Simplex Geometry of Graphs

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in collaboration with Karel Devriendt

Third workshop on Critical and Collective Effects in Graphs and Networks (CCEGN 2018)
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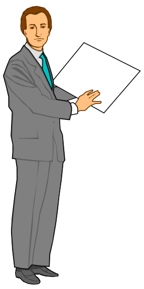
Outline



Background:

Electrical matrix equations

Geometry of a graph

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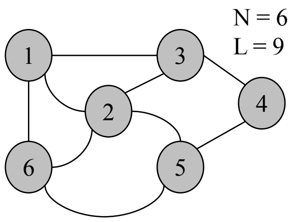
Adjacency matrix A



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

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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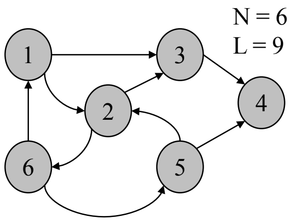
Incidence matrix B



- 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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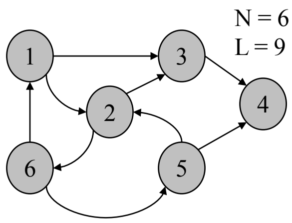
Laplacian matrix Q



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

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

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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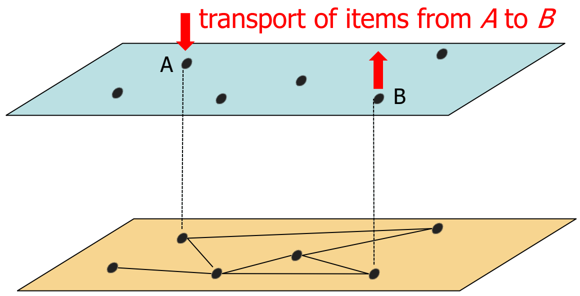
Network: service(s) + topology



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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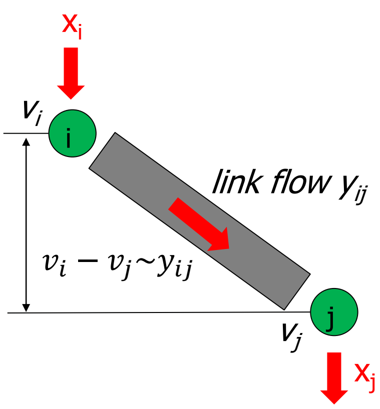
Linear dynamics on networks

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	.	v
injected nodal current vector		weighted Laplacian of the graph		nodal potential vector

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 $\zeta = \left(Q^{\dagger}_{11}, Q^{\dagger}_{22}, \cdots, Q^{\dagger}_{NN}\right)$
An interesting graph metric is the effective graph resistance

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

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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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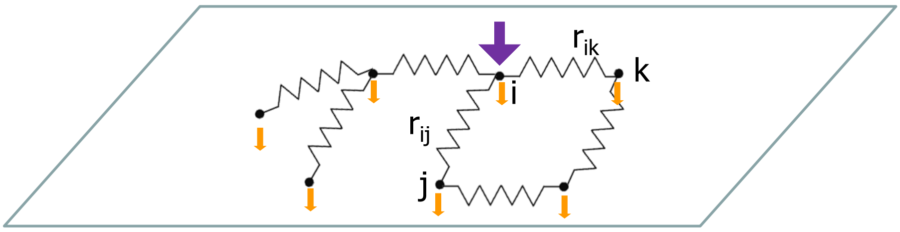

Inverses: $x = Qv \leftrightarrow v = Q^{\dagger} x$ with voltage reference $u^T v = 0$

$Q^{\dagger}$: 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 $v_i = Q^{\dagger}_{ii}$

→ The best spreader is the node k with minimum $Q^{\dagger}_{ii}$

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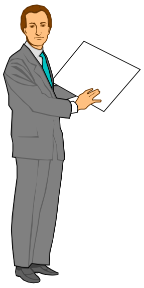

Background:

Electrical matrix equations

Geometry of a graph

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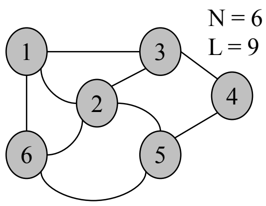
Three representations of a graph

