Asymptotic spectra of large graphs with a uniform local structure

Davide Bianchi

Harbin Institute of Technology (Shenzhen)
School of Science

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Overview

- Preliminaries on graph theory.
- The Poisson problem.
  - Symbol of a sequence of matrices.
- Average sojourn time on a regular d-cycle.
- Refernces

Preliminaries on graph theory

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$$\deg(x) := \sum_{y \in X} w(x, y) + \kappa(x) \quad \text{and} \quad \operatorname{Deg}(x) := \frac{\deg(x)}{\mu(x)}.$$

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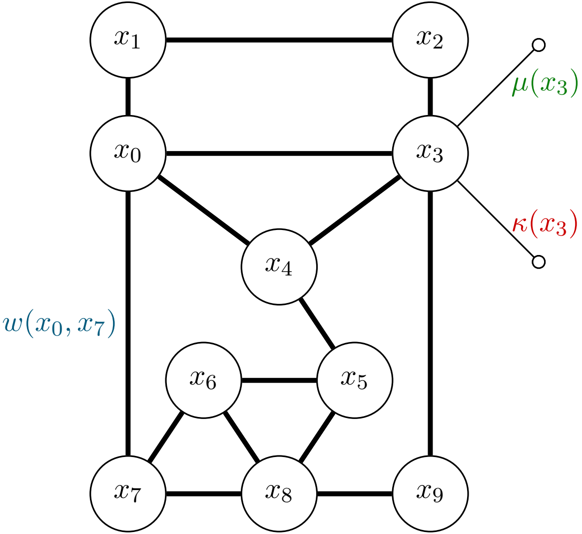
$$C(X) \coloneqq \{u : X \to \mathbb{R}\}.$$

Graphs



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we can write

$$\Delta u(x) \coloneqq \operatorname{Deg}(x)u(x) - \frac{1}{\mu(x)} \sum_{y \in X} w(x,y)u(y).$$

Graph Laplacian - finite case

Let us fix $X = \{x_1, \ldots, x_n\}$ and define

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Then, identifying $u \in C(X)$ with $\boldsymbol{u} \coloneqq (u(x_1), \ldots, u(x_n))^T \in \mathbb{R}^n$, we can write Δ in matrix form,

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W is called adjacency matrix, and D degree matrix.

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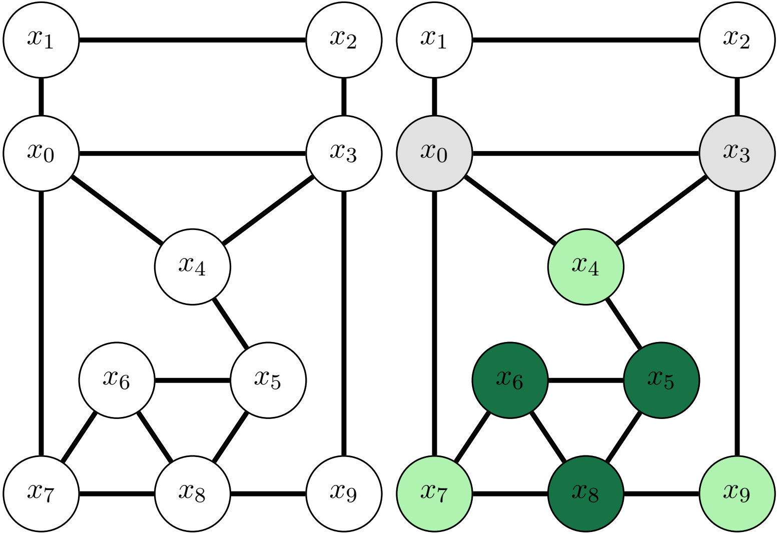
Clearly, $A = \mathring{A} \sqcup \mathring{\partial} A$ and $\dot{\partial} A \subseteq X \setminus A$.

