Simplex Geometry of Graphs

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in collaboration with Karel Devriendt

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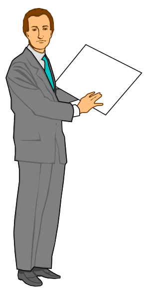
Google matrix: fundamentals, applications and beyond (GOMAX)
IHES, October 15-18, 2018

TU Delft

Outline



Background:

Electrical matrix equations

Geometry of a graph

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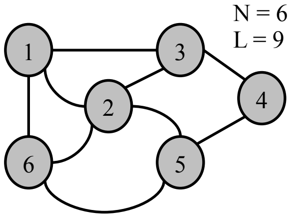
Adjacency matrix A



$$A_{N\times N} = \begin{bmatrix} 0 & 1 & 1 & 0 & 0 & 1 \\ 1 & 0 & 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 & 0 & 1 \\ 1 & 1 & 0 & 0 & 1 & 0 \end{bmatrix}$$

For an undirected graph: $A = A^T$ is symmetric

Number of neighbors of node *i* is the degree: $d_i = \sum_{k=1}^{N} a_{ik}$

if there is a link between node i and j, then $a_{ij} = 1$
else $a_{ij} = 0$

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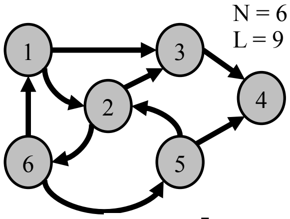
Incidence matrix B



- Label links (e.g.: $l_1 = (1,2)$, $l_2 = (1,3)$, $l_3 = (1,6)$, $l_4 = (2,3)$, $l_5 = (2,5)$, $l_6 = (2,6)$, $l_7 = (3,4)$, $l_8 = (4,5)$, $l_9 = (5,6)$)
- Col *k* for link $l_k = (i,j)$ is zero, except:
  - source node i = 1 → $b_{ik} = 1$
  - destination node j = -1 → $b_{jk} = -1$

$$B_{N\times L} = \begin{bmatrix} 1 & 1 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 1 & -1 & 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & -1 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -1 & -1 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & -1 \\ 0 & 0 & 1 & 0 & 0 & -1 & 0 & 0 & 1 \end{bmatrix}$$

Col sum B is zero: $u^T B = 0$

where the all-one vector $u = (1,1,\ldots,1)$

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B specifies the directions of links

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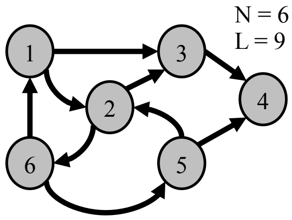
Laplacian matrix Q



$$Q_{N\times N} = \begin{bmatrix} 3 & -1 & -1 & 0 & 0 & -1 \\ -1 & 4 & -1 & 0 & -1 & -1 \\ -1 & -1 & 3 & -1 & 0 & 0 \\ 0 & 0 & -1 & 2 & -1 & 0 \\ 0 & -1 & 0 & -1 & 3 & -1 \\ -1 & -1 & 0 & 0 & -1 & 3 \end{bmatrix}$$

$$Q = BB^T = \Delta - A$$
$$\Delta = diag(d_1 \quad d_2 \quad \dots \quad d_N)$$

Since BB^T is symmetric, so are *A* and *Q*. Although *B* specifies directions, *A* and *Q* lost this info here.

