Chapter 1

Introduction

Questions/confusions:

1. nothing explicit atm.

§1.1. Think about

1. 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?
2. 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.
3. Can use inequalities obtained in the effective resistance literature to obtain inequalities which pertain to all hyperacute simplices. See e.g.,[AALG17]
4. Re-compute the Resistive embedding mentioned in the lecture notes; ensure this isn't the same as our simplex. What properties does it have? Is it a rotation of our simplex? It sits in n-dimensional space, but can it be projected to $\mathbb{R}^{n-1}$?
5. When we tried to shift the normalized Laplacian back, the orthogonality relationships still didn't seem to hold. What if we shift the normalized Laplacian, and then compute the inverse Laplacian?? Before, we were computing the inverse and then shifting.
6. Circumscribed Sphere of simplex (Fiedler talks about this ... I think this is different than the circumscibed ellipsoid?) Also circumsribed ellipsoid of (shifted?) normalized simplex.
7. 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?
8. Embedding approximate distance matrix.
9. Applications of Schur Complement? try next
10. Simplex of the quotient graph? (EEP)
11. Relation of effective resistance to shortest path?
12. Does the simplex structure yield any clues as to possible embeddings of the graph? Pagethickness, planarity, etc? Could start with the high-dimensional simplex, and reduce the dimension one at a time maintaining some invariant of the embedding at each step.
13. Can we estimate diameter, clustering coefficient, average distance, other network properties?

14. Simplex of Hypergraph? Not promising—hypergraph doesn't seem to have common matricial representation.

15. Graph/Spectral sparsification. Can we obtain a good sparsification of a graph by appealing to the simplex? (See Spielman slides).

16. Dimensionality reduction. Can we reduce the dimensionality in specific ways to maintain interesting properties? Started thinking about this; JL lemma, sparsification, etc

17. Graph partitioning via the simplex?

18. Similarity measures between graphs. Projection onto different subspaces??

19. Dynamic Voronoi tesselations and Delauney triangulations. What is the graph(s) of a Delauney triangulation? More generally, is there a set of graphs corresponding to a simplicial complex? Seems hard

20. Diameter, girth? Can't really write these in terms of the quadratic product.

21. Does a clique have any particular structure in the simplex? Do cycles have a structure? Nothing obvious beyond the trivial local connectivity.

22. Is there a geometric way to think about matchings? Edge information is encoded by the dot products between vertices. Yes, answered.

23. Simplex of a directed graph?Directed Laplacian isn't symmetric, so Laplacian in general may not have n orthonormal eigenvectors.

24. Can hypergraphs have simplices? What's the Laplacian of a hypergraph?

25. Is there any connection to the continuous Laplacian operator; can we extract any geometry from this?

26. Simplex of the dual graph?Yes, easy.

27. 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.

28. A simplicial complex is a triangulation of a surface. Each complex corresponds to a graph, and the graphs corresponding to different complexes are connected via the nodes lying on the connected faces of the simplex. This gives a multi-layer graph. This could be interesting to investigate. Connected to Laplacian of hypergraph. Seems a difficult direction.

Chapter 2

Background and Fundamentals

§2.1. General Notation

Let $[n] = \{1, 2, \ldots, n\}$. By $\mathrm{diag}(x_1, x_2, \ldots, x_n)$ 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 $\mathbf{v}_i$. We let $x(i)$ denote the i-th component of a vector $\boldsymbol{x}$. 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 $\|\boldsymbol{x}\|_0$.

§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.

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 complimentary set of vectors $\{\mathbf{u}_i\}$ given by Lemma 2.1 are unique.

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

Let $\mathbf{M} \in \mathbb{R}^{n \times n}$ matrix. We recall that a vector φ satisfying $\mathbf{M}\varphi = \lambda\varphi$ is an *eigenvector* of $\mathbf{M}$, 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 $\mathbf{M}$ is Hermitian, then the Spectral theorem dictates that there exists an orthonormal basis consisting of eigenvectors $\{\varphi_1, \varphi_2, \ldots, \varphi_n\}$ of $\mathbf{M}$ whose corresponding eigenvalues $\{\lambda_1, \ldots, \lambda_n\}$ are all real. Let $\mathbf{\Phi} = (\varphi_1, \varphi_2, \ldots, \varphi_n)$ be the matrix whose i-th column is the i-th eigenvector of $\mathbf{M}$, and set $\mathbf{\Lambda} = \mathrm{diag}(\lambda_1, \ldots, \lambda_n)$. Observe that