Grafi e sottografi



Subgraphs

Definition (Induced subgraph)

$F = (A, w', \kappa', \mu')$ is the canoncial induced subgraph of $G = (X, w, \kappa, \mu)$ if

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If necessary, we will indicate with Δ_F the graph Laplacian associated to the subgraph F.

Subgraphs

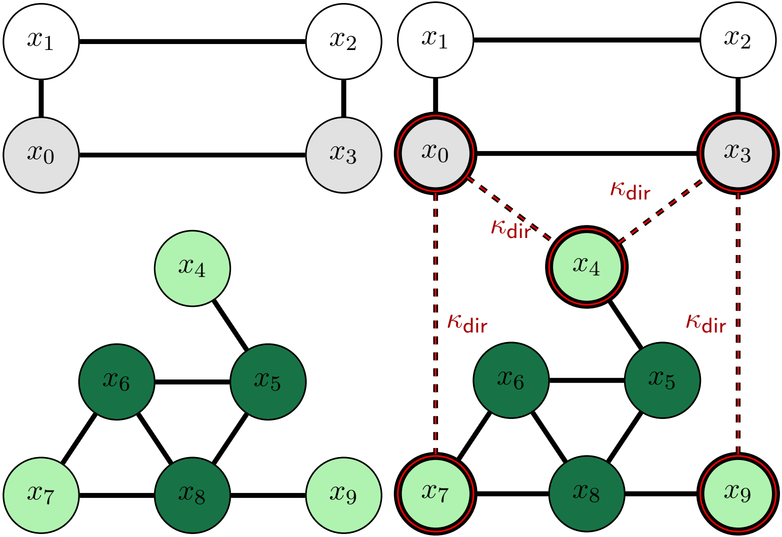
Definition (Dirichlet subgraph)

$F_{\mathsf{dir}} = (A, w', \kappa_{\mathsf{dir}}, \mu')$ is the Dirichlet subgraph of $G = (X, w, \kappa, \mu)$ if

- $A \subset X$;
- $w' \equiv w_{|A \times A}$;
- $\mu' \equiv \mu_{|A}$;
- $\kappa_{\mathsf{dir}}(x) = \kappa(x) + \sum_{y \in X \setminus A} w(x, y)$.

We will indicate with Δ_{dir} the graph Laplacian associated to F_{dir}.

Sottografi


x_1
x_2
x_0
x_3
x_4
x_6
x_5
x_7
x_8
x_9
x_1
x_2
x_0
x_3
κ_{dir}
κ_{dir}
x_4
κ_{dir}
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x_9

Graph Laplacian of a Dirichlet subgraph

Let $\mathbf{i}\colon C(A) \hookrightarrow C(X)$ be the canonical embedding

$$\mathbf{i}v(x) = \begin{cases} v(x) & \text{if } x \in A, \\ 0 & \text{if } x \in X \setminus A. \end{cases}$$

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The Dirichlet graph Laplacian Δ_{dir} can be viewed as the restriction of Δ having imposed (zero) Dirichlet conditions on the exterior boundary $\dot{\partial} A$.

The Poisson problem

Solving the Poisson problem on (finite) graphs

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on $F_{\mathsf{dir}} = (A, w_{|A \times A}, \kappa_{\mathsf{dir}}, \mu_{|A})$.There exists a unique solution for every $g \in C(A)$.

Simple example of a graph with locally uniform structure

The path graph:

$$G = (X_{n+2}, w, \kappa, \mu)$$

where

- $X_{n+2} = \{x_i \mid i = 0, \ldots, n+1\}$,
- $w(x_i, x_j) = \begin{cases} 1 & \text{if } |i-j| = 1, \\ 0 & \text{otherwise.} \end{cases}$
- $\kappa(x_i) = 0$ and $\mu(x_i) = 1$ for every $i = 0, \ldots, n+1$.