Basic property: $Qu = 0$

u is an eigenvector of *Q*
Belonging to eigenvalue μ = 0

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$Qu = BB^T u = 0$ because $0 = u^T B = B^T u$

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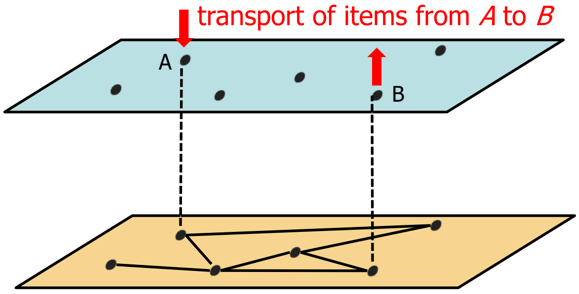
Network: service(s) + topology



Service (function)

software, algorithms

Topology (graph)

hardware, structure

Service and topology
- own specifications
- both are, generally, time-variant
- service is often designed independently of the topology
- often more than 1 service on a same topology

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Function of network

- Usually, the function of a network is related to the *transport of items over its underlying graph*
- In man-made infrastructures: two major types of transport
  - Item is a flow (e.g. electrical current, water, gas,…)
  - Item is a packet (e.g. IP packet, car, container, postal letter,…)
- Flow equations (physical laws) determine transport (Maxwell equations (Kirchhoff & Ohm), hydrodynamics, Navier-Stokes equation (turbulent, laminar flow equations, etc.)
- Protocols determine transport of packets (IP protocols and IETF standards, car traffic rules, etc.)

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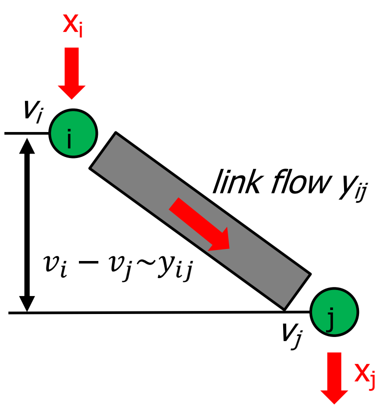
Linear dynamics on networks

Linear dynamic process: "proportional to" (~) graph of network



Examples:

- water (or gas) flow ~ pressure
- displacement (in spring) ~ force
- heat flow ~ temperature
- electrical current ~ voltage

$$x = Q \cdot v$$

x	Q	v
injected nodal current vector	weighted Laplacian of the graph	nodal potential vector

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P. Van Mieghem, K. Devriendt and H. Cetinay, 2017, "Pseudoinverse of the Laplacian and best spreader node in a network", Physical Review E, vol. 96, No. 3, p 032311.

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Pseudoinverse of the Laplacian (review)

The inverse of the current-voltage relation $x = Qv$
is the voltage-current relation $v = Q^{\dagger}x$
subject to $u^T x = 0$ and $u^T v = 0$

The spectral decomposition

$$\tilde{Q} = \sum_{k=1}^{N-1} \tilde{\mu}_k z_k z_k^T$$

allows us to compute the pseudoinverse (or Moore-Penrose inverse)

$$Q^{\dagger} = \sum_{k=1}^{N-1} \frac{1}{\tilde{\mu}_k} z_k z_k^T$$

The effective resistance N x N matrix is $\tilde{\Omega} = u\zeta^T + \zeta u^T - 2Q^{\dagger}$,
where the N x 1 vector $\zeta = (Q_{11}^{\dagger}, Q_{22}^{\dagger}, \cdots, Q_{NN}^{\dagger})$
An interesting graph metric is the effective graph resistance

$$R_G = N u^T \zeta = N \text{trace}(Q^{\dagger}) = N \sum_{k=1}^{N-1} \frac{1}{\mu_k}$$

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P. Van Mieghem, K. Devriendt and H. Cetinay, 2017, "Pseudo-inverse of the Laplacian and best spreader node in a network", Physical Review E, vol. 96, No. 3, p 032311.