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

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

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

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

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

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

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 $\mathbf{M} \in \mathbb{C}^{n\times m}$ for some $n, m \in \mathbb{N}$. We call a matrix $\mathbf{M}^+ \in \mathbb{C}^{m\times n}$ satisfying both

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

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

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

Lemma 2.2 ([BH12]). Let $\mathbf{M} \in \mathbb{C}^{n\times m}$. There exists a unique Pseudoinverse of $\mathbf{M}^+$ of $\mathbf{M}$. Moreover, the following properties hold:

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

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

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

$$\boldsymbol{L}_G(\boldsymbol{L}_G)^+ = (\boldsymbol{L}_G)^+\boldsymbol{L}_G = \mathbf{I} - \frac{1}{n}\mathbf{1}\mathbf{1}^t, | \tag{2.3}$$

and

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

Lemma 2.3. Suppose $\mathbf{M} \in \mathbb{C}^{m\times m}$ admits the eigendecomposition

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

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

$$\mathbf{M}^+ = \sum_{i=1}^k \frac{1}{\lambda_i} \varphi_i \varphi_i^t. \tag{2.4}$$

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,

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

Performing a similar computation then demonstrates that

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

and similarly, $\mathbf{QMQ} = \mathbf{Q}$. 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

$$(\mathbf{QM})^t = (\mathbf{MQ})^t = \left(\sum_{i=1}^k \varphi_i \varphi_i^t)\right)^t = \sum_{i=1}^k (\varphi_i \varphi_i^t)^t = \sum_{i=1}^k \varphi_i \varphi_i^t = \mathbf{MQ} = \mathbf{QM},$$

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

§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

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

a set we call that *neighbourhood* of i. The *degree of* i if $\deg(i) \overset{\text{def}}{=} |\delta(i)|$. The *weight of* i if $w(i) \overset{\text{def}}{=} \sum_{j\in\delta(i)} w(i, j)$. Note that if G is unweighted, then $w(i) = \deg(i)$.

Abusing notation, we extend the weight function w to sets of edges or vertices by setting $w(A) = \sum_{a\in A} w(a)$.

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, $\sum_{i\sim j} = \sum_{(i,j)\in E}$.

For a vertex $i \in V$, we let $\delta(i)$ denote the neighbours of i, i.e., $\delta(i) = \{j \in V : (i, j) \in E\}$.

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., $\boldsymbol{W} = \mathrm{diag}(w(1), w(2), \ldots, w(n))$. The *degree matrix* of G is $\mathrm{diag}(\deg(1), \deg(2), \ldots, \deg(n))$. The *adjacency matrix* of G encodes the edge relations, namely, $\boldsymbol{A}_G(i,j) = w((i,j))$ for all $i \neq j$, and $\boldsymbol{A}_G(i,i) = 0$ for all i. Notice that (for undirected graphs) $\boldsymbol{A}_G$ is symmetric. 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

$$\boldsymbol{L}_G = \sum_{i \sim j} \boldsymbol{L}_{i,j}. \tag{2.5}$$

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

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

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

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

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 precisely what ensures that the orientation we chose for the edges is inconsequential). Consequently,

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

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

$$\boldsymbol{L}_G = \boldsymbol{B}_G^t \boldsymbol{B}_G. \tag{2.6}$$

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 2.5 yields

$$\mathcal{L}_G(f) = f^t\left(\sum_{i\sim j}\boldsymbol{L}_{i,j}\right)f = \sum_{i\sim j} f^t\boldsymbol{L}_{i,j}f = \sum_{i\sim j} w(i,j)(f(i)-f(j))^2. \tag{2.7}$$

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 2.5 for the normalized Laplacian:

$$\widehat{\boldsymbol{L}}_G = \sum_{i\sim j}\widehat{\boldsymbol{L}}_{i,j}. \tag{2.8}$$

Likewise, defining $\widehat{\boldsymbol{B}}_G \in \mathbb{R}^{E\times V}$ by $\widehat{\boldsymbol{B}}_G = \boldsymbol{B}_G\boldsymbol{W}_G^{-1/2}$ gives

