect this transformation. 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:

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

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

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

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

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., $f(\boldsymbol{L}_G) = \boldsymbol{\Phi} f(\boldsymbol{\Lambda})\boldsymbol{\Phi}^t = \sum_i f(\lambda_i)\varphi_i\varphi_i^t$ 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).

4.3.1. 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:

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

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

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

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

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

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

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

combined with the facts that $\left\| \boldsymbol{\mu}_i - \boldsymbol{\mu}_j \right\|_2^2 = r^{\mathrm{eff}}(i, j)$ 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 $\mathcal{R} = \mathrm{conv}(\boldsymbol{\mu}_1, \ldots, \boldsymbol{\mu}_n)$ 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 $\mathbb{R}^n$:

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

Lemma 4.2. *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,

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

since $\varphi_i \in \mathrm{span}(\mathbf{1})^\perp$ 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 (3.6). 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 $\boldsymbol{L}_G^{1/2}\boldsymbol{\chi}_i$.

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