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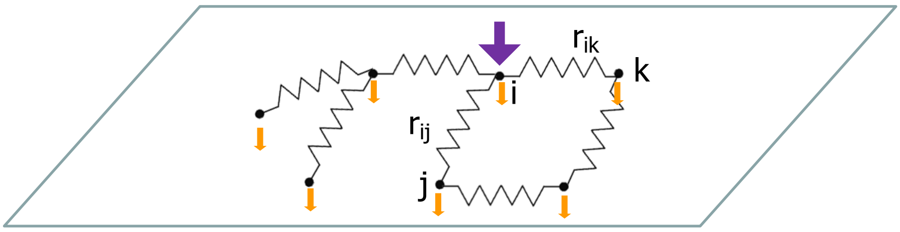

Inverses: $x = Qv$ ⟺ $v = Q^{\dagger}x$ with voltage reference $u^T v = 0$

$Q^{\dagger}$: pseudoinverse of the weighted Laplacian obeying $QQ^{\dagger} = Q^{\dagger}Q = I - \frac{1}{N}J$
$J = uu^T$: all-one matrix u : all-one vector

Unit current injected in node i
$x = e_i - 1/N\, u$

→

nodal potential of i
$v_i = Q_{ii}^{\dagger}$

→ The best spreader is node k with $Q_{kk}^{\dagger} \leq Q_{ii}^{\dagger}$ for $1 \leq i \leq N$

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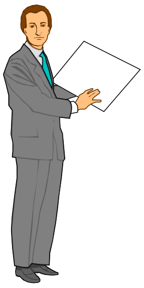
Outline



Background:

Electrical matrix equations

Geometry of a graph

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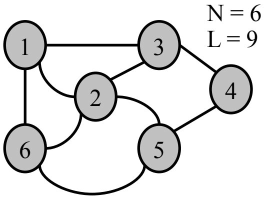
Three representations of a graph

Topology domain



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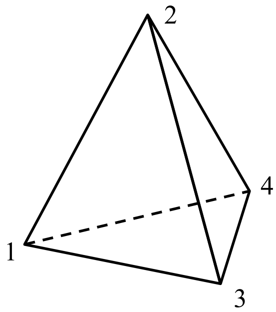
Spectral domain

$$A = A^T = X\Lambda X^T$$

$X_{N\times N}$: orthogonal eigenvector matrix

$\Lambda_{N\times N}$: diagonal eigenvalue matrix

Geometric domain



Undirected graph on *N* nodes
= simplex in Euclidean *(N-1)*-dimensional space

Devriendt, K. and P. Van Mieghem, 2018, "The Simplex Geometry of Graphs", Delft University of Technology, report20180717. (http://arxiv.org/abs/1807.06475).

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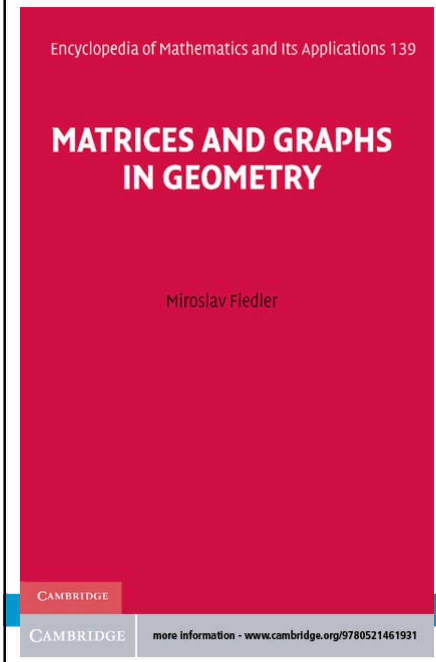

appeared in 2011

Miroslav Fiedler (1926-2015)

Father of “algebraic connectivity”

His 1972 paper: > 3400 citations

"This book comprises, in addition to auxiliary material, the research on which I have worked for over 50 years."

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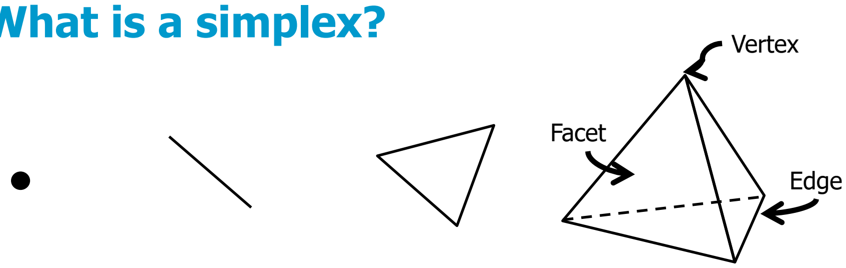
What is a simplex?