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

As we've done here, we will typically emphasize the associate of elements associated to the normalized Laplacian with a hat. Using Equation (2.8), we see that the quadratic form $\widehat{\mathcal{L}}_G$ associated with $\widehat{\boldsymbol{L}}_G$ acts as

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

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 2.6 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 $\boldsymbol{L}\varphi = \mathbf{0}$. 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

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

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

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

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

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

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

so $\boldsymbol{W}^{1/2}\boldsymbol{\chi}_{V_1}, \dots, \boldsymbol{W}^{1/2}\boldsymbol{\chi}_{V_k}$ lie in the kernel of $\widehat{\boldsymbol{L}}$. Conversely, if $\varphi \in \ker(\widehat{\boldsymbol{L}})$, 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

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

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

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

Why did I do this?

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 (2.3) 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. ⊠

§2.4. Simplices

TODO Introduce simplex with defns, etc.

Define hyperplane $\mathcal{H}_i$ (maybe $\mathcal{H}_{\{i\}^c}$) which contains $\mathcal{S}_{\{i\}^c}$ and corresponding halfspaces $\mathcal{H}_i^+$ and $\mathcal{H}_i^-$.

DEFINITION 2.2. A set of points $\boldsymbol{x}_1, \dots, \boldsymbol{x}_k$ are said to be *affinely independent* if, for each j, the set $\{\boldsymbol{x}_j - \boldsymbol{x}_i\}_{i \neq j}$ is linearly independent.

DEFINITION 2.3. A *simplex* $\mathcal{S}$ in $\mathbb{R}^{n-1}$ is the convex hull of n affinely independent vectors $\boldsymbol{\sigma}_1, \dots, \boldsymbol{\sigma}_n$. That is,

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

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

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

Given a point $\boldsymbol{p} = \mathbf{\Sigma}\boldsymbol{x} \in \mathcal{S}$, $\boldsymbol{x}$ 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

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

We will typically omit the restriction symbol from the notation and simply write $\mathcal{S}_U = \mathcal{S} \restriction_U$.

Bunch of stuff commented out here. No sure what's needed.

2.4.1. Dual Simplex

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

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

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

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

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

Therefore, the set $\{\boldsymbol{\gamma}_1, \ldots, \boldsymbol{\gamma}_n\}$ determines a simplex, which we call the *dual simplex* of $\mathcal{S}$.

Definition 2.4. Given a simplex $\mathcal{S}_1 \subseteq \mathbb{R}^{n-1}$ with vertex set $\mathbf{\Sigma}(\mathcal{S}_1) = (\boldsymbol{\sigma}_1, \ldots, \boldsymbol{\sigma}_n)$, a simplex $\mathcal{S}_2 \subseteq \mathbb{R}^{n-1}$ with vertex vectors $\mathbf{\Sigma}(\mathcal{S}_2) = (\boldsymbol{\gamma}_1, \ldots, \boldsymbol{\gamma}_n)$ is called a *dual simplex* of $\mathcal{S}_1$ if $\boldsymbol{\gamma}_i$ is normal to $\mathcal{S}_{\{i\}^c}$ for all $i \in [n]$.

Lemma 2.5. 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. The second part of the statement is clear by construction. ⊠

Claim 2.2. For each $i \in [n]$, $\boldsymbol{\gamma}_i$ is perpendicular to $\mathcal{S}_{\{i\}^c}$.

Proof. We begin with 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

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

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. ⊠

CHAPTER 3

The Graph-Simplex Correspondence

Fiedler Book [Fie11].

§3.1. Convex Polyhedra of Matrices

Consider an arbitrary real and symmetric matrix $\mathbf{M} \in \mathbb{R}^{n\times n}$ which admits the eigendecomposition $\mathbf{M} = \sum_{i=1}^{d} \lambda_i \varphi_i \varphi_i^t$ for some $d \leq n$ (i.e., $\mathbf{M}$ has eigenvalue zero with multiplicity $n-d$) where the eigenvectors $\{\varphi_i\}_{i=1}^{d}$ are orthonormal.

