Spectral partitions of quantum graphs

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(joint work with J.B. Kennedy, P. Kurasov, and C. Léna)

February, 2019

Partitioning domains

Goal: subdivide $\Omega \subset \mathbb{R}^2$ in 2 subsets as homogeneous as possible

- nodal: find two subsets on which smooth functions are "almost constant", with most of the gradient at their mutual boundary.
- Cheeger: find two subsets of size as close as possible, penalizing size of their mutual boundary.

Idea: supports of positive and negative part of the first sign-changing eigenfunction of (Dirichlet) Laplacian or 1-Laplacian on Ω

Goal: subdivide $\Omega \subset \mathbb{R}^2$ in **k** subsets as homogeneous as possible

- Courant 1923: the k-th eigenfunction of Δ_Ω^D has at most k nodal domain.
- Pleijel 1956: only finitely many eigenfunctions attain this bound, asymptotically #nodal domains of k-th eigenfunction is rather $\approx \frac{2}{3}k$.
- Cheeger: ???

Spectral partitions on domains

Goal: find a partition $\mathcal{P}$ of $\Omega \subset \mathbb{R}^n$ in **precisely** k open, connected, disjoint subdomains $\omega_1, \ldots, \omega_k$.

$\mathcal{P} \equiv (\omega_1, \omega_2) \mapsto \max\left\{\lambda_1^D(\omega_1), \lambda_1^D(\omega_2)\right\}$ has a minimum given by a nodal partition.

Idea: Consider the functional

$$\Lambda_{k,\infty} : \mathcal{P} \mapsto \max_{1 \le i \le k} \lambda_1^D(\omega_i)$$

or

$$\Lambda_{k,p} : \mathcal{P} \mapsto \left(\frac{1}{k}\sum_{i=1}^{k}(\lambda_1^D(\omega_i))^p\right)^{\frac{1}{p}}, \qquad p > 0.$$

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Rationale

Faber–Krahn: the first Dirichlet eigenvalue on ω is minimal (among all domains of $\mathbb{R}^n$ with same volume) precisely when ω is a Euclidean ball.

$\rightsquigarrow$ In order to minimize $\Lambda_{k,p}$, each ω_i tends to get as close as possible to a ball.

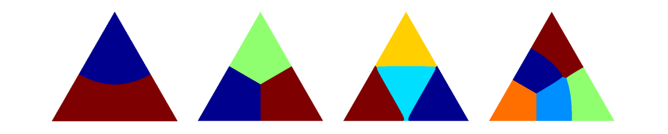


Figure: Minimal partitions for $p = 50$ and $k = 2, 3, 4, 5$ (Bogosel–Bonnaillie-Noël 2017)

Existence of p-minimal k-partitions

Theorem (Conti–Terracini–Verzini, Calc. Var. 2005)

$\Lambda_{k,p}$ has a minimum over a (reasonable) class of k-partitions, for all $p > 0$ and $k \geq 2$.

(proof based on abstract variational results for free boundary problems)

Further properties of planar partitions

Theorem (Helffer–Hoffmann-Ostenhoff–Terracini, Ann. H. Poincaré AN 2009)

Let $n = 2$ and $\mathcal{P}^*$ be an ∞-minimal k-partition.

- *If $n = 2$ and the dual graph of $\mathcal{P}^*$ is bipartite, then there is u s.t.*

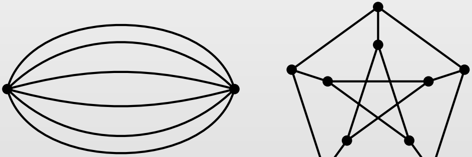
$$-\Delta_\Omega^D u = \Lambda_{k,p}(\mathcal{P}^*)u$$

  and whose nodal set agrees with $\mathcal{P}^*$.
- *$\mathcal{P}^*$ is an equipartition, i.e., $\lambda_1^D(\omega_i) = \lambda_1^D(\omega_j)$ for all i, j.*

Graphs and metric graphs

$G = (V, E)$, with

- $V = \{v_1, \dots, v_n\}$ finite
- $E = \{e_1, \dots, e_m\}$ finite



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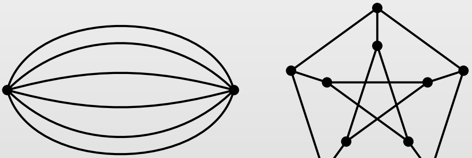

A metric graph $\mathcal{G}$ is obtained by associating an interval $[0, \ell_e]$ with each edge e of G; G is the **discrete graph underlying** $\mathcal{G}$.