Point Line Segment Triangle Tetrahedron

Roughly : a simplex is generalization of a triangle to *N* dimensions

Potential : Euclidean geometry is the oldest, mathematical theory

T. L. Heath, *The Thirteen Books of Euclid's Elements*, Vol. 1-3, Cambridge University Press, 1926

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Spectral decomposition weighted Laplacian (1)

Spectral decomposition: $Q = ZMZ^T$

where $M = diag(\mu_1, \mu_2, \cdots, \mu_{N-1}, 0)$, because $Q\,u = 0$

and the eigenvector matrix Z obeys $Z^T Z = Z\,Z^T = I$ with structure

node →

$$Z = \begin{bmatrix} (z_1)_1 & (z_2)_1 & \cdots & (z_N)_1 \\ (z_1)_2 & (z_2)_2 & \cdots & (z_N)_2 \\ \vdots & \vdots & \ddots & \vdots \\ (z_1)_N & (z_2)_N & \cdots & (z_N)_N \end{bmatrix} = \begin{bmatrix} (z_1)_1 & (z_2)_1 & \cdots & 1/\sqrt{N} \\ (z_1)_2 & (z_2)_2 & \cdots & 1/\sqrt{N} \\ \vdots & \vdots & \ddots & \vdots \\ (z_1)_N & (z_2)_N & \cdots & 1/\sqrt{N} \end{bmatrix}$$

↑ frequencies (eigenvalues)

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$Q = \sum_{k=1}^{N-1} \mu_k z_k z_k^T$

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Spectral decomposition weighted Laplacian (2)

Only for a positive semi-definite matrix, it holds that

$$Q = ZMZ^T = \left(Z\sqrt{M}\right)\left(Z\sqrt{M}\right)^T$$

The matrix $S = \left(Z\sqrt{M}\right)^T$ obeys $Q = S^T S$ and has rank *N-1*
(row $N = 0$ due to $\mu_N = 0$)

$$S = \begin{bmatrix} \sqrt{\mu_1}(z_1)_1 & \sqrt{\mu_1}(z_1)_2 & \cdots & \sqrt{\mu_1}(z_1)_N \\ \sqrt{\mu_2}(z_2)_1 & \sqrt{\mu_2}(z_2)_2 & \cdots & \sqrt{\mu_2}(z_2)_N \\ \vdots & \vdots & \ddots & \vdots \\ \sqrt{\mu_{N-1}}(z_{N-1})_1 & \sqrt{\mu_{N-1}}(z_{N-1})_2 & \cdots & \sqrt{\mu_{N-1}}(z_{N-1})_N \\ 0 & 0 & & 0 \end{bmatrix}$$

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$Q = \sum_{k=1}^{N-1} \mu_k z_k z_k^T$

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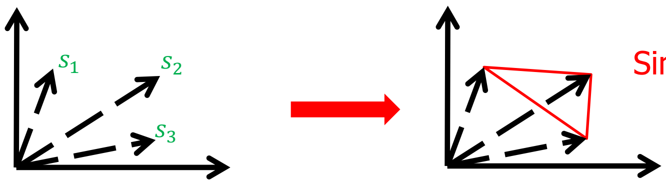
Geometrical representation of a graph

$$S = \begin{bmatrix} \sqrt{\mu_1}(z_1)_1 & \sqrt{\mu_1}(z_1)_2 & \cdots & \sqrt{\mu_1}(z_1)_N \\ \sqrt{\mu_2}(z_2)_1 & \sqrt{\mu_2}(z_2)_2 & \cdots & \sqrt{\mu_2}(z_2)_N \\ \vdots & \vdots & \ddots & \vdots \\ \sqrt{\mu_{N-1}}(z_{N-1})_1 & \sqrt{\mu_{N-1}}(z_{N-1})_2 & \cdots & \sqrt{\mu_{N-1}}(z_{N-1})_N \\ 0 & 0 & & 0 \end{bmatrix}$$