We define the polyhedron $\mathcal{S}(\mathbf{M}) \subseteq \mathbb{R}^{d-1}$ on the vertices $\boldsymbol{\sigma}_1, \ldots, \boldsymbol{\sigma}_n$ by setting

$$\boldsymbol{\sigma}_i(j) = \varphi_j(i)\lambda_j^{1/2},$$

and

$$\mathcal{S}(\mathbf{M}) = CH(\boldsymbol{\sigma}_1, \ldots, \boldsymbol{\sigma}_n) = \left\{ \sum_{\boldsymbol{\sigma}\in\boldsymbol{\Sigma}} \boldsymbol{\sigma} \cdot x(i) : \sum_i x(i) = 1, x(i) \geq 0 \right\} = \{\boldsymbol{\Sigma}\boldsymbol{x} : \|\boldsymbol{x}\|_1 = 1, \boldsymbol{x} \geq \mathbf{0}\}.$$

Letting $\boldsymbol{\Sigma} = [\boldsymbol{\sigma}_1, \ldots, \boldsymbol{\sigma}_n] \in \mathbb{R}^{d\times n}$ be the matrix whose i-th column is the i-th vertex $\boldsymbol{\sigma}_i$, one can verify that

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

where $\boldsymbol{\Phi} = (\varphi_1, \ldots, \varphi_d)$ and $\boldsymbol{\Lambda} = \mathrm{diag}(\lambda_1, \ldots, \lambda_d)$. Hence,

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

That is, $\mathbf{M}$ is the Gram matrix of the vertex vectors of $\mathcal{S}(\mathbf{M})$. Observe that the polytope $\mathcal{S}(\mathbf{M})$ is indeed d-dimensional:

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

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

$$\mathbf{M}^+ = \sum_{i=1}^{d} \lambda_i^{-1}\varphi_i\varphi_i^t.$$

We can thus associated with $\mathbf{M}^+$ as simplex $\mathcal{S}_{\mathbf{M}^+}$, which has as its vertex matrix $\boldsymbol{\Sigma}_{\mathbf{M}^+} = (\boldsymbol{\Phi}\boldsymbol{\Lambda}^{-1/2})^t$; that is, the vertices are defined by $\boldsymbol{\sigma}_i(j) = \varphi_j(i)/\lambda_j^{1/2}$.

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 $\mathcal{S}_G \stackrel{\text{def}}{=} \mathcal{S}_{\boldsymbol{L}_G}$ and $\widehat{\mathcal{S}}_G \stackrel{\text{def}}{=} \mathcal{S}_{\widehat{\boldsymbol{L}}_G}$ corresponding to G's combinatorial and normalized Laplacians. We let $\boldsymbol{\Sigma}_G = (\boldsymbol{\sigma}_1, \dots, \boldsymbol{\sigma}_n)$ and $\widehat{\boldsymbol{\Sigma}}_G = (\widehat{\boldsymbol{\sigma}}_1, \dots, \widehat{\boldsymbol{\sigma}}_n)$ denote the vertices of $\mathcal{S}_G$ and $\widehat{\mathcal{S}}_G$, respectively. Since $\text{rank}(\boldsymbol{L}_G) = \text{rank}(\widehat{\boldsymbol{L}}_G) = n-1$, the polytopes $\mathcal{S}_G$ and $\widehat{\mathcal{S}}_G$ are in fact simplices. Consequently, we will often refer to $\mathcal{S}_G$ as the *simplex of* G, and to $\widehat{\mathcal{S}}_G$ as the *normalized simplex of* G. If G is clear from context we will often drop it from the subscript.

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

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

For the inverse simplex and normalized simplex of G we have

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

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

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

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

§3.2. The Graph of a Simplex

In this section we demonstrate that each hyperacute 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

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

and

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

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

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

Let $\mathcal{S}^+$ be a hyperacute simplex, and $\mathcal{S}$ its dual. The vertex matrix $\boldsymbol{\Sigma}$ of $\mathcal{S}$ contains the outer normals of $\mathcal{S}^+$ (see discussion on dual simplex in Section 2.4.1). Hence, taking $\boldsymbol{Q} = \boldsymbol{\Sigma}^t\boldsymbol{\Sigma}$ in the above Lemma applied to the simplex $\mathcal{S}^+$, we obtain explicit entries for the gram matrix $\boldsymbol{\Sigma}^t\boldsymbol{\Sigma}$:

