GREEN MATRICES OF WEIGHTED GRAPHS WITH PENDANT VERTICES

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joint work with
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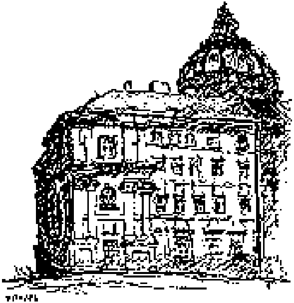

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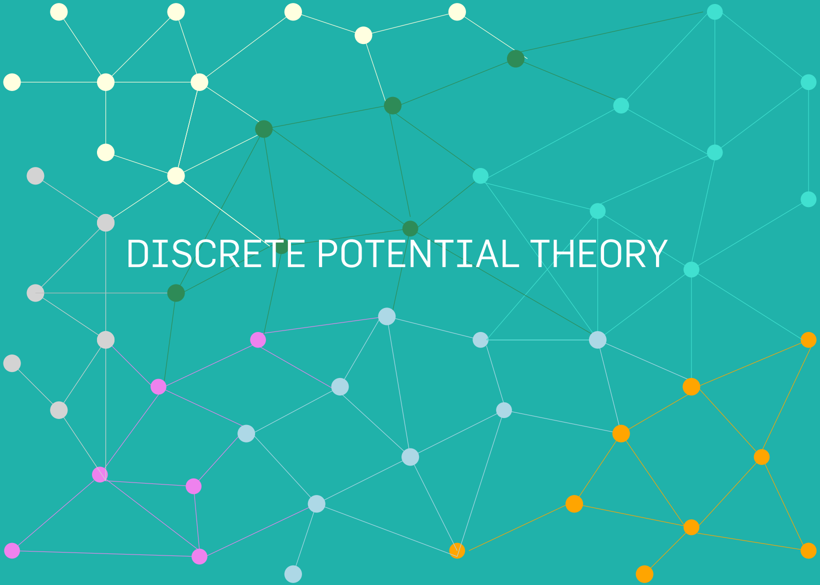
SPAIN

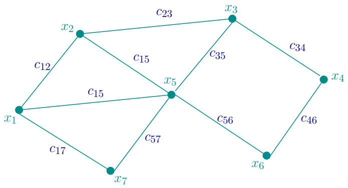
OUTLINE

DISCRETE POTENTIAL THEORY



DEFINITIONS AND CONCEPTS

- A weighted graph $\Gamma = (V, E, c)$ is composed by:
  - V is a set of elements called vertices.
  - E is a set of elements called edges.
  - $c : V \times V \longrightarrow [0, \infty)$ is an application named conductance associated to the edges.
- u, v are adjacent, $u \sim v$ iff $c(u, v) = c_{uv} \neq 0$.
- The degree of a vertex u is $d_u = \sum\limits_{v \in V} c_{uv}$.



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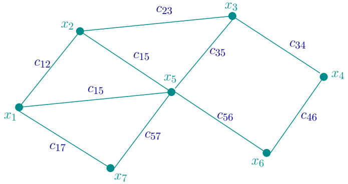

- Consider the set of real-valued functions on V, $\mathcal{C}(V)$, where every function on V is a vector in $\mathbb{R}^n$.

$$\begin{array}{ccc} \mathcal{C}(V) & \longleftrightarrow & \mathbb{R}^n \\ u & \longleftrightarrow & [u(x_1), \ldots, u(x_n)]^T. \end{array}$$

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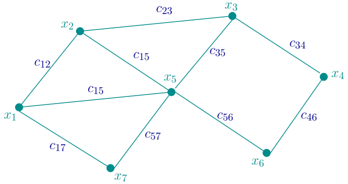

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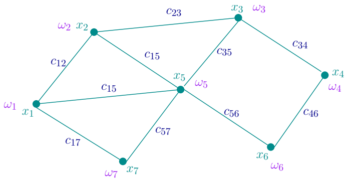

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- A weight is a positive function $\omega : V \longrightarrow (0, +\infty)$. The set of weights is denoted by $\Omega(V)$.

