The Graph-Simplex Correspondence and its Algorithmic Implications

Ben Chugg, Supervisor: Renaud Lambiotte

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Background: Spectral Graph Theory

Graph $G = (V, E, w)$.

- Vertex set $V = \{1, 2, \ldots, n\}$;
- Edge set $E \subset V \times V$;
- Edge weights given by $w : E \to \mathbb{R}_{\geq 0}$. (Graph is unweighted if $w(i,j) \in \{0, 1\}$ for all i, j).

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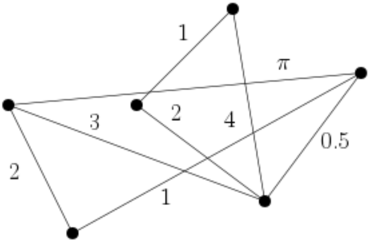
Weight of vertex i, $w(i) = \sum_j w(i, j)$.



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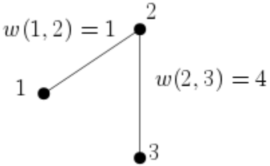
- Laplacian matrix $\boldsymbol{L}_G = \boldsymbol{W}_G - \boldsymbol{A}_G$.



$$\boldsymbol{A}_G = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 4 \\ 0 & 4 & 0 \end{pmatrix} \quad \boldsymbol{W}_G = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 5 & 0 \\ 0 & 0 & 4 \end{pmatrix}$$

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- If G is connected, then $\lambda_i > 0$ for all $i < n$.
- Set $\boldsymbol{\Phi} = (\boldsymbol{\varphi}_1 \ \ldots \ \boldsymbol{\varphi}_{n-1})$ and $\boldsymbol{\Lambda} = \mathrm{diag}(\lambda_1, \ldots, \lambda_{n-1})$. Then

$$\boldsymbol{L}_G = \boldsymbol{\Phi} \boldsymbol{\Lambda} \boldsymbol{\Phi}^*.$$

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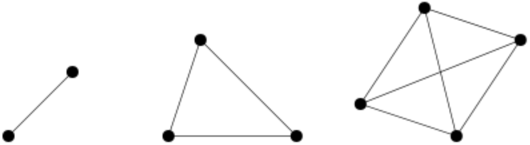
Simplices! Just high-dimensional triangles.



R^1: Line $\quad$ R^2: Triangle $\quad$ R^3: Tetrahedron

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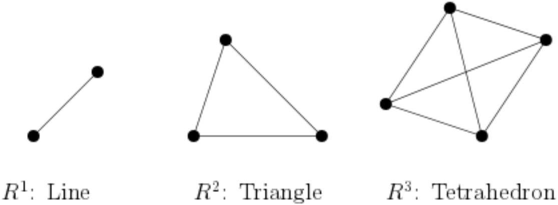

Simplex $\mathcal{S} \subset \mathbb{R}^{n-1}$ is the convex hull of n vertex vectors $\boldsymbol{\sigma}_1, \ldots, \boldsymbol{\sigma}_n$.
Technical note: Vertex vectors must be affinely independent.

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Formalisms (boooo).

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Vertex matrix $\boldsymbol{\Sigma} = (\boldsymbol{\sigma}_1 \ \ldots \ \boldsymbol{\sigma}_n)$.

$$\begin{aligned}\mathcal{S} &= \left\{ \sum_i x(i)\boldsymbol{\sigma}_i : \sum_i x(i) = 1, x(i) \geq 0 \right\} \\ &= \{\boldsymbol{\Sigma}\boldsymbol{x} : \|\boldsymbol{x}\|_1, \boldsymbol{x} \geq 0\}\end{aligned}$$

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Each face of a simplex is a lower-dimensional simplex.
For $U \subset [n]$, face corresponding to vertices $\{\boldsymbol{\sigma}_i\}_{i\in U}$ is

$$\mathcal{S}_U = \{\mathbf{\Sigma}\boldsymbol{x} : \|\boldsymbol{x}\|_1, \boldsymbol{x} \geq 0, x(i) = 0 \; \forall i \in U^c\}$$

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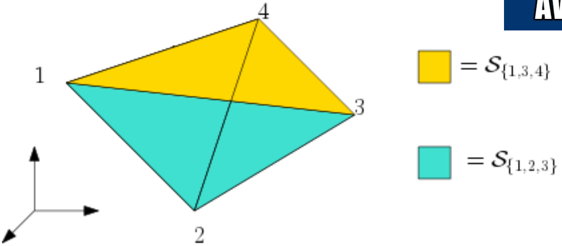
Pictures! (Yaaaaaay)



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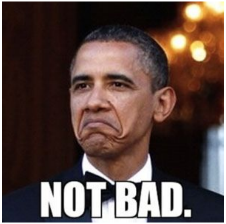

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Connected, weighted, graph G with non-zero eigenvalues $\lambda_1, \dots, \lambda_{n-1}$ and corresponding eigenvectors $\boldsymbol{\varphi}_1, \dots, \boldsymbol{\varphi}_{n-1}$.