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Fix $X_n := \{x_i \mid i = 1, \dots, n\} \subset X_{n+2}$ and

$$F_{\mathsf{dir}} = (X_n, w_{|X_n \times X_n}, \kappa_{\mathsf{dir}}, \mu_{|X_n}) \subset G$$

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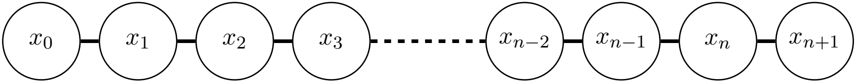

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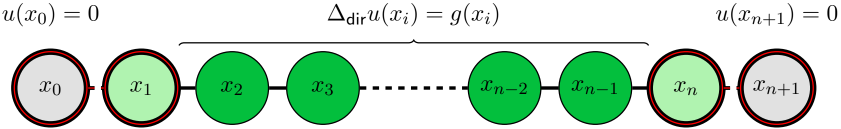

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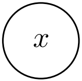
Let us complexify the example

From a single node



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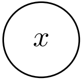
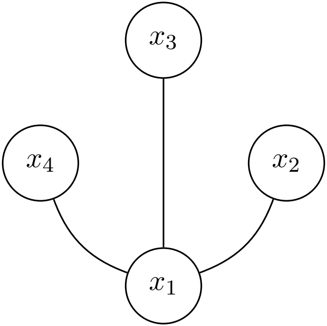


To a “mold/diamond” graph



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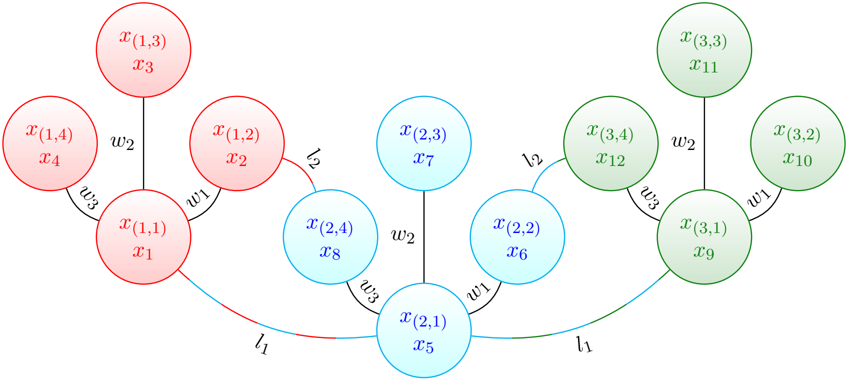
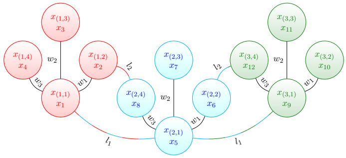


Let us complexifying the example

$$W = \begin{pmatrix} 0 & w_1 & w_2 & w_3 \\ w_1 & 0 & 0 & 0 \\ w_2 & 0 & 0 & 0 \\ w_3 & 0 & 0 & 0 \end{pmatrix}$$

$$L = \begin{pmatrix} l_1 & 0 & 0 & 0 \\ 0 & 0 & 0 & l_2 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

	x_1	x_2	x_3	x_4	x_5	x_6	x_7	x_8	x_9	x_{10}	x_{11}	x_{12}
x_1	0	w_1	w_2	w_3	l_1	0	0	0	0	0	0	0
x_2	w_1	0	0	0	0	0	0	l_2	0	0	0	0
x_3	w_2	0	0	0	0	0	0	0	0	0	0	0
x_4	w_3	0	0	0	0	0	0	0	0	0	0	0
x_5	l_1	0	0	0	0	w_1	w_2	w_3	l_1	0	0	0
x_6	0	0	0	0	w_1	0	0	0	0	0	0	l_2
x_7	0	0	l_2	0	w_2	0	0	0	0	0	0	0
x_8	0	0	0	0	w_3	0	0	0	0	0	0	0
x_9	0	0	0	0	l_1	0	0	0	0	w_1	w_2	w_3
x_{10}	0	0	0	0	0	0	0	0	w_1	0	0	0
x_{11}	0	0	0	0	0	0	l_2	0	w_2	0	0	0
x_{12}	0	0	0	0	0	0	0	0	w_3	0	0	0