The i-th column vector $s_i = \left(\sqrt{\mu_1}(z_1)_i, \sqrt{\mu_2}(z_2)_i, \cdots, \sqrt{\mu_N}(z_N)_i = 0\right)$ represents a point p_i in (N-1)-dim space (because S has rank N-1)



Simplex geometry: omit zero row, $S_{N\times N} \to S_{(N-1)\times N}$

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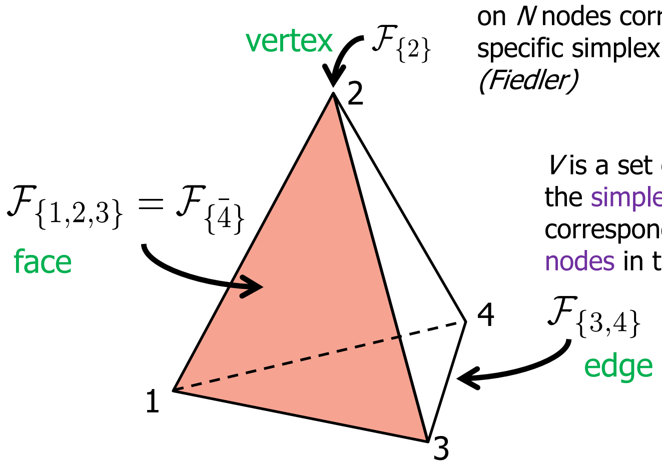
Faces of a simplex

Each connected, undirected graph on N nodes corresponds to 1 specific simplex in N-1 dimensions *(Fiedler)*



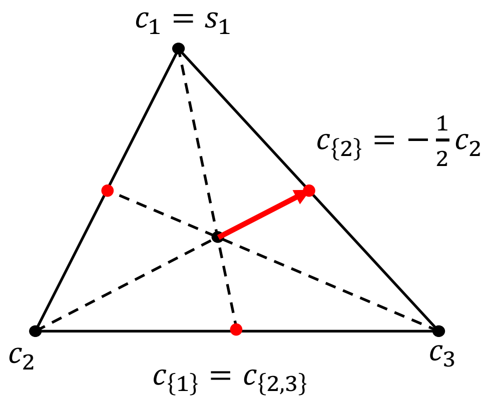
V is a set of vertices of the simplex in $\mathbb{R}^{N-1}$, corresponding to a set of nodes in the graph G

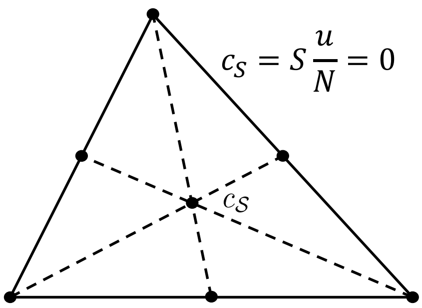
A face $F_V = \{p \in \mathbb{R}^{N-1} | p = Sx_V \; with \; (x_V)_i \geq 0 \; and \; u^T x_V = 1\}$

The vector $x_V \in \mathbb{R}^N$ is a barycentric coordinate with $\begin{cases} (x_V)_i \in \mathbb{R} & if\; i \in V \\ (x_V)_i = 0 & if\; i \notin V \end{cases}$