DEFINITIONS AND CONCEPTS

- Any matrix $K \in \mathcal{M}_{n\times n}$ is the kernel of the endomorphism $\mathcal{K}$ of $\mathcal{C}(V)$ that assigns to any $u \in \mathcal{C}(V)$ the function v.

$$\begin{array}{rccc} \mathcal{K}: & \mathcal{C}(V) & \longrightarrow & \mathcal{C}(V) \\ & u & \longrightarrow & \mathcal{K}(u) = Ku = v. \end{array}$$

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Common used operators

	Operator	Kernel
Identity	$\mathcal{I}$	I
Projector on σ along τ	$\mathcal{P}_{\sigma,\tau}(u) = \langle \tau, u \rangle \sigma$	$P_{\sigma,\tau} = \sigma \otimes \tau$
Projector on ω	$\mathcal{P}_{\omega}(u) = \langle \omega, u \rangle \omega$	$P_{\omega} = \omega \otimes \omega$

LAPLACIAN OPERATOR AND LAPLACIAN MATRIX

- The Laplacian operator $\mathcal{L}$ is

$$\begin{array}{rccc} \mathcal{L}: & \mathcal{C}(V) & \longrightarrow & \mathcal{C}(V) \\ & u & \longrightarrow & \mathcal{L}(u) = \sum_{x,y\in V} c_{xy}[u(x)-u(y)]. \end{array}$$

- The corresponding Laplacian matrix is

$$(L)_{ij} = \begin{cases} d_i & if \quad i=j, \\ -c_{ij} & if \quad i\neq j. \end{cases}$$

- For a simple graph, $c_{ij}=1$ for any $i,j\in V$ and the applications of its spectrum have been widely studied in Spectral Graph Theory (The Laplacian Spectrum of Graphs, B. Mohar).
- The general case has not been so well studied.

DISCRETE POTENTIAL THEORY

Definition

The Schrödinger $\mathcal{L}_q$ operator on a network with potential q is a generalization of the Laplacian operator $\mathcal{L}$ defined as

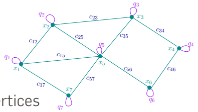
$$\begin{array}{rccc} \mathcal{L}_q : & \mathcal{C}(V) & \longrightarrow & \mathcal{C}(V) \\ & u & \longrightarrow & \mathcal{L}_q(u) = \mathcal{L}(u) + qu, \end{array}$$

where $qu \in \mathcal{C}(V)$ is defined as $qu(x) = q(x)u(x)$, for all $x \in V$.

- The Schrödinger matrix of a network Γ with potential Q is defined as

$$L_q = L + Q, \quad Q = diag(q_1, \dots, q_n).$$

Observe that $\mathcal{L}_q$ can be also considered as the Laplacian operator of a network with loops of value q_i associated of each vertex.



DISCRETE POTENTIAL THEORY

- Any Schrödinger operator $\mathcal{L}_q$ is selfadjoint.
- If $\mathcal{L}_q$ is positive definite, then it is invertible and its inverse is called Green's operator.
- However we are interested in those Schrödinger operators $\mathcal{L}_q$ who are positive semi-definite.
- Now consider $q_\omega = -\frac{1}{\omega}\mathcal{L}(\omega) \in \mathcal{C}(V)$, it is called the potential determined by a weight $\omega \in \Omega(V)$.

Proposition

The Schrödinger operator $\mathcal{L}_q$ with potential q is positive semidefinite iff there exists a weight $\omega \in \Omega(V)$ and a real number $\lambda \geq 0$ such that $q = q_\omega + \lambda$.
In this case λ is the lowest eigenvalue and its associated eigenfunctions are multiples of ω.

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THE POISSON EQUATION

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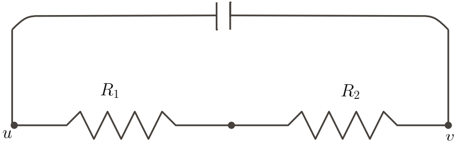
- Our goal is to solve the Poisson equation for $\mathcal{F}$ on V with data $f \in V$, that is to find $u \in V$ such that
$$\mathcal{L}_q(u) = f.$$
- It $\mathcal{L}_q$ is positive semidefinite, then the operator that assigns to each function $f \in \mathcal{C}(V)$ the unique $u \in \mathcal{C}(V)$ such that
$$\mathcal{L}_q(u) = f - \mathcal{P}_\omega(f),$$
is called orthogonal Green's operator $\mathcal{G}_q$, and its kernel G_q is called Green's matrix.
- Notice that
$$\mathcal{G}_q(\omega) = \begin{cases} \frac{1}{\lambda} & \text{if} \quad \lambda \neq 0 \\ 0 & \text{if} \quad \lambda = 0. \end{cases}$$
- Some applications: by knowing the Green's matrix G_q we can compute the effective resistances and the Kirchhoff index of the weighted graph.