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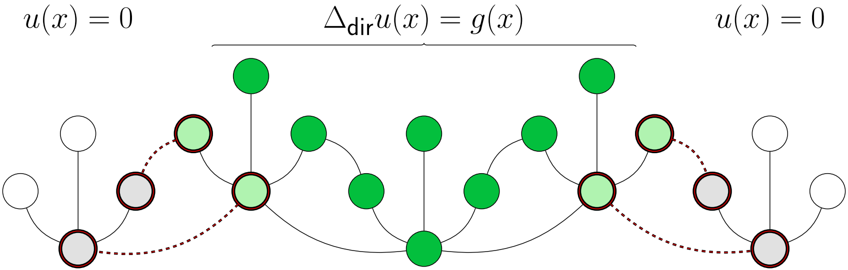

$$F_{\mathsf{dir}} = (X_n, w_{|X_n \times X_n}, \kappa_{\mathsf{dir}}, \mu_{|X_n})$$

Solving the Poisson problem on (finite) graphs

Suppose $|X_n| = d_n$. We need to solve the linear system

$$\Delta_{\mathsf{dir}} \boldsymbol{u} = \boldsymbol{g}. \tag{1}$$

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$$\boldsymbol{u}^{(j+1)} := S(\Delta_{\mathsf{dir}}, \boldsymbol{g}, \boldsymbol{u}^{(j)})$$

be an iterative method for the solution of system (1).

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$$w_1 = 1, \quad w_2 = 2, \quad w_3 = 3, \quad l_1 = 10, \quad l_2 = 1, \quad g(x_{k,i}) = \sin(ki).$$

d_n	Gauss-Seidel
1016	96
4088	> 100
16376	> 100

Solving the Poisson problem on (finite) graphs: TGM

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A Two-Grid Method (TGM) is defined by the following algorithm

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&2.\ \boldsymbol{r}_m = (P_n^m)^H \boldsymbol{r}_n\\
&3.\ \Delta'_{\mathsf{dir}} = (P_n^m)^H \Delta_{\mathsf{dir}} (P_n^m)\\
&4.\ \text{Solve}\, \Delta'_{\mathsf{dir}}\boldsymbol{y} = \boldsymbol{r}_m\\
&5.\ \hat{\boldsymbol{u}}^{(j)} = \boldsymbol{u}^{(j)} - P_n^m \boldsymbol{y}\\
&6.\ \boldsymbol{u}^{(j+1)} = S(\Delta_{\mathsf{dir}}, \hat{\boldsymbol{u}}^{(j)}, \boldsymbol{g})
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where $P_n^m \in \mathbb{C}^{d_n} \times \mathbb{C}^m$, with $m < d_n$, is a full-rank matrix.

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We need to find a “good” P_n^m.

Symbol of a sequence of matrices

Asymptotic spectrum

Definition (Spectral symbol)

Let $\{A_{\boldsymbol{n},\nu}\}_{\boldsymbol{n}}$ be a sequence of matrices and let $\mathfrak{f} : D \to \mathbb{C}^{\nu\times\nu}$ be a measurable Hermitian matrix-valued function defined on the measurable set $D \subset \mathbb{R}^m$, with $0 < \mu_m(D) < \infty$.
We say that $\{A_{\boldsymbol{n},\nu}\}_{\boldsymbol{n}}$ is distributed like $\mathfrak{f}$ in the sense of eigenvalues, in symbols $\{A_{\boldsymbol{n},\nu}\}_{\boldsymbol{n}} \sim_\lambda \mathfrak{f}$, if

$$\lim_{\boldsymbol{n}\to\infty} \frac{1}{d_{\boldsymbol{n}}} \sum_{k=1}^{d_{\boldsymbol{n}}} F(\lambda_k(A_{\boldsymbol{n},\nu})) = \frac{1}{\mu_m(D)} \int_D \sum_{k=1}^{\nu} F\left(\lambda_k(\mathfrak{f}(\boldsymbol{y}))\right) d\mu_m(\boldsymbol{y})$$

