# Graph-based learning

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**The Mathematics of Scientific Machine Learning and Digital Twins @ Erice, Italy**

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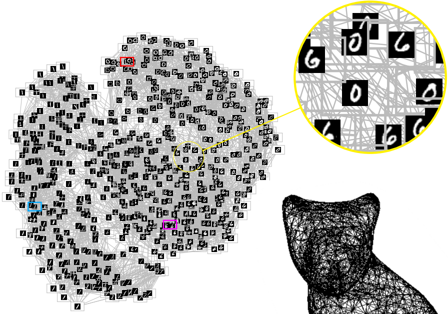
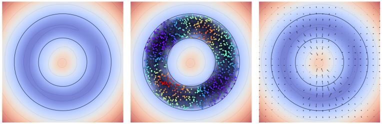
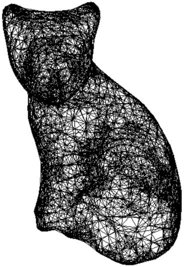
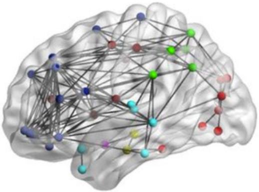
# Outline

# Graph-Structured Data is Omnipresent



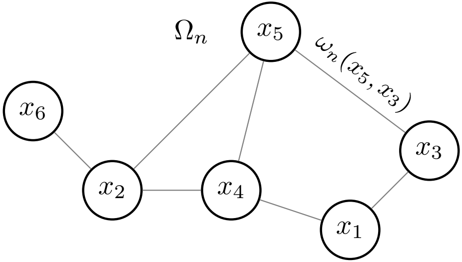






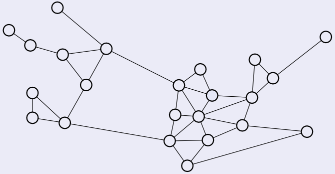
## Definition

A finite weighted graph is a tuple $G = (\Omega, \omega)$, where $\Omega$ is a finite vertex set and $\omega : \Omega \times \Omega \to [0, \infty)$ is a (symmetric) weight function.
We define $E := \{(x, y) \subset \Omega \ : \ \omega_{xy} > 0\}$ to be the set of edges of the graph.

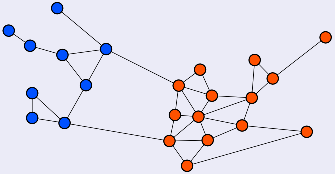


# Graph-Based Learning

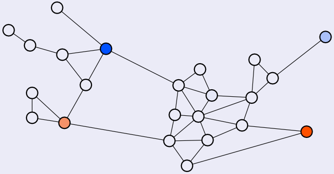
## Unsupervised



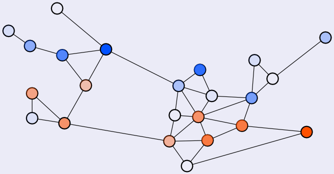
**Partition the data into clusters**



## Semi-supervised



**Extend labels to the whole dataset**



What are the challenges with graph-based learning?

## What are the challenges with graph-based learning?

- Convex relaxations
- Labeling guarantees
- Robustness and regularity
- Large data / continuum limits

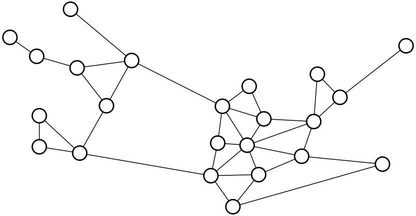
1 Motivation

2 Graph Clustering

3 Semi-Supervised Learning

4 Conclusion

**Idea:** Subdivide the graph into two groups by means of a graph cut.



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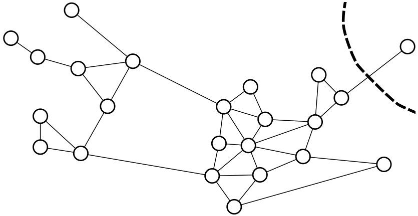

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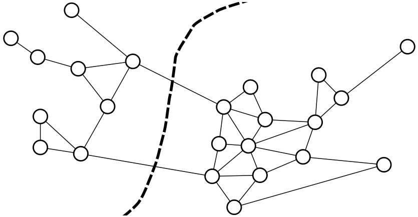