Centroids

$c_V = S\frac{u_V}{|V|}$ is the centroid of face F_V with $(u_V)_i = 1_{i\in V}$





a centroid of a face is a vector

centroid of simplex is origin

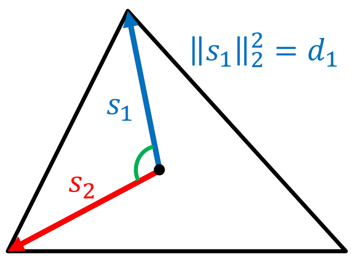
$u_{V} = u - u_V$ ⟶ $|V|c_V = S(u - u_V) = -(N - V)c_V$

Geometric representation of a graph

$\|s_i\|_2^2 = d_i$ $\quad \|s_i - s_j\|_2^2 = (s_i - s_j)^T(s_i - s_j) = s_i^T s_i + s_j^T s_j - 2s_i^T s_j$

$= Q_{ii} + Q_{jj} - 2Q_{ij}$

$= d_i + d_j + 2a_{ij}\ for\ i \neq j, else\ zero$



$s_1^T s_2 = Q_{12} = -a_{12}$

The matrix with off-diagonal elements $d_i + d_j + 2a_{ij}$ is a distance matrix (if the graph G is connected)

The geometric graph representation is not unique (node relabeling changes Z)

$s_i^T s_j = \sum_{k=1}^{N-1}\sqrt{\mu_k}(z_k)_i\sqrt{\mu_k}(z_k)_j = \sum_{k=1}^{N-1}\mu_k(z_k z_k^T)_{ij} = Q_{ij}$

$Q = \sum_{k=1}^{N-1}\mu_k z_k z_k^T$ and $Q = S^T S$

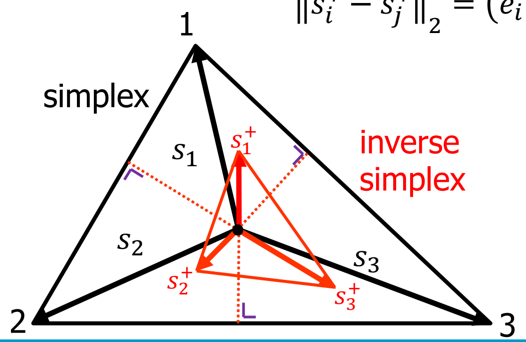
Geometry of a graph (dual representation)

Spectral decomposition: $Q^\dagger = ZM^\dagger Z^T = \left(Z\sqrt{M^\dagger}\right)\left(Z\sqrt{M^\dagger}\right)^T$

The matrix $S^\dagger = \left(Z\sqrt{M^\dagger}\right)^T$ has rank *N-1* and $Q^\dagger = \left(S^\dagger\right)^T S^\dagger$

The *i*-th column vector $s_i^\dagger$ obeys

$$\left\|s_i^\dagger - s_j^\dagger\right\|_2^2 = \left(e_i - e_j\right)^T Q^\dagger \left(e_i - e_j\right) = \omega_{ij}$$



From $S^T S^\dagger = I - \frac{uu^T}{N}$:

$$\begin{cases} s_j^T s_i^+ = -\frac{1}{N} \\ s_i^T s_i^+ = 1 - \frac{1}{N} \end{cases}$$

$\Rightarrow$ $\left(s_k - s_j\right)^T s_i^+ = 0$

ω_{ij} is the effective resistance between node *i* and *j*

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Volume of simplex and inverse simplex of a graph

Volume of the simplex $\quad V_G = \frac{N}{(N-1)!}\sqrt{\xi}$

where the number of (weighted) spanning trees ξ is $\xi = \frac{1}{N}\prod_{k=1}^{N-1}\mu_k$