for all $F \in C_c(\mathbb{R})$, where $\lambda_1(\mathfrak{f}(\boldsymbol{y})), \ldots, \lambda_\nu(\mathfrak{f}(\boldsymbol{y}))$ are the eigenvalues of $\mathfrak{f}(\boldsymbol{y})$ and $\lambda_1(X_{\boldsymbol{n},\nu}), \ldots, \lambda_{d_{\boldsymbol{n}}}(X_{\boldsymbol{n},\nu})$ are the eigenvalues of $\{X_{\boldsymbol{n},\nu}\}$, sorted in non-decreasing order.

Definition (Monotone rearrangment)

Let $f : \Omega \subset \mathbb{R}^d \to \mathbb{R}$ be measurable on a set Ω with $0 < \mu_d(\Omega) < \infty$. The monotone rearrangement of f is the function denoted by $f^\dagger$ and defined as follows:

$$f^\dagger : (0,1) \to \mathbb{R}, \qquad f^\dagger(y) = \inf\left\{ u \in \mathbb{R} : \frac{\mu_d\{f \leq u\}}{\mu_d(\Omega)} \geq y \right\}.$$

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$$\max_{k=1,\dots,n} \left\{ \left|\lambda_k(A_n) - f^\dagger\left(\frac{k}{n+1}\right)\right| \right\} \to 0 \quad \text{as } n \to \infty.$$

See:

- D. Bianchi, *Analysis of the spectral symbol associated to discretization schemes of linear self-adjoint differential operators*. Calcolo 58.38 (2021): pp. 1–47.
- G. Barbarino, D. Bianchi, and C. Garoni, *Constructive approach to the monotone rearrangement of functions.* Expositiones Mathematicae 40.1 (2021).

Asymptotic spectrum: Examples

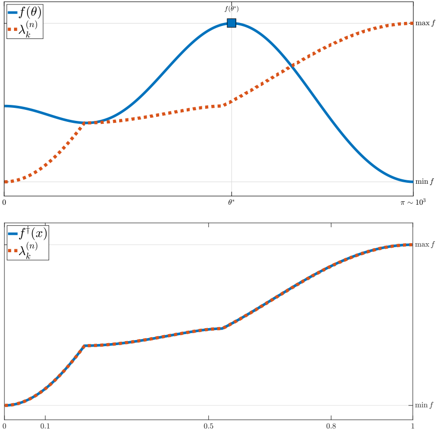
Toeplitz matrix $T_n \in \mathbb{C}^{n\times n}$:

$$T_n = \begin{pmatrix} t_0 & t_{-1} & \cdots & t_{1-n} \\ t_1 & t_0 & \ddots & \vdots \\ \vdots & \ddots & \ddots & t_{-1} \\ t_{n-1} & \cdots & t_1 & t_0 \end{pmatrix},$$

$$\{T_n\}_n \sim t_0 + \sum_{k=1}^{n-1} (t_k + t_{-k}) \cos(k\theta) + (t_k - t_{-k})\imath \sin(k\theta) \; \theta \in [-\pi, \pi].$$

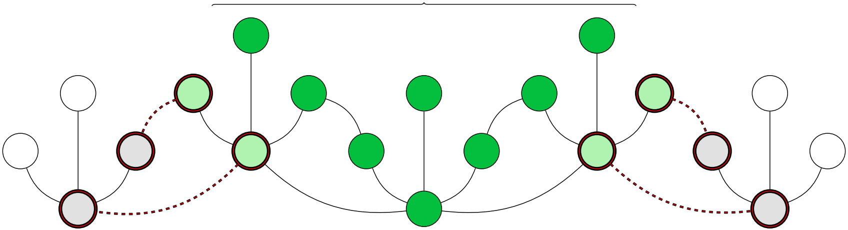
Fix: $t_1 = t_{-1} = 1, \quad t_2 = t_{-2} = -6, \quad t_3 = t_{-3} = 1, \quad t_4 = t_{-4} = 1,$
and 0 all the other coefficients. Then

$$\mathfrak{f}(\theta) = 2\cos(\theta) - 12\cos(2\theta) + 2\cos(3\theta) + 2\cos(4\theta).$$