For $i \leq n$ and $j \leq n-1$, define

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

so

$$\boldsymbol{\Sigma} = (\boldsymbol{\sigma}_1 \ \dots \ \boldsymbol{\sigma}_n) = \boldsymbol{\Lambda}^{1/2}\boldsymbol{\Phi}^*.$$

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Denote this simplex $\mathcal{S}_G$.

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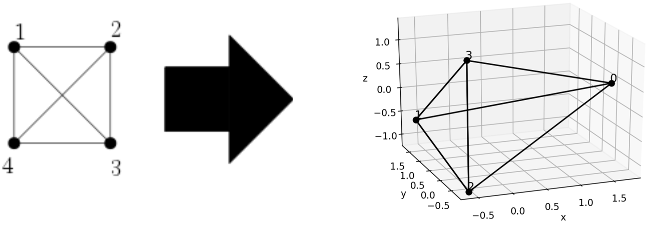

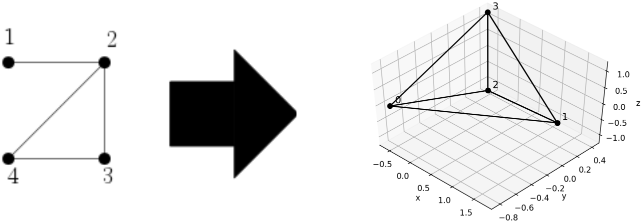

Dual Simplex

We can also define the "dual" vertices

$$\boldsymbol{\sigma}_i^+(j) = \boldsymbol{\varphi}_j(i)\lambda_j^{-1/2},$$

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Denote this simplex $\mathcal{S}_G^+$.

Pseudo-whaaaaat?

Pseudoinverse relationship:

$$\boldsymbol{L}_G^+ \boldsymbol{L}_G = \boldsymbol{L}_G \boldsymbol{L}_G^+ = \boldsymbol{I} - \frac{1}{n}\boldsymbol{J} = \text{Projection onto span}(\mathbf{1})^\perp.$$

$\boldsymbol{J}$ is the all 1's matrix.

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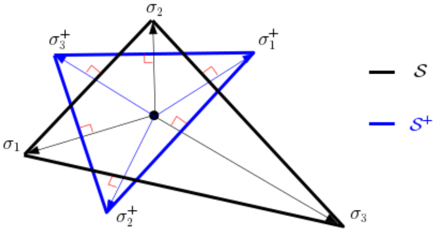
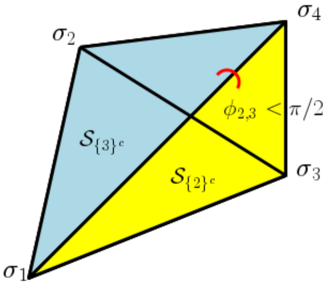
Yields orthogonality relationships between simplex and inverse simplex: $\mathcal{S}^+_{U^c}$ orthogonal to $\mathcal{S}_U$.



Graph of a Simplex?

The simplex of a graph is hyperacute: Angle $\theta_{i,j}$ between $\mathcal{S}_{\{i\}^c}$ and $\mathcal{S}_{\{j\}^c}$ (these are hyperplanes) is $< \pi/2$.



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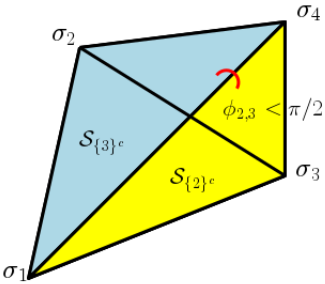

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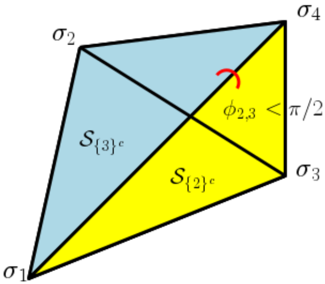

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Why? (Needs another half an hour).

Recap

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Defines hyperacute simplex $\mathcal{S}_G$ where $\boldsymbol{\Sigma}^*\boldsymbol{\Sigma} = \boldsymbol{L}_G$.