Volume of the inverse simplex $\quad V_G^+ = \frac{1}{(N-1)!\sqrt{\xi}}$

Hence: $$\frac{V_G}{V_G^+} = N\xi = \prod_{k=1}^{N-1}\mu_k$$

K. Menger, "New foundation of Euclidean geometry", American Journal of Mathematics, 53(4):721-745, 1931

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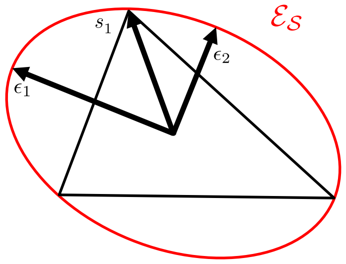
Steiner ellipsoid of simplex



projection $s_1^T \epsilon_2 = \mu_2 (z_2)_1$

semi-axis: $\|\epsilon_2\| = \sqrt{\frac{N}{N-1}\mu_2}$

volume:

$$V_{\mathcal{E}_S} = \frac{\pi^{N/2}}{\Gamma(N/2+1)} \frac{N^{N/2}}{(N-1)^{N/2}} \sqrt{\prod_{k=1}^{N} \mu_k}$$

Hence,

$$V_{\mathcal{E}_S}^2 = \frac{(N\pi)^N}{\left(\Gamma(N/2+1)\right)^2 (N-1)^N} \prod_{k=1}^{N} \mu_k$$

$$V_{N-ellipsoid} = \frac{\pi^{N/2}}{\Gamma(N/2+1)} \prod_{k=1}^{N} \epsilon_k$$

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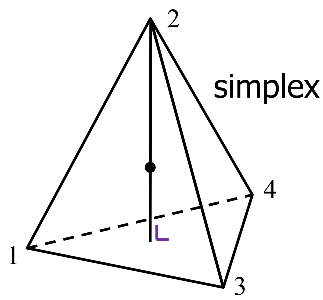
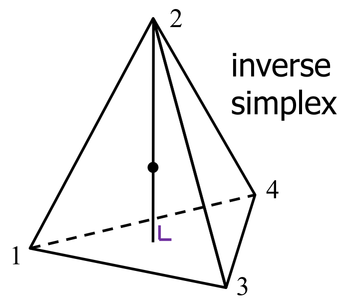
altitude(s) in a simplex

Fiedler





$$\|a_{\{2\}}\|^2 = \frac{1}{Q_{22}^{\dagger}} \qquad \|a_2^+\|^2 = \frac{1}{d_2}$$

The altitude from a vertex s_i^+ to the complementary face $F_{\{i\}}^+$ in the inverse simplex (dual graph representation) has a length equal to the inverse degree of node i

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recall that $Q_{ii}^{\dagger} = v_i$ (nodal potential, best spreader)

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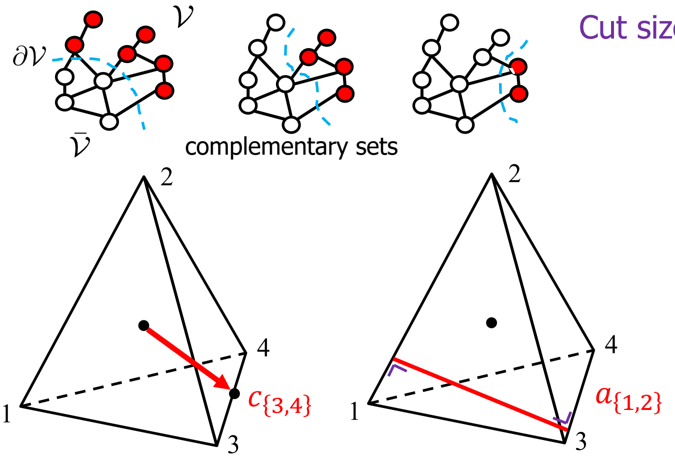
Cut size of graph and altitude of simplex



$\|c_{\{3,4\}}\|^2 = \frac{\partial\{3,4\}}{4}$ $\|a_{\{1,2\}}\|^2 = \frac{1}{\partial^+\{1,2\}}$

Cut size: $|\partial V| = u_V^T Q u_V$

$Q = S^T S$

$$|\partial V| = u_V^T S^T S u_V = \|S u_V\|_2^2 = \|c_V\|_2^2 V^2$$

altitude:
vector from face F_V to face $F_{\bar{V}}$ and orthogonal to both faces