Asymptotic spectrum: Examples

$u(x) = 0$ $\quad$ $\Delta_{\mathsf{dir}}^{(n)} u(x) = g(x)$ $\quad$ $u(x) = 0$



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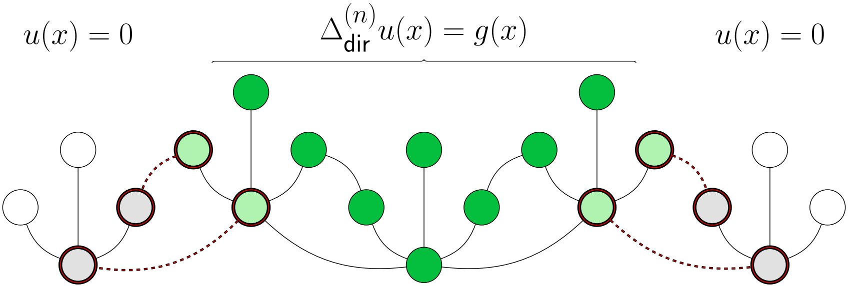
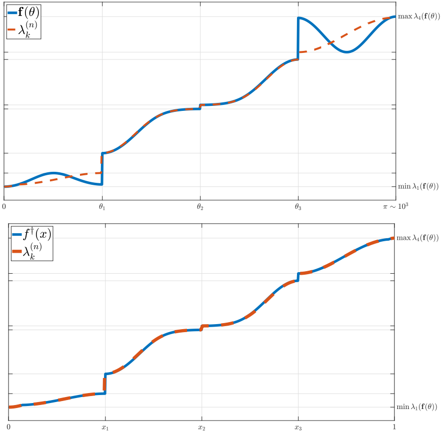


$\{\Delta^{(n)}_{\mathsf{dir}}\}_n \sim_\lambda \boldsymbol{f}(\theta) = D - \left[W + (L + L^T)\cos(\theta) + (L - L^T)\imath\sin(\theta)\right] \in \mathbb{R}^{4\times 4}$, where $\theta \in [-\pi, \pi]$. See

- A. Adriani, D. Bianchi, and S. Serra-Capizzano, *Asymptotic Spectra of Large (Grid) Graphs with a Uniform Local Structure (Part I): Theory*. Milan Journal of Mathematics 88 (2020): pp. 409–454.
- A. Adriani, D. Bianchi, P. Ferrari, S. Serra-Capizzano, *Asymptotic Spectra of Large (Grid) Graphs with a Uniform Local Structure (Part II): Numerical Applications*. Preprint (2021), arXiv: 2111.13859.



It is possible to check that $0 \leq \lambda_1(\boldsymbol{f}(\theta)) < \lambda_2(\boldsymbol{f}(\theta)) < \lambda_3(\boldsymbol{f}(\theta)) < \lambda_4(\boldsymbol{f}(\theta))$ for all $\theta \in [-\pi, \pi]$, and

$$\det(\boldsymbol{f}(\theta)) = 292 - 292\cos(\theta).$$

Hence, we deduce that both the determinant and $\lambda_1(\boldsymbol{f}(\theta))$ have a zero of order 2 in $\theta = 0$.

Solving the Poisson problem on (finite) graphs: TGM

Once we know that $\lambda_1(\boldsymbol{f}(\theta))$ has only one zero of order 2 in $\theta = 0$, that is, $\boldsymbol{f}^\dagger(\theta)$ has only one zero of order 2 in $\theta = 0$, we can prescribe a suitable grid transfer operator P_n^m for the TGM.