No boundary conditions can be imposed on functions in

$$L^2(\mathcal{G}) := \bigoplus_{e \in E} L^2(0, \ell_e)$$

so **functions in $L^2(\mathcal{G})$ do not see the combinatorics of $\mathcal{G}$.**

Introduce

$$C(\mathcal{G}) := \{f \in \bigoplus_{e \in E} C[0, \ell_e] : f \text{ is continuous at each } v \in V\}$$

and

$$H^1(\mathcal{G}) := \{f = (f_e)_{e \in E} \in L^2(\mathcal{G}) \cap C(\mathcal{G}) : f_e \in H^1(0, \ell_e)\ \forall e \in E\}$$

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Spectral gap of quantum graphs

Consider

$$\lambda_1(\mathcal{G}) := \inf_{\substack{f\in H^1(\mathcal{G})\\ f\perp 1}} \frac{\|f'\|^2_{L^2(\mathcal{G})}}{\|f\|^2_{L^2(\mathcal{G})}}$$

$\lambda_1(\mathcal{G})$ is the spectral gap of $\Delta_{\mathcal{G}}$, the self-adjoint, positive semidefinite operator on $L^2(\mathcal{G})$ associated with

$$a(f) := \sum_{\mathrm{e}\in\mathrm{E}} \int_0^{\ell_{\mathrm{e}}} |f'|^2, \quad f \in H^1(\mathcal{G})$$

Nicaise, Bull. Sc. 1987;... Berkolaiko–Kennedy–Kurasov–M. 2018; ...

Partitioning metric graphs

Goal: subdivide $\mathcal{G}$ in k subsets as homogeneous as possible

- Cheeger

  Nicaise, Bull. Sc. math. 1987; Kurasov, Acta Phys. Pol. 2013; Kennedy–M., PAMM 2016; Del Pezzo–Rossi, Mich. Math. J. 2016

- nodal

  Gnutzmann–Smilansky–Weber, Waves Random Media 2004; Berkolaiko Comm. Math. Phys. 2008

Energy functional on partitions

For a given partition $\mathcal{P}$ of $\mathcal{G}$ into k **clusters** $\mathcal{G}_1, \ldots, \mathcal{G}_k$ consider

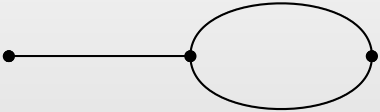
$$\Lambda_{k,\infty} : \mathcal{P} \mapsto \max_{1 \le i \le k} \lambda_1(\mathcal{G}_i).$$

or

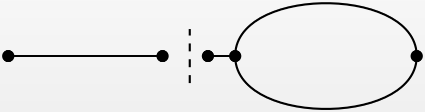
$$\Lambda_{k,p} : \mathcal{P} \mapsto \left(\frac{1}{k} \sum_{i=1}^{k} (\lambda_1(\mathcal{G}_i))^p \right)^{\frac{1}{p}}, \qquad p > 0.$$

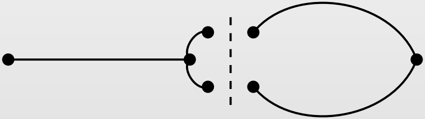
Goal: Minimize these functionals over all partitions of $\mathcal{G}$.

How to partition a quantum graph?