Topology domain



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

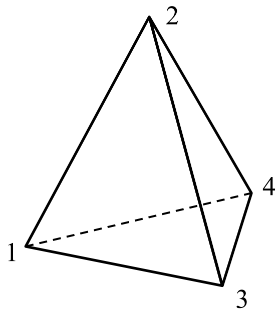
Spectral domain

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

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

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

Geometric domain



Simplex in Euclidean *N*-dimensional space

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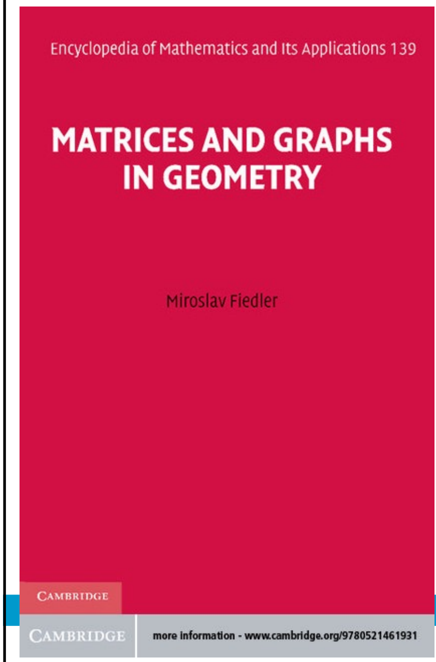


appeared in 2011

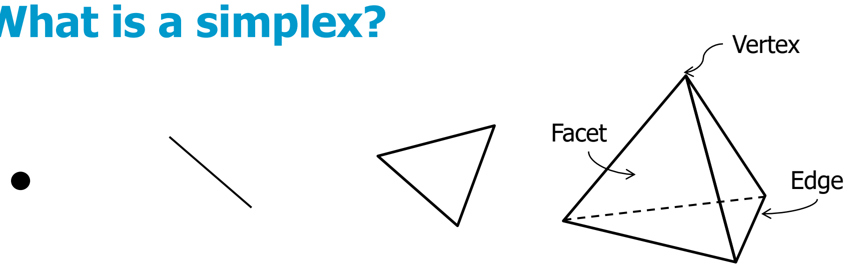
Miroslav Fiedler (1926-2015)

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."

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

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 $Z^TZ = Z\,Z^T = I$ 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)

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

Spectral decomposition weighted Laplacian (2)

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

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

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

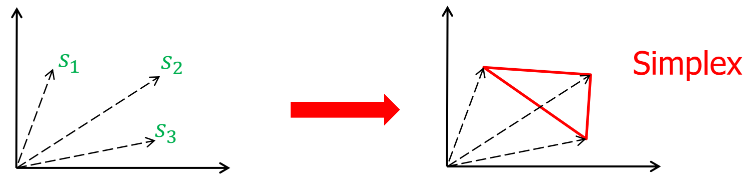
$$S = \begin{bmatrix} \sqrt{\mu_1}(z_1)_1 & \sqrt{\mu_1}(z_1)_2 & \cdots & \sqrt{\mu_1}(z_1)_N \\ \sqrt{\mu_2}(z_2)_1 & \sqrt{\mu_2}(z_2)_2 & \cdots & \sqrt{\mu_2}(z_2)_N \\ \vdots & \vdots & \ddots & \vdots \\ \sqrt{\mu_{N-1}}(z_{N-1})_1 & \sqrt{\mu_{N-1}}(z_{N-1})_2 & \cdots & \sqrt{\mu_{N-1}}(z_{N-1})_N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