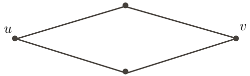
APPLICATIONS: EFFECTIVE RESISTANCES

Klein and Rándic (93) proposed a distance measure between two vertices of electrical networks called the effective resistance

$d(u,v) = 2$



$$R_{uv} = \frac{1}{\frac{1}{R_1}+\frac{1}{R_2}}$$



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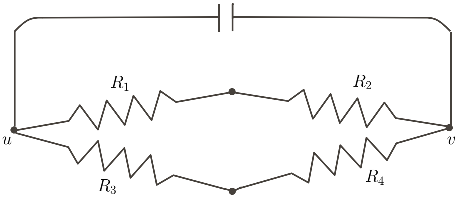

$$R_{uv} = \frac{1}{\frac{1}{R_1+R_2}+\frac{1}{R_3+R_4}}$$

APPLICATIONS: EFFECTIVE RESISTANCES

- Bendito, Carmona, Encinas, Gesto (2008) proved that the resistance distance between any pair of vertices $x, y \in V$ can be computed as the solution of the following linear problem

$$\mathcal{L}(u) = \pi_{x,y},$$

where $\mathcal{L}$ is the Laplacian operator of the weighted graph and $\pi_{x,y} = \varepsilon_x - \varepsilon_y$ is called the dipole between x and y.

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Proposition [Bendito, Carmona, Encinas, Gesto (2009)]

For any $x, y \in V$ it is verified that

$$R_{\lambda,\omega}(x,y) = \frac{(G_q)_{x,x}}{\omega_x^2} + \frac{(G_q)_{y,y}}{\omega_y^2} - \frac{2(G_q)_{x,y}}{\omega_x \omega_y}.$$

APPLICATIONS: KIRCHHOFF INDEX

- Introduced in Chemistry as a better alternative to other parameters for discriminating among different molecules with similar shapes and structures.
- The Kirchhoff index or Total Resistance of the weighted graph is the sum of all the effective resistances between any pair of vertices of the weighted graph.

Corollary [Bendito, Carmona, Encinas, Gesto (2009)]

For any $x, y \in V$ it is verified that

$$k(\lambda,\omega) = trace(G_q) - \begin{cases} \frac{1}{\lambda} & \text{if} \quad \lambda \neq 0 \\ 0 & \text{if} \quad \lambda = 0. \end{cases}$$

PREVIOUS RESULTS

PREVIOUS RESULTS

The Green matrix has been computed for

- Cluster graphs
- Some composite weighted graphs
- Generalized linear polyominoes
- Join graphs
- Perturbations of an edge

PERTURBING THE CONDUCTANCE OF AN EDGE

Corollary [Carmona, Encinas, Mitjana]

Consider $\sigma \in \mathcal{C}(V)$, the perturbation of $\mathcal{F}$ by σ and the operator

$$\mathcal{H}_\sigma = \mathcal{F} + \mathcal{P}_\sigma$$

then when $\langle \sigma, \omega \rangle = 0$

$$\mathcal{G}^{\mathcal{H}} = \mathcal{G} - \frac{1}{1 + \langle \mathcal{G}(\sigma), \sigma \rangle} \mathcal{P}_{\mathcal{G}(\sigma)},$$

whereas, when $\langle \sigma, \omega \rangle \neq 0$

$$\mathcal{H}^{-1} = \mathcal{G} - \frac{1}{\beta} \Big[\lambda \mathcal{P}_{\mathcal{G}(\sigma)} - \langle \sigma, \omega \rangle \left(\mathcal{P}_{\mathcal{G}(\sigma),\omega} - \mathcal{P}_{\omega,\mathcal{G}(\sigma)} \right) - (1 + \langle \sigma, \omega \rangle) \, \mathcal{P}_\omega \Big],$$

where $\beta = \lambda(1 + \langle \mathcal{G}(\sigma), \sigma \rangle) + \langle \sigma, \omega \rangle^2$.

ADDING PENDANT VERTICES

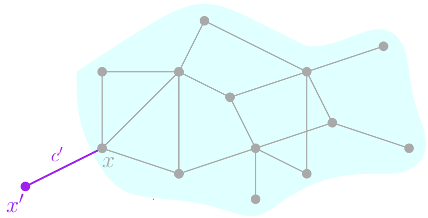
Goal

To study the perturbation of the Green matrix of a weighted graph caused by the perturbation due to add a pendant vertex, relating both Green matrices.