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$$P_n^m = T_n(p)K_n$$

where $T_n(p)$ is the Toeplitz matrix generated by the Fourier coefficients of the polynomial p and K_n is the cutting matrix

$$K_n = [\delta_{i-\mathfrak{g}j}]_{i,j}, \quad i = 0, \dots, n-1;\ j = 0, \dots, k-1, \qquad \delta_\ell = \begin{cases} 1 & \text{if } \ell \equiv 0 \pmod{n}, \\ 0 & \text{otherwise} \end{cases}.$$

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Choose $p : [0,\pi] \to \mathbb{R}$ such that

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Then the TGM is optimal. See

- A. Adriani, D. Bianchi, P. Ferrari, S. Serra-Capizzano, *Asymptotic Spectra of Large (Grid) Graphs with a Uniform Local Structure (Part II): Numerical Applications*. Preprint (2021), arXiv: 2111.13859. (And all references therein.)

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Asymptotic spectrum: Examples

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- G_i and G_j are connected if and only if $|i-j| \in \{t_1, \ldots, t_r\}$.

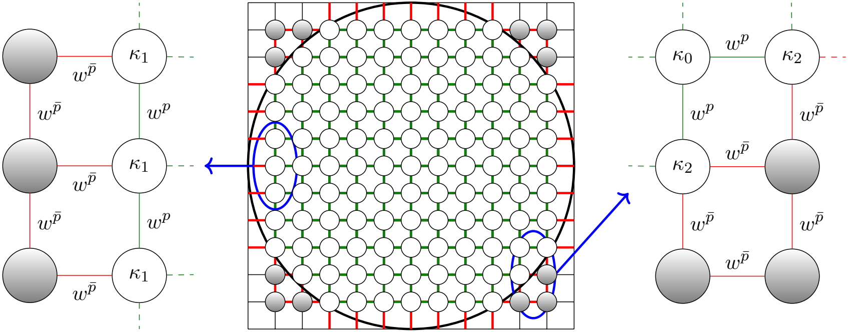
Then $\{W^{(n)}\} \sim_\lambda \boldsymbol{f}(\theta)$,

$$\boldsymbol{f}(\theta) = W + \sum_{k=1}^{r} \left(L_{t_k} + L_{t_k}^T\right) \cos(t_k\theta) + \sum_{k=1}^{m} \left(L_{t_k} - L_{t_k}^T\right) \imath \sin(t_k\theta).$$

Asymptotic spectrum: Examples

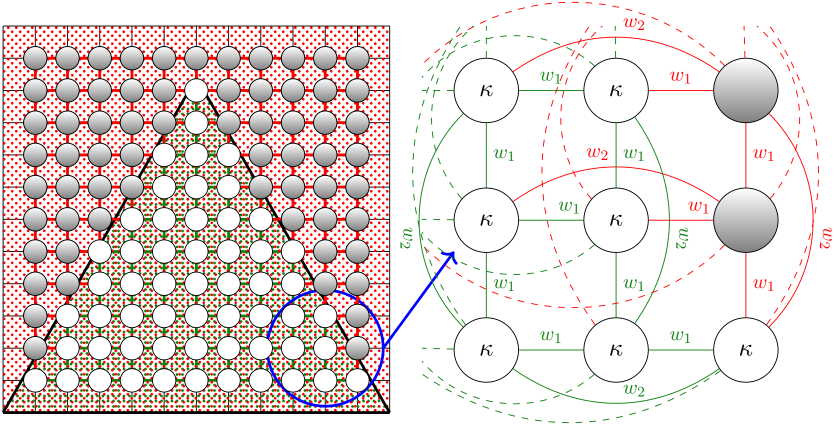
It is possible to compute explicitly the symbol functions for subgraphs too.