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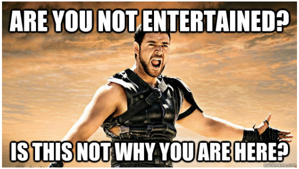
Recap



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Dual simplex $\mathcal{S}_G^+$ where $(\boldsymbol{\Sigma}^+)^*\boldsymbol{\Sigma}^+ = \boldsymbol{L}_G^+$.

Given hyperacute simplex $\mathcal{S}_0$, there is a graph G such that $\mathcal{S}_G^+ = \mathcal{S}_0$.

Basic Properties

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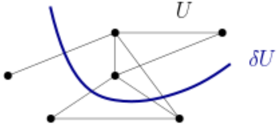
- Cut set of $U \subset V$: $\delta U \equiv \{(i,j) \in E : i \in U, j \in U^c\}$. Centroid of face $\mathcal{S}_U$ related to weight of cut:

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

(Weight of set A is $w(A) = \sum_{i \in A} w(i)$).



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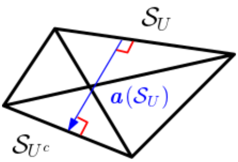
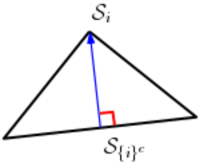
- Altitude $\boldsymbol{a}(\mathcal{S}_U)$ points from $\mathcal{S}_U$ to $\mathcal{S}_{U^c}$ and is orthogonal to both.





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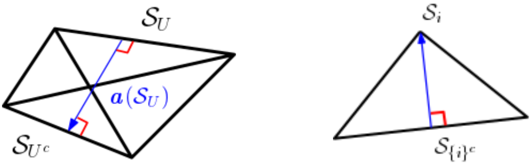

- Altitudes of $\mathcal{S}_G$ relate to centroids of $\mathcal{S}_G^+$:

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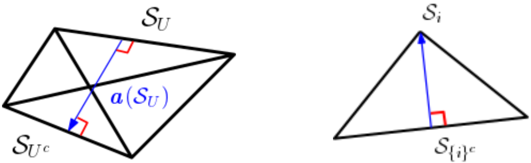

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- Altitudes of inverse simplex describe cut weights:

$$\|\boldsymbol{a}^+(\mathcal{S}_U)\|_2^2 = \frac{1}{w(\delta U)}.$$

Insights?

Simplex geometry yields new Laplacian inequalities. E.g., for $\boldsymbol{x} \perp \mathbf{1}$,

$$\boldsymbol{x}^* \boldsymbol{L}_G \boldsymbol{x} \cdot \boldsymbol{\chi}_A^* \boldsymbol{L}_G^+ \boldsymbol{\chi}_A \geq \frac{\|\boldsymbol{x}\|_1^2}{4},$$

where $A = \{i : x(i) \geq 0\}$ and $\boldsymbol{\chi}_A$ is indicator vector.

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Spectral theory yields new geometric inequalities. E.g., for any U,

$$\|\boldsymbol{\Sigma}\boldsymbol{\chi}_U\|_2^2 \geq \frac{|U|}{2} \min_j \|\Pi_j(\boldsymbol{\Sigma})\|_2^2,$$

where Π_j is projection onto j-th axis.

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Algorithmic Graph Theory understood very well. Obtain immediate results in Algorithmic Simplex Theory.

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Algorithmic Graph Theory understood very well. Obtain immediate results in Algorithmic Simplex Theory.

Relationship $\|\boldsymbol{a}^+(\mathcal{S}_U)\|_2^2 = \frac{1}{w(\delta U)}$ implies the problem **compute the minimum altitude of a hyperacute simplex** is NP hard.

On the other hand, given $s, t \in V$,

$$\begin{aligned} \max_U \quad & \left\|\boldsymbol{a}^+(\mathcal{S}_U)\right\|_2^2 \\ \text{s.t.} \quad & s \in U, t \in U^c, \end{aligned}$$

admits a polynomial time algorithm (via max-flow min-cut theorem).

Questions

- Can we apply random graph theory to gain insights about random simplices?
- Given G, can we compute $\mathcal{S}_G$ and/or $\mathcal{S}_G^+$ faster than $O(n^3)$? Can we approximate $\mathcal{S}_G$? This keeps me up at night.
- Do low dimensional approximations of $\mathcal{S}_G$ converse graph properties? (E.g., communities?)
- A probability distribution over the vertices is a barycentric coordinate. The distribution of a random walk therefore gives a path in the simplex. Does this path have any significance?
- The normalized Laplacian $\widehat{\boldsymbol{L}}_G = \boldsymbol{W}_G^{-1/2}\boldsymbol{L}_G\boldsymbol{W}_G^{-1/2}$ also admits a corresponding simplex. What are its properties?