- **proper** partitions
  (Band–Berkolaiko–Raz–Smilanski, Comm. Math. Phys. 2012)





- **faithful** partitions

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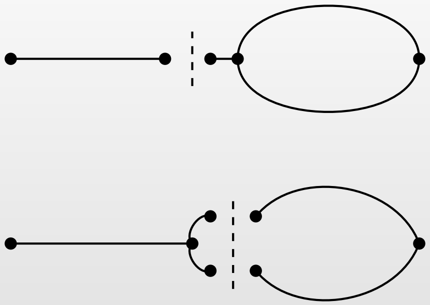
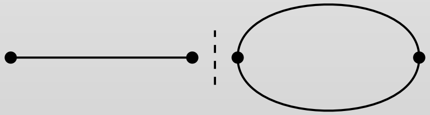
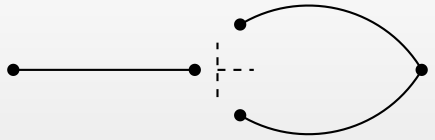


- **faithful** partitions



- **rigid** partitions



- **lax** partitions

Lax partitions are the most general ones: $\mathfrak{P}_k$;
rigid partitions are better behaved: $\mathfrak{R}_k$.

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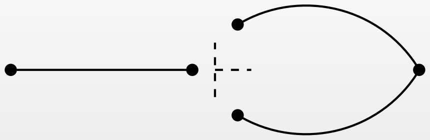

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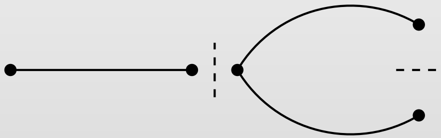
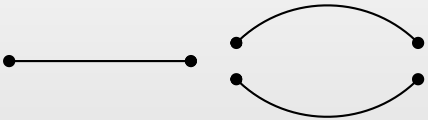


Lax partitions are the most general ones: $\mathfrak{P}_k$;
rigid partitions are better behaved: $\mathfrak{R}_k$.

An *invalid* 2-partition...



...but a valid (and faithful) 3-partition.

Theorem

1) For each k and each p there is

- *a* **lax** *partition* $\mathcal{P}^*_{lax}$ *minimizing* $\Lambda_{k,p} : \mathfrak{P}_k \to \mathbb{R}$, $\tilde{\mathcal{P}}$ *is generally not rigid;*
- *a* **rigid** *partition* $\mathcal{P}^*$ *minimizing* $\Lambda_{k,p}|_{\mathfrak{R}_k} : \mathfrak{R}_k \to \mathbb{R}$.

2) The restrictions of $\Lambda_{k,p}$ to the classes of **proper** *or* **faithful** *partitions don't generally have minima.*

We call

- $\Lambda_{k,p}(\mathcal{P}^*_{\text{lax}})$ **lax** (k,p)-**energy**;
- $\Lambda_{k,p}(\mathcal{P}^*)$ **rigid** (k,p)-**energy**.

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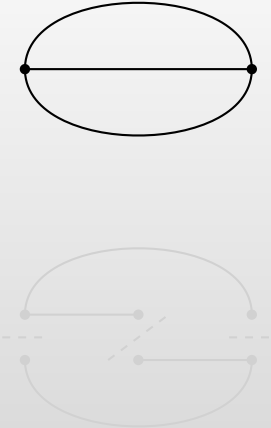
When is a rigid partition minimal?

Proposition

If $\mathcal{P}^* \in \mathfrak{R}_k$ s.t. $\Lambda_{k,\infty}(\mathcal{P}^*) = \frac{\pi^2 k^2}{|\mathcal{G}|^2}$, then $\mathcal{P}^*$ is the minimizer of $\Lambda_{k,\infty}$.

3-pumpkin and a rigid ∞-minimal 2-partition



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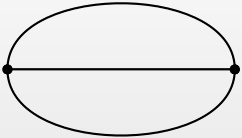
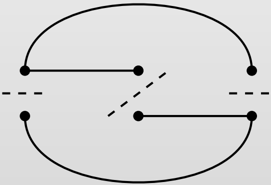
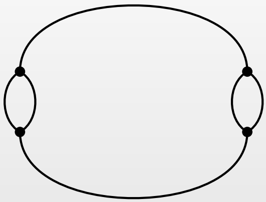




Headphone graph: its lax $(2,\infty)$-energy is given by one rigid and one lax partition.