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

(Here $\theta^+ i, j$ is the angle between $\mathcal{S}^+_{\{i\}^c}$ and $\mathcal{S}^+_{\{j\}^c}$.) We claim that $\boldsymbol{\Sigma}^t\boldsymbol{\Sigma}$ is the Laplacian matrix of some graph G. First, the matrix is symmetric. Second, for each i, $(\boldsymbol{\Sigma}^t\boldsymbol{\Sigma})(i,i) = \left\|\boldsymbol{a}_i^+\right\|_2^{-2} > 0$, and for $i\neq j$, $(\boldsymbol{\Sigma}^t\boldsymbol{\Sigma})(i,j) < 0$ since $\theta_{i,j}^+ < \pi/2$ by assumption (note therefore the importance that $\mathcal{S}^+$ is hyperacute). Finally, denote $\boldsymbol{\Sigma} = (\boldsymbol{\sigma}_1, \dots, \boldsymbol{\sigma}_n)$, and recall from the construction of the dual simplex in Section 2.4.1 that $\boldsymbol{\sigma}_n = -\sum_{i<n}\boldsymbol{\sigma}_i$. Therefore, for $i\neq n$,

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

hence $\mathbf{\Sigma}^t\mathbf{\Sigma}\mathbf{1} = \mathbf{0}$, 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 3.2 with the following theorem.

THEOREM 3.1. There exists a bijection between hyperacute simplices in $\mathbb{R}^{n-1}$ centered at the origin and connected, weighted graphs on n vertices.

§3.3. Simplices of Special Graphs

Subgraphs Let $H \subseteq G$, in the sense that $w_H(i,j) \leq w_G(i,j)$ for all $i,j \in [n]$. Then, for any $f : V \to \mathbb{R}$ we see that

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

Therefore,

$$\|\mathbf{\Sigma}_H f\|_2^2 \leq \|\mathbf{\Sigma}_G f\|_2^2.$$

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

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:

$$(\boldsymbol{L}_{G\times H} f_{uv})(ij) = \deg_{G\times H}((i,j))f_{uv}(ij) - \sum_{(k,\ell)\in\delta((i,j))} f_{uv}(k\ell)$$

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

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

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

3.3.1. Examples

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

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

since $\sum_i \varphi(i) = \langle\varphi, \mathbf{1}\rangle = 0$. **TODO** Find orthonormal basis of eigenvectors.

§3.4. Properties of $\mathcal{S}_G$

Fix a graph $G=(V,E)$ with $|V|=n$.

Unclear whether this stuff holds for $\mathcal{S}_G$ or whether it does for every simplex? If the latter, then move into previous 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 $\boldsymbol{x}_{\boldsymbol{p}}$ and $\boldsymbol{x}_{\boldsymbol{q}}$ respectively, write

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

where we've employed Equation (3.1). Now, $\boldsymbol{x}_{\boldsymbol{p}}(i) = 0$ for all $i\in U^c$ and $\boldsymbol{x}_{\boldsymbol{q}}(j)=0$ for all $j\in U$. Therefore, $\langle\boldsymbol{x}_{\boldsymbol{p}},\boldsymbol{x}_{\boldsymbol{q}}\rangle = 0$. Moreover, $\|\boldsymbol{x}_{\boldsymbol{p}}\|_1 = \|\boldsymbol{x}_{\boldsymbol{q}}\|_1 = 1$ 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,

$$\mathcal{S} = \left\{ \boldsymbol{x} \in \mathbb{R}^{n-1} : \boldsymbol{x}^t \boldsymbol{\Sigma}^+ + \frac{\mathbf{1}^t}{n} \geq \mathbf{0}^t \right\}. \tag{3.3}$$

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 (3.3).