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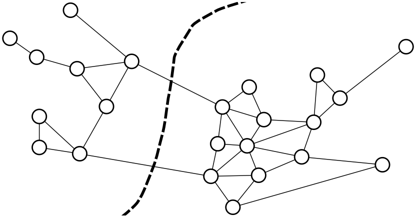

**Aim:** Minimize the normalized cut energy

$$\mathrm{NCut}(A) := \frac{\mathrm{Per}(A)}{\mathrm{vol}(A)} + \frac{\mathrm{Per}(A^c)}{\mathrm{vol}(A^c)},$$

where $\mathrm{Per}(A) := \sum_{x\in A, y\in A^c} \omega_{xy}$ is the perimeter of $A$, $\deg(x) := \sum_{y\in\Omega} \omega_{xy}$ is the degree of $x \in \Omega$, and $\mathrm{vol}(A) := \sum_{x\in A} \deg(x)$ is the volume of $A$.

The cut minimization problem $\min_{A\subset\Omega} \mathrm{NCut}(A)$ is a combinatoric optimization problem and NP-hard (Von Luxburg, 2007).

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Convex relaxation

$$\min_{u:\Omega\to\mathbb{R}} \left\{ \sum_{x,y\in\Omega} \omega_{xy} \left| \frac{u(x)}{\sqrt{\deg(x)}} - \frac{u(y)}{\sqrt{\deg(y)}} \right|^2 \,:\, \left\langle u, \sqrt{\deg} \right\rangle = 0,\ \|u\|^2 = 1 \right\},$$

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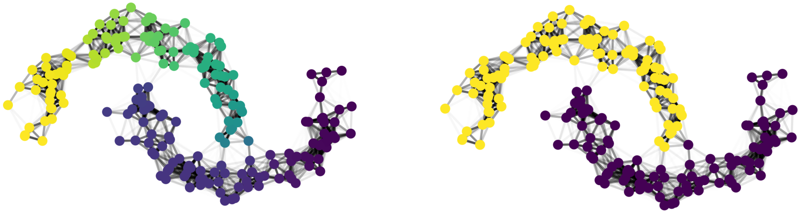
is equivalent to eigenvalue problem $-Lu=\lambda u$ for the normalized graph Laplacian

$$Lu(x):=\frac{1}{\sqrt{\deg(x)}}\sum_{y\in\Omega}\omega_{xy}\left(\frac{u(y)}{\sqrt{\deg(y)}}-\frac{u(x)}{\sqrt{\deg(x)}}\right).$$

**Spectral clustering:** Threshold the second eigenvector of the graph Laplacian.



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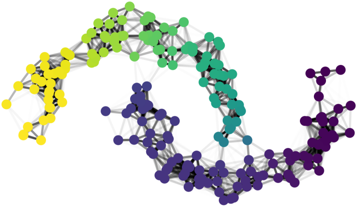

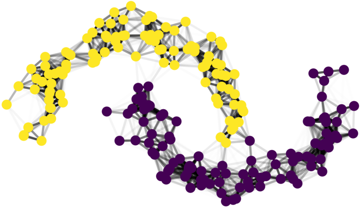

**Theorem (Cheeger inequality, Chung, 2007)**

*Let* $G = (\Omega, \omega)$ *be such that* $\deg(x) > 0$ *for all* $x \in \Omega$*, and let* $\lambda_2 \geq 0$ *denote the second eigenvalue of* $-L$*. Then it holds*

$$\frac{\lambda_2}{2} \leq \min_{A \subset \Omega} \mathrm{NCut}(A) \leq \sqrt{8\lambda_2}.$$

### Graph-Based Learning

- **Given:** Weighted graph $G_n = (\Omega_n, \omega_n)$ with $\#\Omega_n = n \in \mathbb{N}$.
- **Goal:** $\mathbf{u}_n : \Omega_n \to \mathbb{R}$ solving a clustering or labeling task
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graph PDE $\to$ continuum PDE, as $n \to \infty$.

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Real data often lies on unions of manifolds $\mathcal{M} := \mathcal{M}^{(1)} \cup \mathcal{M}^{(2)}$ with (potentially different) dimensions $d^{(1)} \leq d^{(2)}$.