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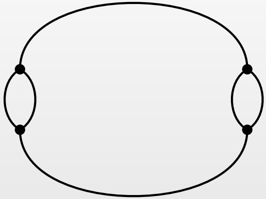
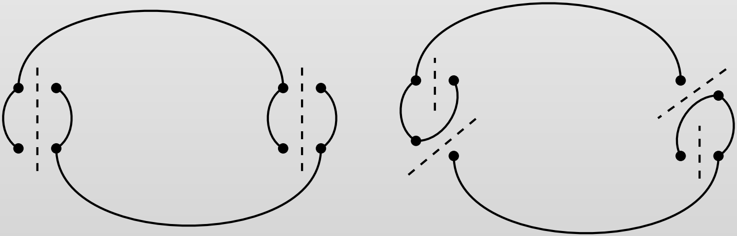
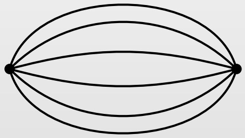




6-pumpkin: its lax $(2, \infty)$-energy is given by a rigid partition.



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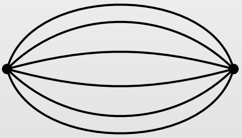
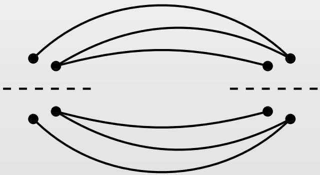
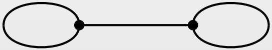
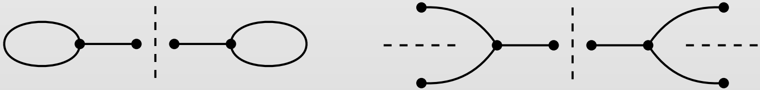




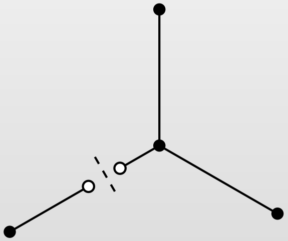
A dumbbell: lax $(2,\infty)$-energy and rigid $(2,\infty)$ do not agree.





Dirichlet problems

An **internally connected** partition is a rigid partition whose clusters are still connected after removal of separation points between clusters.



One can likewise study

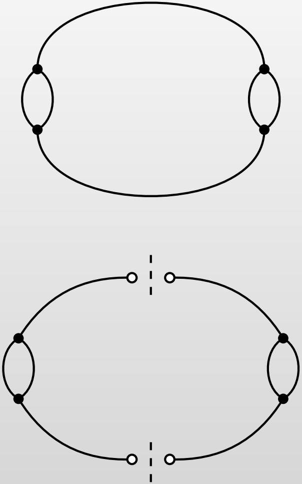
$$\Lambda^D_{k,\infty} : \mathcal{P} \mapsto \max_{1\le i\le k} \lambda^D_1(\mathcal{G}_i).$$

or

$$\Lambda^D_{k,p} : \mathcal{P} \mapsto \left(\frac{1}{k}\sum_{i=1}^k (\lambda^D_1(\mathcal{G}_i))^p\right)^{\frac{1}{p}}, \qquad p > 0;$$

Dirichlet conditions are imposed in each separation point; the restriction of $\Lambda^D_{k,p}$ to the class of internally connected partitions doesn't generally have a minimum.

Headphone graph: a minimal, internally connected Dirichlet partition



Monotonicity properties

Denote

$$\mathcal{L}_{k,p} := \min\{\Lambda_{k,p}(\mathcal{P}) : \mathcal{P} \in \mathfrak{R}_k\}$$

Proposition

1) $\mathcal{L}_{k,p}$ *is monotonically increasing in* p *for any* k*.*
2) $\mathcal{L}_{k,p}$ *is eventually monotonically increasing in* k *for any* p*.*

Conjecture

Every $\mathcal{G}$ admits a rigid 2-partition $\mathcal{P} = \{\mathcal{G}_1, \mathcal{G}_2\}$ such that

$$\lambda_1(\mathcal{G}) \le \min\{\lambda_1(\mathcal{G}_1), \lambda_1(\mathcal{G}_2)\}.$$

The conjecture is true for loops.