Recovering G from its simplices. The (normalized) Laplacian of a graph naturally encodes all of the graph's information. By means of the relationships $\mathbf{\Sigma}^t\mathbf{\Sigma} = \boldsymbol{L}$ and $\widehat{\mathbf{\Sigma}}^t\widehat{\mathbf{\Sigma}} = \widehat{\boldsymbol{L}}$, so too do the simplices $\mathcal{S}$ and $\widehat{\mathcal{S}}$. More precisely, given the simplices, the edge information can be recovered using inner products:

$$\langle \boldsymbol{\sigma}_i, \boldsymbol{\sigma}_j \rangle = \begin{cases} w(i), & \text{if } i = j, \\ -w(i,j), & \text{otherwise,} \end{cases} \quad \text{and} \quad \langle \widehat{\boldsymbol{\sigma}}_i, \widehat{\boldsymbol{\sigma}}_j \rangle = \begin{cases} 1, & \text{if } i = j, \\ -1/\sqrt{w(i)w(j)}, & \text{otherwise.} \end{cases}$$

In particular, the edge (i,j) belongs to E iff $\langle \boldsymbol{\sigma}_i, \boldsymbol{\sigma}_j \rangle$ and $\langle \widehat{\boldsymbol{\sigma}}_i, \widehat{\boldsymbol{\sigma}}_j \rangle$ are strictly less than zero. Each simplex takes space $O(n^2)$ to store, regardless of the number of edges in G. If G is sparse, then this does not constitute an improvement. If G is dense on the other hand—say $|E| = \omega(n^2)$—then storing n vectors in $\mathbb{R}^{n-1}$ could be advantageous. Of course, in order to compute the simplex we need to first obtain an eigendecomposition of the Laplacian which can be infeasible for large graphs.

Centroids. The *centroid* $c(\mathcal{S})$ of a simplex $\mathcal{S}$ is the point $\S\mathbf{1}/n$, where $\S = \S(\mathcal{S})$ are the vertices of $\mathcal{S}$. Intuitively, it constitutes the center of mass of the simplex; an equal linear combination of all vertices. If $\mathcal{S} = \mathcal{S}(\mathbf{M})$ is the simplex corresponding to the matrix $\mathbf{M}$ with $(\varphi_1, \ldots, \varphi_n)$ and eigenvalues $\lambda_1, \ldots, \lambda_n$ then we have

$$\mathbf{\Lambda}^{1/2}\mathbf{\Phi}^t\mathbf{1} = (\sqrt{\lambda_1}\langle \varphi_1, \mathbf{1}\rangle, \ldots, \sqrt{\lambda_n}\langle \varphi_n, \mathbf{1}\rangle)^t,$$

and so

$$c(\mathcal{S}) = \left(\sqrt{\lambda_1}\frac{\langle \varphi_1, \mathbf{1}\rangle}{n}, \ldots, \sqrt{\lambda_n}\frac{\langle \varphi_{n-1}, \mathbf{1}\rangle}{n} \right)^t.$$

Similarly,

$$c(\mathcal{S}^+) = \left(\frac{\langle \varphi_1, \mathbf{1}\rangle}{n\sqrt{\lambda_1}}, \ldots, \frac{\langle \varphi_{n-1}, \mathbf{1}\rangle}{n\sqrt{\lambda_{n-1}}} \right)^t.$$

For an eigenvector φ of $\boldsymbol{L}$ we have $\varphi\mathbf{1} = 0$, implying that $\mathbf{\Phi}^t\mathbf{1} = \mathbf{0}$. Therefore,

$$c(\mathcal{S}) = \frac{1}{n}\S\mathbf{1} = \frac{1}{n}(\mathbf{\Lambda}^{1/2})^t\mathbf{\Phi}^t\mathbf{1} = \mathbf{0},$$

and likewise, $c(\mathcal{S}^+) = \mathbf{0}$.

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

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

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

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

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

$$\|c(\mathcal{S}_U)\|_2^2 = \frac{w(\delta U)}{|U|^2}. \tag{3.4}$$

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

$$\left\|c(\mathcal{S}_U^+)\right\|_2^2 = \frac{w(\delta^+ U)}{|U|^2}, \tag{3.5}$$

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

For the normalized Laplacian on the other hand,

$$\begin{aligned}
\widehat{\mathcal{L}}(\chi_U) &= \sum_{i \sim j} w(i,j) \left(\frac{\chi_U(i)}{\sqrt{w(i)}} - \frac{\chi_U(j)}{\sqrt{w(j)}} \right)^2 \\
&= \sum_{i \in U, j \in U^c} w(i,j) \left(\frac{\chi_U(i)}{\sqrt{w(i)}} - \frac{\chi_U(j)}{\sqrt{w(j)}} \right)^2 \\
&= \sum_{i \in U, j \in U^c} w(i,j) \frac{\chi_U(i)}{w(i)} \\
&= \sum_{i \in U} \frac{W(\delta(i) \cap U^c)}{w(i)}.
\end{aligned} \tag{3.6}$$

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,

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

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

Altitudes

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 $\mathbf{\Sigma}(\boldsymbol{x}_{U^c} - \boldsymbol{x}_U)$ where $\boldsymbol{x}_{U^c}$ and $\boldsymbol{x}_U$ are the barycentric coordinates of $\boldsymbol{p}$ and $\boldsymbol{q}$.