A grid graph inside a sphere



Asymptotic spectrum: Examples

A graph inside a triangle



Average sojourn time on a regular d-cycle

Consider a sequence of graphs $\{G_n\}_n$ with number of nodes n_d and zero killing term, and the correspondent sequence of graph Laplacians $\{\Delta_n\}_n$. Fix $\alpha \in (0, 2]$.

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then

$$\{\Delta_n^{\alpha/2}\}_n \sim_\lambda \frac{1}{(f(\boldsymbol{\theta}))^{\alpha/2}}, \qquad \boldsymbol{\theta} \in [0,\pi]^d$$

and

$$\lim_{n_d\to\infty} \frac{1}{n_d} \sum_{k=2}^{n_d} \frac{1}{\lambda_k^{\alpha/2}} = \frac{1}{\pi^d} \int_{[0,\pi]^d} \frac{1}{(f(\boldsymbol{\theta}))^{\alpha/2}} \, d\boldsymbol{\theta}.$$

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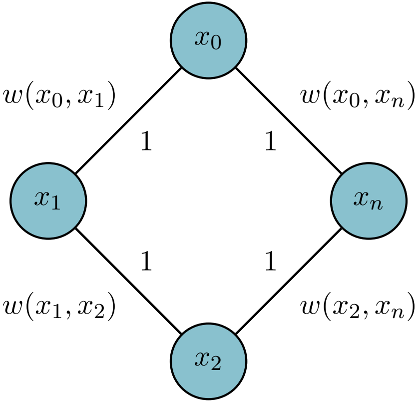
This can be helpful to compute the average sojourn time, on a departure node x_0, of a discrete random walk for a regular graph,

$$T_0 = \lim_{n_d \to \infty} \frac{1}{n_d} \sum_{k=2}^{n_d} \frac{1}{\lambda_k^{\alpha/2}}.$$

See

- T. M. Michelitsch, B. A. Collet, A. P. Riascos, A. F. Nowakowski, and F. C. G. A. Nicolleau. *Recurrence of random walks with long-range steps generated by fractional Laplacian matrices on regular networks and simple cubic lattices*. Journal of Physics A: Mathematical and Theoretical 50 (2017): 505004.

Consider a cycle G_n with n nodes



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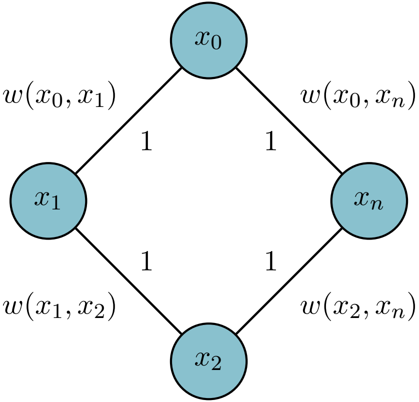

and G_n^d be the d-dimensional cycle, with $d \in \mathbb{N}$. Then

$$(f(\boldsymbol{\theta}))^{\alpha/2} = \left(\sum_{j=1}^{d} 2 - 2\cos(\theta_j) \right)^{\frac{\alpha}{2}}.$$

T_0 is then finite if and only if

$$\int_{[0,\pi]^d} \frac{1}{\left(\sum_{j=1}^{d} 2 - 2\cos(\theta_j)\right)^{\frac{\alpha}{2}}} \, d\boldsymbol{\theta} < \infty.$$

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Therefore, by standard calculus, T_0 is finite if and only if

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that is, by passing to spherical coordinates, if and only if

$$\int_0^\pi \frac{\rho^{d-1}}{(\rho^2)^{\frac{\alpha}{2}}}\, d\rho < \infty,$$

which is true if and only if $0 < \alpha < d$. It follows then that we have recurrence if and only if $\alpha \geq d$ and transience if and only if $0 < \alpha < d$.

Possible future directions of research

- Study the nonlinear Poisson equation $\Delta\Phi u = g$ on large/infinite graphs;
- Study recurrence properties of "diamond" graphs with complex structures;
- Applications? Chemistry, Biology, etc.

References

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