Proposition

The conjecture is true whenever $\mathcal{G}$ has a cutvertex.

If the conjecture fails for $\mathcal{G}$, then $\mathcal{L}_{1,p} > \mathcal{L}_{2,p}$ for any p.

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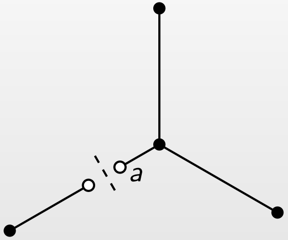
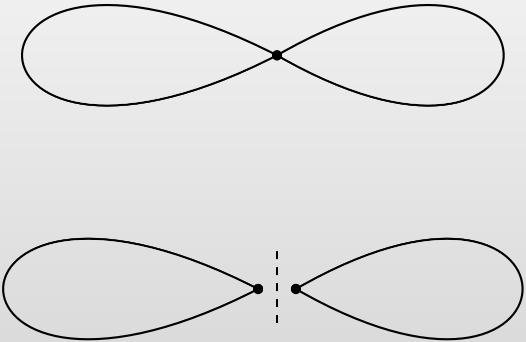
Example: the minimal partition may depend on p.



- Each internally connected 2-partition is parametrized by $a \in (0, 1)$.
- For all $p > 0$ there is one $a_p \in (0, 1)$ whose corresponding partition $\mathcal{P}_{a_p}$ achieves the minimum of $\Lambda^D_{2,p}$; $p \mapsto a_p$ is real analytic, $a_p > 0$, $\frac{d}{dp} a_p < 0$, and $\lim_{p\to\infty} a_p = 0$.

Example: minimal *rigid* partitions need not be equipartitions.



Metrizing spaces of graphs

Given G, let

$$\Gamma_{\mathsf{G}} := \{\mathcal{G} : \text{underlying discrete graph of } \mathcal{G} \text{ is } \mathsf{G}\} \ ;$$

each $\mathcal{G} \in \Gamma_{\mathsf{G}}$ is uniquely determined by $(\ell_{\mathsf{e}})_{\mathsf{e}\in\mathsf{E}}$.

- Γ_{G} is a (non-complete) metric space wrt

$$d_{\Gamma_{\mathsf{G}}}(\mathcal{G},\tilde{\mathcal{G}}) := d_{\mathbb{R}^m}((\ell_{\mathsf{e}}),(\ell_{\tilde{\mathsf{e}}})) \ ;$$

- denote its completion by $\overline{\Gamma_{\mathsf{G}}}$.

Metrizing spaces of partitions

- For a given k, call two lax partitions $\mathcal{P}, \tilde{\mathcal{P}}$ "color equivalent" if $\tilde{\mathcal{P}}$ can be obtained from $\mathcal{P}$ by shifting the separation points inside edges' interiors;
- Color equivalence is an equivalence relation on $\mathfrak{P}_k$;
- Two partitions in the same equivalence class are defined by clusters $\mathcal{G}_1, \ldots, \mathcal{G}_k$ having same underlying discrete graphs $\mathsf{G}_1, \ldots, \mathsf{G}_k$.
- Given two lax k-partitions in the same equivalence class, define

$$d_{\mathfrak{P}_k}(\mathcal{P}_1, \mathcal{P}_2) := \sum_{i=1}^{k} d_{\Gamma_{\mathsf{G}_i}}(\mathcal{G}_i, \tilde{\mathcal{G}}_i).$$

- $\mathfrak{P}_k$ is a (non-complete) metric space wrt $d_{\mathfrak{P}_k}$;
- the limit of a sequence of partitions in the completion $\overline{\mathfrak{P}_k}$ is an m-partition for some $m \leq k$;
- the set of rigid k-partitions is closed in $\overline{\mathfrak{P}_k}$;
- the sets of proper, faithful, or internally connected partitions are not.