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

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

where we've used that $\mathbf{\Sigma 1} = \mathbf{0}$. 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 $\mathbf{\Sigma}^+ x_{U^c}$. 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

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

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

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

Proof. By definition of the altitude there exists barycentric coordinates $\boldsymbol{x}_U$ and $\boldsymbol{x}_{U^c}$ such that $a^+U = \mathbf{\Sigma}^+(\boldsymbol{x}_U - \boldsymbol{x}_{U^c})$. Combining this representation of a_U^+ with that given by Lemma 3.7, write

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

where the final equality comes from using the definition of the centroid in the numerator, and Equation 3.4 in the denominator. Recalling the relation between $\mathbf{\Sigma}$ and $\mathbf{\Sigma}^+$ given by Equation 3.1 and that $\boldsymbol{x}_U$ and $\boldsymbol{x}_{U^c}$ are barycentric coordinates, we can rewrite the above as

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

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

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

⊠

Corollary 3.1. 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. ☒

Lemma 3.9. The vectors $\boldsymbol{\sigma}_i^+$ and $\boldsymbol{a}(\mathcal{S}_i)$ are antiparallel.

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

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

where the penultimate and final inequalities follow from Equation (3.5) and Lemma 3.8, respectively. Let $\boldsymbol{x} = \boldsymbol{x}_{\{i\}^c}$ be the barycentric coordinate of the face $\S_{\{i\}^c}$ such that $\boldsymbol{a}_i = \boldsymbol{\Sigma}(\boldsymbol{x} - \boldsymbol{\chi}_i)$. Then,

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

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

Lemma 3.10. For any non-empty $U \subseteq V$,

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

Proof. This is a consequence of identities (3.4) and (3.5) 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

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

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

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

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

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

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

§3.6. Construction via Extended Menger and Gramian

Will include this after the proof is sorted

§3.7. Inequalities

LEMMA 3.12. 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 3.13. For any f with $\langle f, \mathbf{1}\rangle = 0$,

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

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

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

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

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

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

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

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

LEMMA 3.14. Let $G = (V, E, w)$ be a weighted graph and let $U \subseteq V$ obey $\mathrm{vol}(U) < \mathrm{vol}(V)/2$ and

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

§3.8. Steiner Circumscribed Ellipsoid

Fiedler derivation: [Fie05]. More Fiedler geometry: [Fie93]. A *quadric* in $\mathbb{C}^d$ is a hypersurface of dimension $d-1$ of the form

$$\boldsymbol{Q}(\boldsymbol{Q}, \boldsymbol{r}, s) \stackrel{\text{def}}{=} \{\boldsymbol{x} \in \mathbb{C}^d : \boldsymbol{x}^t \boldsymbol{Q} \boldsymbol{x} + \boldsymbol{r}^t \boldsymbol{x} + s = 0\}.$$

Definition 3.2. 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 3.15 ([Fie05]). The Steiner circumscribed Ellipsoid of $\mathcal{S} = \mathcal{S}(G)$ satisfies

$$\mathcal{E}(\mathcal{S}) = \left\{ \boldsymbol{x} : \boldsymbol{x}^t \boldsymbol{\Sigma}^+ (\boldsymbol{\Sigma}^+)^t \boldsymbol{x} - \frac{n-1}{n} = 0 \right\}. \tag{3.7}$$

Proof. Set $\mathbf{M} = \boldsymbol{\Sigma}^+(\boldsymbol{\Sigma}^+)^t$ and $E = \{\boldsymbol{x} : \boldsymbol{x}^t \mathbf{M} \boldsymbol{x} = (n-1)/n\}$. 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

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

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

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

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

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

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

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

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

Perhaps a more insightful representation of $\mathcal{E}(\mathcal{S})$ comes from noticing that

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

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

Hence, by (3.7),

$$\mathcal{E}(\mathcal{S}) = \left\{\boldsymbol{x} : \boldsymbol{x}^t\mathbf{\Lambda}^{-1}\boldsymbol{x} = \frac{n-1}{n}\right\}. \tag{3.8}$$

Simplex 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

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

§3.9. Random Walks

Very unclear if there's anything interesting here.