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$$E_n(u) := \frac{1}{n^2 \varepsilon^2} \sum_{i,j=1}^{n} \eta\left(\frac{|x_i - x_j|}{\varepsilon_n}\right) \left| \frac{u(x_i)}{\sqrt{\deg_n(x_i)}} - \frac{u(x_j)}{\sqrt{\deg_n(x_j)}} \right|^2$$

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**Theorem (LB and Slepčev, 2025)**

*If* $\left(\frac{\log n}{n}\right)^{1/d^{(2)}} \ll \varepsilon_n \ll 1$, *almost surely the* $\Gamma$*-limit of the functionals* $E_n$ *is given by*

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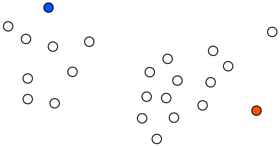
*where* $H^1_{\sqrt{\rho}}(\mathcal{M})$ *is a tensorized Sobolev space with a trace condition on the intersection if* $d^{(1)} = d^{(2)} = \dim(\mathcal{M}^{(1)} \cap \mathcal{M}^{(2)}) + 1$.

**Given:**

- a data set $\Omega_n \subset \mathbb{R}^d$,
- with labels $g : \mathcal{O}_n \subset \Omega_n \to \mathbb{R}$.



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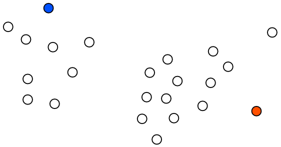

**Goal:**

a "smooth" function $\mathbf{u}_n : \Omega_n \to \mathbb{R}$
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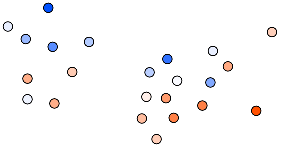

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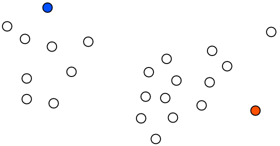

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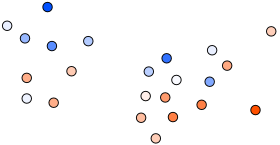

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**Model:**

construct a weighted graph $G_n = (\Omega_n, \omega_n)$
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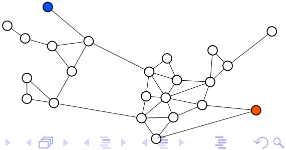

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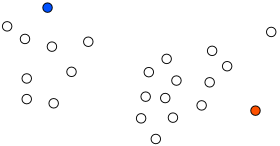

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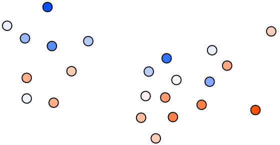

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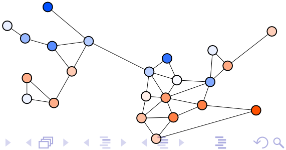
Compute $\mathbf{u}_n$ via graph PDE.



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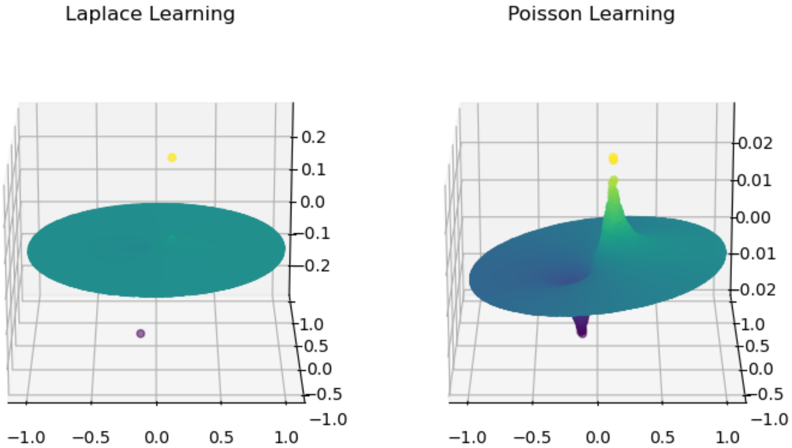

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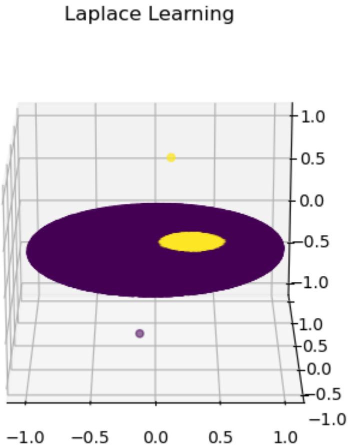