Unfortunately, $\overline{\mathfrak{P}_k}$ or $\overline{\mathfrak{R}_k}$ are NOT compact. And yet:

Theorem

$J : A \to \mathbb{R}$ attains its minimum at a lax (resp., rigid) m-partition, $m \leq k$, if

- *$A \subset \overline{\mathfrak{P}_k}$ (resp., $A \subset \overline{\mathfrak{R}_k}$)*
- *J is lsc*

If additionally

- *[coercivity-/monotonicity-type techn. assumpt.]*

then the minimizer is actually a k-partition.

Back to $\Lambda_{k,p}$

Meaning of the "coercivity" conditions:
$\Lambda_{k,p}(\mathcal{P}) = +\infty$ if $\mathcal{P}$ is an m-partition with $m < k$.

Indeed, $\Lambda_{k,p}$ satisfies it by Nicaise' inequality

$$\lambda_1(\mathcal{G}) \geq \frac{\pi^2}{|\mathcal{G}|^2}$$

(Same for $\Lambda^D_{k,p}$, since $\lambda^D_1(\mathcal{G}) \geq \frac{\pi^2}{4|\mathcal{G}|^2}$)

Clustering vertices/data

Goal: given a graph $G = (V, E)$, subdivide V in k subsets as homogeneous as possible

- nodal

  Fiedler, Czech. Math. J. 1975;

  Davies–Gladwell–Leydold–Stadler, LAA 2001

- Cheeger

  Dodziuk, TAMS 1984; Alon–Milman, J. Comb. Th. 1985; Bühler–Hein, Proc. ICML 2009;

  Lee–Oveis Gharan–Trevisan, JACM 2012

- spectral

  Osting–White–Oudet, SIAM J. Sci. Comp. 2014

A von Below-like inequality

Proposition (Amini–Cohen-Steiner, Comment. Math. Helv. 2018)

$$\frac{\lambda_k(\mathsf{G}_{\mathcal{P}})\ \Theta(\mathcal{P})}{2} \leq \lambda_k(\mathcal{G})$$

where

- $\lambda_k(\mathcal{G})$ k-th eigenvalue of $\Delta_{\mathcal{G}}$;
- $\lambda_k(\mathsf{G}_{\mathcal{P}})$ k-th eigenvalue of the normalized Laplacian of a proximity graph based on $\hat{\mathcal{P}} := \mathcal{P}_1 \cup \mathcal{P}_2$ ($\mathcal{P}_1, \mathcal{P}_2$ any lax partitions of $\mathcal{G}$);
- $\Theta(\mathcal{P}) := \min \lambda_1(\mathcal{G}_i)$

Heat content

Given an open domain $\Omega \subset \mathbb{R}^n$:

$$Q_\Omega(t) := \int_\Omega e^{t\Delta_D}\mathbf{1}(x)\ dx = \sum_{j=1}^{\infty} e^{t\lambda_j^\Omega}\left(\int_\Omega \phi_j^\Omega(x)\ dx\right)^2$$

- $Q_\Omega(t) = |\Omega| - \frac{2t}{\pi}|\partial(\Omega)| + o(t) \quad \text{as } t \to 0$
  (v.d. Berg–Davies, Math. Z. 1989)
- Further terms of the asymptotics depend on the geometry of $\partial\Omega$
  (v.d. Berg–Le Gall, Math. Z. 1994, v.d. Berg–Gilkey, JFA 1994)

Idea: Consider a parametrized version of spectral partitioning by studying

$$\Xi_{k,\infty}(\mathcal{P},t) := \max_{1\le i\le k} Q_{\mathcal{G}_i}(t), \quad t \ge 0,$$

for any given $\mathcal{P} = (\mathcal{G}_1, \ldots, \mathcal{G}_k) \in \mathfrak{P}_k$.

Conference advertisement

On mathematical aspects of interacting systems in low dimension

Hagen, Germany, June 24 to 27, 2019

Organizers:

- Joachim Kerner (joachim.kerner@fernuni-hagen.de)
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Thank you for your attention!