ADDING NEW PENDANT VERTICES

ADDING ONE PENDANT VERTEX X'

- New network: $\Gamma' = (V', E', c')$, $V' = V \cup \{x'\}$, $E' = E \cup \{e_{x,x'}\}$, $c' = c'(x, x') > 0$
- New weight: $\omega_{x'} \in \Omega(V')$, such that $\omega'_{x_i} = \omega_{x_i} / \sqrt{1 + \omega_{x'}^2}$ for any $x_i \in V'$, $i = 0, \dots, n$



- It holds $\omega'_i / \omega'_j = \omega_i / \omega_j$ for any $i, j \in V'$.

ADDING ONE PENDANT VERTEX X'

- The Schrödinger operator of Γ' is

$$\mathcal{L}'_q(u) = \mathcal{L}'(u) + q'u,$$

with $q' = q'_{\omega'} + \lambda$ and $q'_{\omega'} = -\frac{1}{\omega'}\mathcal{L}'(\omega') \in \mathcal{C}(V')$.

- The relation between the kernels of both Schrödinger operators is given by

$$L'_{q'} = \begin{pmatrix} L'_q & -c'\varepsilon_x \\ -c'\varepsilon_x^{\mathsf{T}} & q'_{x,x'} \end{pmatrix},$$

where $L'_q = L_q + c'\frac{\omega_{x'}}{\omega_x}P_{\varepsilon_x}$ is the kernel of the perturbed operator $\mathcal{L}'_q = \mathcal{L}_q + \mathcal{P}_{\sigma_{x,x'}}$, with $\sigma_{x,x'} = \sqrt{c'\frac{\omega_{x'}}{\omega_x}}\varepsilon_x$ and $q'_{x,x'} = c'\frac{\omega_x}{\omega_{x'}} + \lambda \in \mathbb{R}$.

ADDING ONE PENDANT VERTEX

Proposition

The kernel of ${\mathcal{L}'}_{q'}^{-1}$ is

$$(L'_{q'})^{-1} = \begin{pmatrix} H^{-1} & \frac{c'}{q'_{x,x'}} H^{-1}\varepsilon_x \\ \frac{c'}{q'_{x,x'}} \varepsilon_x^{\mathsf{T}} H^{-1} & \frac{1}{q'_{x,x'}} - \frac{c'}{(q'_{x,x'})^2} \varepsilon_x^{\mathsf{T}} H^{-1} \varepsilon_x \end{pmatrix}, \qquad (1)$$

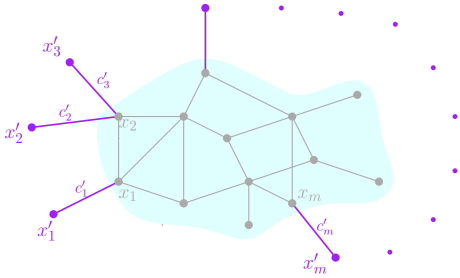
where H^{-1} is the kernel of the operator

$$\mathcal{H}^{-1} = \mathcal{G}_{\lambda,\omega} - \frac{1}{\beta}\Big[\lambda \mathcal{P}_{\mathcal{G}_{\lambda,\omega}(\sigma_{x,x'})} - \langle \sigma_{x,x'}, \omega\rangle \left(\mathcal{P}_{\mathcal{G}_{\lambda,\omega}(\sigma_{x,x'}),\omega} - \mathcal{P}_{\omega,\mathcal{G}_{\lambda,\omega}(\sigma_{x,x'})}\right) - (1 + \langle \sigma_{x,x'}, \omega\rangle)\, \mathcal{P}_\omega\Big],$$

and $\beta = \lambda(1 + \langle \mathcal{G}_{\lambda,\omega}(\sigma_{x,x'}), \sigma_{x,x'}\rangle) + \langle \sigma_{x,x'}, \omega\rangle^2$.

ADDING SEVERAL PENDANT VERTICES $X'_1, \dots, X'_M$

- New network: $\Gamma' = (V', E', c')$, $V' = V \cup \{x'_1, \dots, x'_m\}$, $E' = E \cup \{e_{x_1,x'_1}, \dots, e_{x_m,x'_m}\}$ and $c'_i = c'(x_i, x'_i) > 0$ for $i = 1, \dots, m$
- New weight: $\omega_{x'} \in \Omega(V')$, such that $\omega'_x = \omega_x / \sqrt{1 + \sum_{i=1}^m \omega^2_{x'_i}}$ for any $x_i \in V'$, $i = 0, \dots, n$