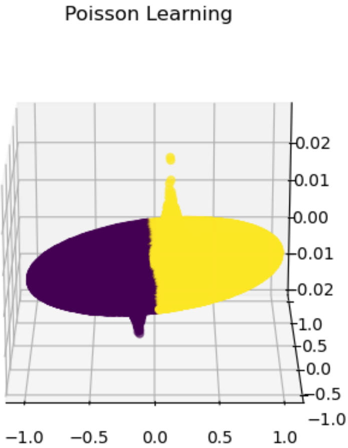

## Poisson Learning

Find $\mathbf{u}_n : \Omega_n \to \mathbb{R}$ such that

$$-L_n \mathbf{u}_n = \sum_{x \in \mathcal{O}_n} (g(x) - \overline{g})\delta_x,$$

subject to $\sum_{x \in \Omega_n} \deg_n(x) u(x) = 0$.

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## Continuum Problem

Find $u \in W^{1,1}(\Omega)$, distributional solution of

$$-\operatorname{div}(\rho^2 \nabla u) = \sum_{x \in \mathcal{O}} (g(x) - \overline{g})\delta_x,$$

subject to $\frac{\partial u}{\partial \nu} = 0$ and $\int_\Omega u \rho^2 \, \mathrm{d}x = 0$.

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- $g : \mathbb{R}^d \to \{-1, 1\}$ are binary labels, $\overline{g} := \frac{1}{|\mathcal{O}|} \sum_{x \in \mathcal{O}} g(x)$ is the label mean,
- $\Omega_n := \{x_i\}_{i=1}^n$ with *i.i.d.* samples $x_i$ with $\mathrm{Law}(x_i) = \rho$,
- $\mathcal{O}$ is a finite set and $\mathcal{O}_n = \{\pi_n(x) \ : \ x \in \mathcal{O}\}$ where $\pi_n : \Omega \to \Omega_n$ is a closest point projection,
- **Label decision:** $\mathrm{label}(x) = \mathrm{sign}(\mathbf{u}_n(x))$.

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**Poisson Learning**

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**Aims:** convergence rates

# Formal Main Result

**Theorem (Formal, LB, Calder, et al., 2024)**

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*If* $\rho \equiv const$ *this can be improved to*

$$\|\mathbf{u}_n - u\|_{\ell^1(\Omega_n)} \lesssim \varepsilon_n^{\frac{2-\sigma}{d+4}}$$

*for any* $\sigma > 0$.

# Three Levels of Approximation

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## Continuum mollification

Replace continuum data $\sum_{x \in \mathcal{O}}(g(x) - \overline{g})\delta_x$ by $\sum_{x \in \mathcal{O}}(g(x) - \overline{g})\varphi_x$ with $\operatorname{supp} \varphi_x \subset B(x, R)$ obtain quantitative $L^1$-estimates in $R$.

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Prove discrete-to-continuum convergence rates for bounded right hand sides using variational methods (strong convexity).

**NB:** Keeping track of all constants (which blow up) and optimizing over all parameters we obtain the final rate.

**Challenges in graph-based learning:**

- Realistic manifold assumptions
- Convergence rates
- Theoretical guarantees for sparse graphs

**Applications:**

- Data Science
- Grid-free solution of high-dimensional PDEs
- Digital twins?

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# Continuum Mollification

We regularize the continuum equation by approximating the Dirac deltas:

$$-\operatorname{div}(\rho^2 \nabla u) = \sum_{x \in \mathit{\Gamma}} a_x \delta_x \qquad \text{and} \qquad -\operatorname{div}(\rho^2 \nabla u_R) = \sum_{x \in \mathit{\Gamma}} a_x \varphi_x,$$

where $\operatorname{supp} \varphi_x \subset B(x, R)$, $\varphi_x \geq 0$, and $\int_{B(x,R)} \varphi_x(y) \, \mathrm{d}y = 1$.