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

Geometrical representation of a graph

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

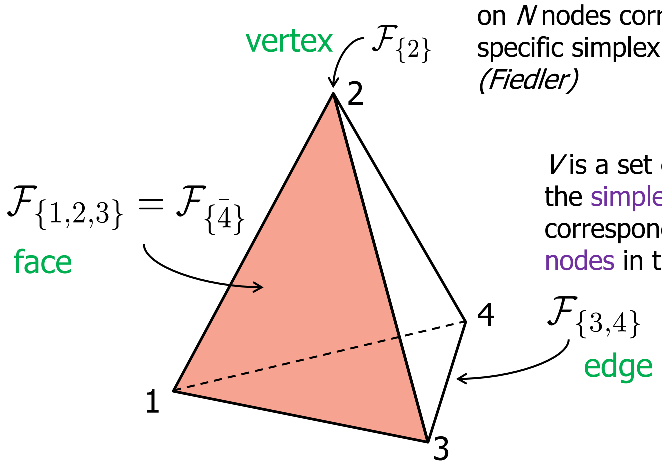
The i-th column vector $s_i = \left(\sqrt{\mu_1}(z_1)_i, \sqrt{\mu_2}(z_2)_i, \cdots, \sqrt{\mu_N}(z_N)_i = 0\right)$ represents a point p_i in (N-1)-dim space (because S has rank N-1)



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

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

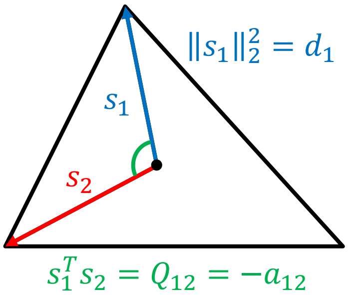
The vector $x_V \in \mathbb{R}^N$ is a barycentric coordinate with $\begin{cases} (x_V)_i \in \mathbb{R} & if \; i \in V \\ (x_V)_i = 0 & if \; i \notin V \end{cases}$

Geometric representation of a graph

$\|s_i\|_2^2 = d_i$ $\qquad \left\|s_i - s_j\right\|_2^2 = \left(s_i - s_j\right)^T\left(s_i - s_j\right) = s_i^T s_i + s_j^T s_j - 2 s_i^T s_j$

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

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



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 *A*!)

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

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

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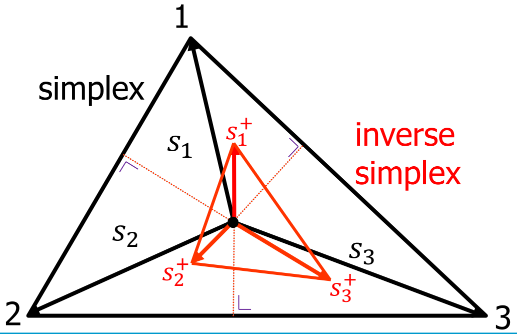
Geometry of a graph (dual representation)

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

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 $\left\|s_i^\dagger - s_j^\dagger\right\|_2^2 = \omega_{ij}$



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

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

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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 $V_G = \frac{N}{(N-1)!}\sqrt{\xi}$

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 $V_G^+ = \frac{1}{(N-1)!\sqrt{\xi}}$

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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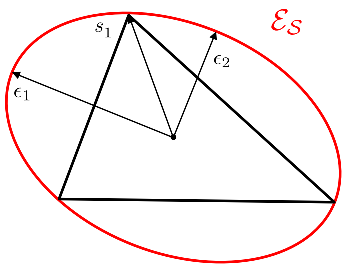
Steiner ellipsoid of simplex



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,

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

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

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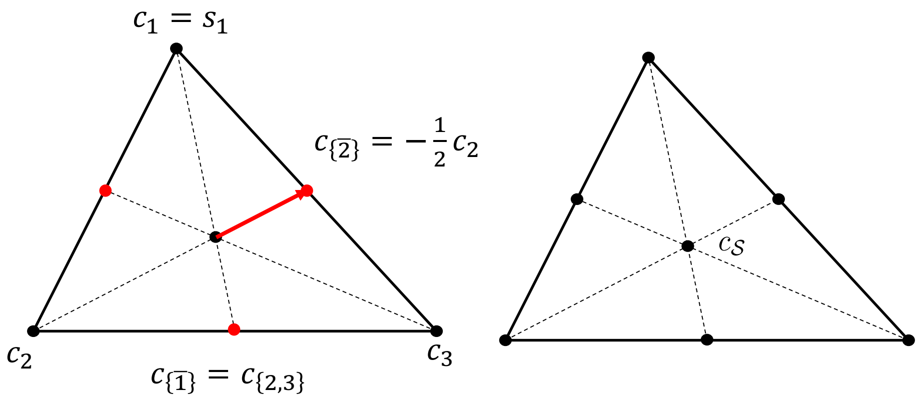
Centroids