$|\partial^+ V| = u_V^T Q^\dagger u_V$

$\|a_V^+\|^2 = \frac{1}{|\partial V|}$

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$c_V = S\frac{u_V}{|V|}$ is the centroid of face F_V with $(u_V)_i = 1_{i\in V}$

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Metrics $\sqrt{\omega_{ij}}$ *and* ω_{ij}

$\|s_i^\dagger - s_j^\dagger\|_2 = \sqrt{\omega_{ij}}$

the Euclidean distance between vertices of inverse simplex $S^\dagger$

⬍

vertices of $S^\dagger$ are an embedding of nodes of the graph G according to the metric $\sqrt{\omega_{ij}}$ (a.o. obeying the triangle inequality)

Also $\|s_i^\dagger - s_j^\dagger\|_2^2 = \omega_{ij}$ *is a metric*

⬍

Inverse simplex $S^\dagger$ of the graph G with positive link weights is hyperacute

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Unpublished recent work with K. Devriendt

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Generalization metrics

$Q^\dagger$ is the Gramm matrix of a hyperacute simplex S^+ → determines a metric

$m_{ij}^{(f)} = (e_i - e_j)^T \, (f(Q))^\dagger \, (e_i - e_j)$ is a metric when f(Q) is a Laplace matrix

"Statistical physics" metrics on a graph

$$m_{ij}^{(stat(g))} = (e_i - e_j)^T \left(e^{(Q+pQ_K)t} - I + gQ_K\right)^\dagger (e_i - e_j) = \sum_{k=1}^{N-1} \frac{\left((z_k)_i - (z_k)_j\right)^2}{e^{(\mu_k + pN)t} + g}$$

with $t = \frac{1}{k_B T}$ and $pN = -E_f$ (chemical potential or Fermi energy)

g = -1 → Bose-Einstein

g = 0 → Maxwell-Boltzmann

g = 1 → Fermi-Dirac

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Unpublished recent work with K. Devriendt

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Summary

- Linearity between process and graph naturally leads to the weighted Laplacian Q and its pseudoinverse $Q^\dagger$
- Spectral decomposition of the weighted Laplacian Q and its pseudoinverse $Q^\dagger$ provides an *N-1* dimensional simplex representation of each graph,
  - allowing computations in the *N-1* dim. Euclidean space (in which a distance/norm is defined)
  - geometry for (undirected) graphs
- Open: "*Which network problems are best solved in the simplex representation?"*

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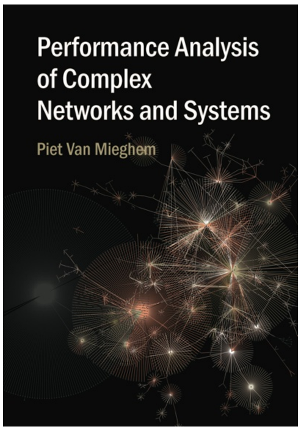
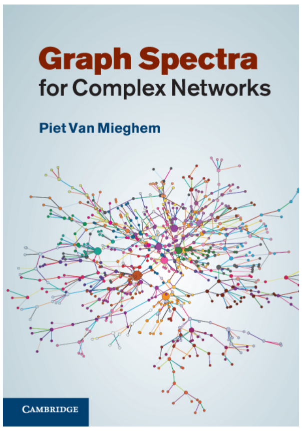
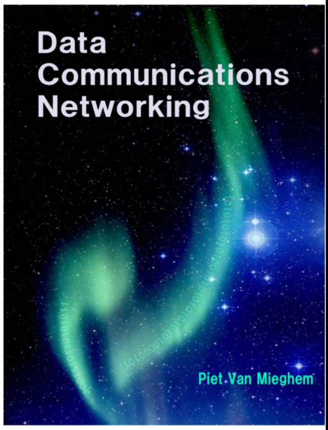
Books







Articles: **http://www.nas.ewi.tudelft.nl**

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