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*If in addition* $\rho \equiv const$ *and* $\varphi_x(y) = R^{-d} \psi(|y - x| / R)$, *then*

$$\|u - u_R\|_{L^1(\Omega)} \lesssim \sum_{x \in \Gamma} |a_x| \, R^2.$$

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We define the random walk graph Laplacian:

$$\widehat{L}_n \mathbf{u}_n(x) := \frac{1}{\varepsilon_n^2 \deg_n(x)} L_n \mathbf{u}_n(x) = \frac{1}{\varepsilon_n^2} \left( \frac{1}{\deg_n(x)} \sum_{y \in \Omega_n} \omega_n(x,y) \mathbf{u}_n(y) - \mathbf{u}_n(x) \right).$$

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The graph heat kernel $\mathcal{H}_k^x$ is the solution of the heat equation, starting with $\delta_x$:

$$\mathcal{H}_{k+1}^x = \mathcal{H}_k^x - \varepsilon_n^2 \widehat{L}_n^T \mathcal{H}_k^x, \qquad \mathcal{H}_0^x = n\delta_x.$$

We define the convolution $\mathcal{H}_k * \mathbf{u}_n(x) := \frac{1}{n} \sum_{y \in \Omega_n} \mathcal{H}_k^x(y) \mathbf{u}_n(y)$.

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**Theorem (LB, Calder, et al., 2024)**

*It holds* $\mathcal{H}_k * (\widehat{L}_n \mathbf{u}_n) = \widehat{L}_n (\mathcal{H}_k * \mathbf{u}_n)$.

# Estimates on Mollified Problem

Let $\mathbf{u}_n$ and $\mathbf{u}_n^{(k)} := \mathcal{H}_k^{\cdot} * \mathbf{u}_n$ solve

$$-\widehat{L}_n \mathbf{u}_n = \sum_{x \in \mathcal{O}} a_x \delta_x \qquad \text{and} \qquad -\widehat{L}_n \mathbf{u}_n^{(k)} = \sum_{x \in \mathcal{O}} a_x \mathcal{H}_k^x.$$

Then it holds

$$\mathbf{u}_n - \mathbf{u}_n^{(k)} = \frac{n\varepsilon_n^2}{\deg_n} \sum_{x \in \mathcal{O}} a_x \sum_{j=0}^{k-1} \mathcal{H}_j^x.$$

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Using that $\deg_n \sim n$ and $\left\| \mathcal{H}_j^x \right\|_{\ell^1(\Omega_n)} = 1$ we get the estimate

$$\left\| \mathbf{u}_n - \mathbf{u}_n^{(k)} \right\|_{\ell^1(\Omega_n)} \lesssim k\varepsilon_n^2 \sum_{x \in \mathcal{O}} |a_x|$$

and will need to choose $1 \ll k \ll \frac{1}{\varepsilon_n^2}$.

# Continuum Limit for Bounded Data

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**Theorem (LB, Calder, et al., 2024)**

*For all $R, \lambda_1, \lambda_2, \varepsilon_n, \delta >$0 sufficiently small, and $q > \frac{d}{2}$ we have with high probability:*

$$\begin{aligned}\|u - \mathbf{u}_n\|^2_{H^1(\mathcal{X}_n)} \lesssim &\left(\|f_n - f\|_{\ell^1(\Omega_n)} + \|\operatorname{osc}_{\Omega\cap B(\cdot,\delta)} f\|_{L^1(\Omega)}\right)\left(\|f\|_{L^q(\Omega)} + \|f_n\|_{\ell^q(\Omega_n)}\right)\\ &+ \|f\|^2_{L^\infty(\Omega)}\lambda_1 + \|f\|^2_{L^\infty(\partial_{4\varepsilon_n}\Omega)}\varepsilon_n + \|f_n\|_{\ell^2(\Omega_n)}\|f_n\|_{\ell^2(\Omega_n\cap\partial_{2R}\Omega)}\\ &+ \left(\|f_n\|^2_{\ell^2(\Omega_n)} + \|f\|^2_{L^2(\Omega)}\right)\left(\frac{\delta}{\varepsilon_n} + \varepsilon_n + \lambda_1^2 + \lambda_2\right).\end{aligned}$$

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We choose $f_n = \sum_{x\in\mathcal{O}} a_x \mathcal{H}_k^x$ and prove discrete-to-continuum convergence rates towards a k-fold convolution $f := \sum_{x\in\mathcal{O}} a_x \rho(x)^{-1}\mathcal{M}_\varepsilon^k(\delta_x)$.