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- The Schrödinger operator of Γ' is $\mathcal{L}'_q(u) = \mathcal{L}'(u) + q'u$, with $q' = q'_{\omega'} + \lambda$ and $q'_{\omega'} = -\frac{1}{\omega'}\mathcal{L}'(\omega')$.
- The relation between the kernels of both Schrödinger operators is given by

$$L'_{q'} = \begin{pmatrix} L'_q & B \\ B^\intercal & D_{q'} \end{pmatrix},$$

where $L'_q = L_q + \sum_{i=1}^m c'_i \frac{\omega_{x'_i}}{\omega_{x_i}} P_{\varepsilon_{x_i}}$, $B = (-c'_{x_1}\varepsilon_{x_1}, \dots, -c'_{x_m}\varepsilon_{x_m})$, and $D_{q'}$ is an invertible diagonal matrix having in the diagonal the potential of the new vertices $q'_{x_i,x'_i} = c'_i \frac{\omega_{x_i}}{\omega_{x'_i}} + \lambda \neq 0$.

ADDING SEVERAL PENDANT VERTICES

Proposition

The kernel of $(\mathcal{L}'_{q'})^{-1}$ is

$$(L'_{q'})^{-1} = \begin{pmatrix} H^{-1} & -H^{-1}BD^{-1} \\ -D^{-1}B^{\intercal}H^{-1} & D^{-1}+D^{-1}B^{\intercal}H^{-1}BD^{-1} \end{pmatrix},$$

where H^{-1} is the kernel of the operator

$$\mathcal{H}^{-1} = \mathcal{G} + \alpha\mathcal{P}_\omega + \sum_{i=1}^{m}\beta_i[\mathcal{P}_{\mathcal{G}(\sigma_i),\omega} - \mathcal{P}_{\omega,\mathcal{G}(\sigma_i)}] - \sum_{i,j=1}^{m}\gamma_{ij}\mathcal{P}_{\mathcal{G}(\sigma_i),\mathcal{G}(\sigma_j)},$$

and $(b_{ij}) = (I + \langle\mathcal{G}(\sigma_j),\sigma_i\rangle)^{-1}$, $\alpha = \left(\lambda + \sum_{r,s} b_{r,s}\langle\mathcal{G}(\sigma_j),\sigma_i\rangle\langle\sigma_s,\omega\rangle\right)^{-1}$,

$$\beta_i = \alpha\sum_{r=1}^{m} b_{ir}\langle\sigma_r,\omega\rangle \quad \text{and} \quad \gamma_{ij} = b_{ij} - \alpha\left(\sum_{r=1}^{m} b_{ir}\langle\sigma_r,\omega\rangle\right)\left(\sum_{r=1}^{m} b_{jr}\langle\sigma_r,\omega\rangle\right).$$

EXAMPLE

Green matrix of a Star graph S_n

We compute the Green matrix of a Star graph S_n with constant weight $\omega = \frac{1}{\sqrt{n}} j$ by adding $n-2$ pendant vertices to a S_2.

$$\text{Starting from} \quad L_{\lambda,2} = \begin{pmatrix} 1+\lambda & -1 \\ -1 & 1+\lambda \end{pmatrix}, \quad B = \begin{pmatrix} -j_{n-2} \\ 0_{n-2} \end{pmatrix},$$

$$H = \begin{pmatrix} \frac{\lambda^2+n\lambda+1}{\lambda+1} & -1 \\ -1 & 1+\lambda \end{pmatrix} \Rightarrow H^{-1} = \begin{pmatrix} \frac{1+\lambda}{\lambda^2+n\lambda} & \frac{1}{\lambda^2+n\lambda} \\ \frac{1}{\lambda^2+n\lambda} & \frac{\lambda^2+n\lambda+1}{(\lambda+1)(\lambda^2+n\lambda)} \end{pmatrix}.$$

$$G_{\lambda,n} = \begin{pmatrix} \frac{n-1}{n(\lambda+n)} & \frac{-1}{n(\lambda+n)} & \cdots & \frac{-1}{n(\lambda+n)} \\ \frac{-1}{n(\lambda+n)} & \frac{(n-1)\lambda+(n^2-n-1)}{n(\lambda+1)(\lambda+n)} & \cdots & -\frac{\lambda+n+1}{n(\lambda+n)(\lambda+1)} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{-1}{n(\lambda+n)} & -\frac{\lambda+n+1}{n(\lambda+n)(\lambda+1)} & \cdots & \frac{(n-1)\lambda+(n^2-n-1)}{n(\lambda+1)(\lambda+n)} \end{pmatrix}$$

TO KNOW MORE ABOUT THIS TOPIC ....

Advanced Course on Combinatorial Matrix Theory

Date: February 2015

Location: Centre de Recerca Matemàtica (CRM), Barcelona

Thanks for your attention

Děkuji za pozornost

Gracias por su atención