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.

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

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

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

3.9.2. Continuous Time Random Walks

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

$$\frac{d\boldsymbol{\pi}(t)}{dt} = -\boldsymbol{\pi}(t)^t \boldsymbol{W}^{-1}\boldsymbol{L}, \tag{3.9}$$

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 (3.9) 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, $\boldsymbol{W}^{-1}\boldsymbol{\pi} \in \text{span}\{\boldsymbol{1}\}$, i.e., $\boldsymbol{\pi} \in \text{span}\{\boldsymbol{w}\}$. 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 $\boldsymbol{\pi} = (\pi_1, \ldots, \pi_n)$ corresponds to a point in the simplex, namely $\boldsymbol{p}_\pi = \S\boldsymbol{\pi}$. It is thus natural to wonder whether this point tells us anything interesting about the dynamics of the walk.

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

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

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

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

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

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

We have

Chapter 4

Algorithmic Implications

§4.1. Computational Complexity

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 (3.6) 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. 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 $\boldsymbol{x}, \boldsymbol{y} \in \{\boldsymbol{\sigma}_1^+, \ldots, \boldsymbol{\sigma}_n^+, \boldsymbol{o}\}$. 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:

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

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

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

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. 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,

$$\boldsymbol{B}^t \boldsymbol{f} = \boldsymbol{e}. \tag{4.1}$$

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

$$\boldsymbol{f} = \boldsymbol{W}\boldsymbol{B}\boldsymbol{\rho}. \tag{4.2}$$

Combining (4.1) and (4.2) we see that $\boldsymbol{e} = \boldsymbol{B}^t\boldsymbol{f} = \boldsymbol{B}^t\boldsymbol{W}\boldsymbol{B}\boldsymbol{\rho} = \boldsymbol{L}_G\boldsymbol{\rho}$, and so $\boldsymbol{\rho} = \boldsymbol{L}_G^+\boldsymbol{e}$ whenever $\langle \boldsymbol{e}, \mathbf{1}\rangle$ (recall that $\boldsymbol{L}_G^+$ is the inverse of $\boldsymbol{L}_G$ in the space $\mathrm{span}(\mathbf{1})^t$).

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

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

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

Definition 4.1. The *effective resistance* between nodes i and j is $r_{\text{eff}}(i, j) \stackrel{\text{def}}{=} \mathcal{L}_G^+(\boldsymbol{\chi}_i - \boldsymbol{\chi}_j)$.

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.

4.3.1. Resistive Embedding

Consider the vertices $\boldsymbol{\mu}_i = \boldsymbol{L}_G^{+/2}\boldsymbol{\chi}_i \in \mathbb{R}^n$, for $i \in [n]$. This yields n points in $\mathbb{R}^n$, also with pairwise squared distances equal to the effective resistance of the graph:

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

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

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

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

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

combined with the facts that $\left\|\boldsymbol{\mu}_i - \boldsymbol{\mu}_j\right\|_2^2 = r_{\text{eff}}(i,j)$ and $\|\boldsymbol{\mu}_i\|_2^2 = \boldsymbol{L}_G^{+}(i,i)$.

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 $\mathcal{R} = \operatorname{conv}(\boldsymbol{\mu}_1, \ldots, \boldsymbol{\mu}_n)$ 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 4.1. 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 $\varphi_i \in \operatorname{span}(\mathbf{1})^\perp$ for all $i < n$. Hence $\langle \mathbf{1}, \boldsymbol{p}\rangle = 0$ meaning that $\langle \mathbf{1}, \boldsymbol{p} - \boldsymbol{q}\rangle = 0$ as well. ⊠

The relationship between $\mathcal{R}$ and $\mathcal{S}$ gives us an alternate way to prove equalities such as (3.4). 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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