a centroid of a face is a vector

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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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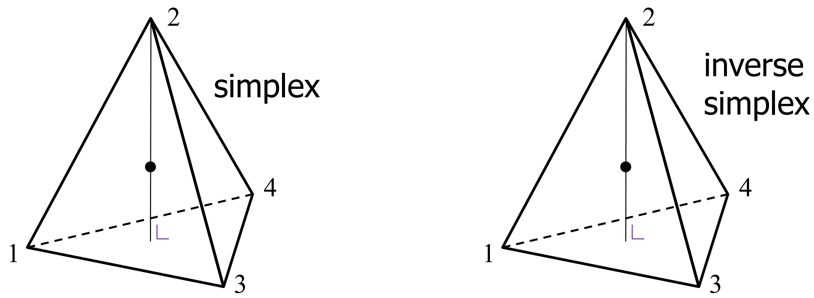
altitude(s) in a simplex

Fiedler



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

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

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

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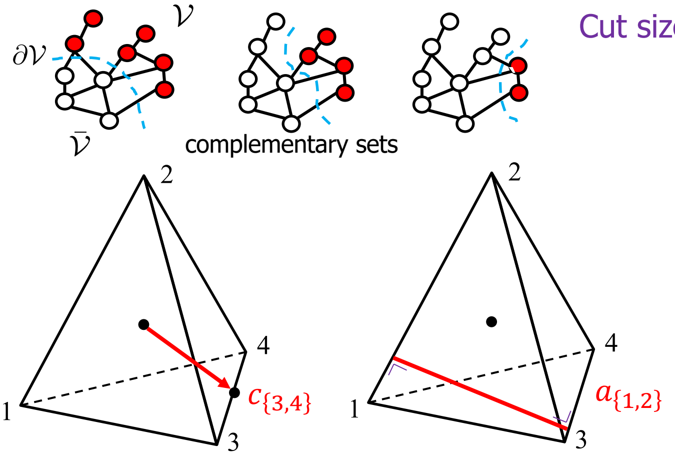
Cut size of graph and altitude of simplex



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

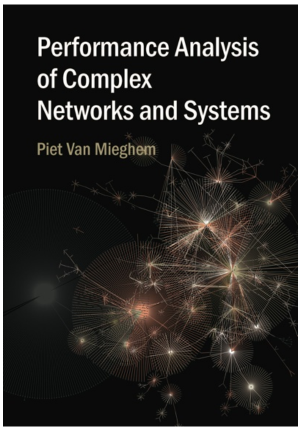
$$\|c_{\{3,4\}}\|^2 = \frac{\partial\{3,4\}}{4} \qquad \|a_{\{1,2\}}\|^2 = \frac{1}{\partial^+\{1,2\}} \qquad |\partial^+ V| = u_V^T Q^\dagger u_V$$

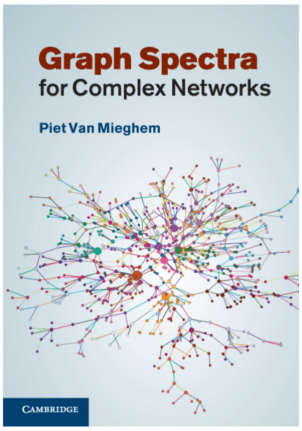
$c_V = S\frac{u_V}{|V|}$ is the centroid of face F_V with $(u_V)_i = 1_{i\in V}$

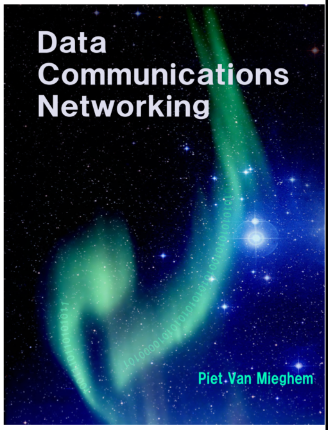
Summary

- 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)
- Open: "*Which network problems are most suitably solved in the simplex representation?"*

Books







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

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