

Eigenvalue problems on graphs and hypergraphs

Machine Learning and PDEs Workshop

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FAU Erlangen-Nürnberg

April 28th, 2025



Outline

Weighted graphs in data science and machine learning

- ▶ Data modeling with graphs
- ▶ Differential operators on graphs

Eigenvalue problems on graphs

- ▶ Linear eigenvalue problems
- ▶ Nonlinear eigenvalue problems

Extension to hypergraphs

- ▶ Data modeling with hypergraphs
- ▶ Differential operators on hypergraphs
- ▶ Eigenvalue problems on hypergraphs

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Eigenvalue problems on graphs

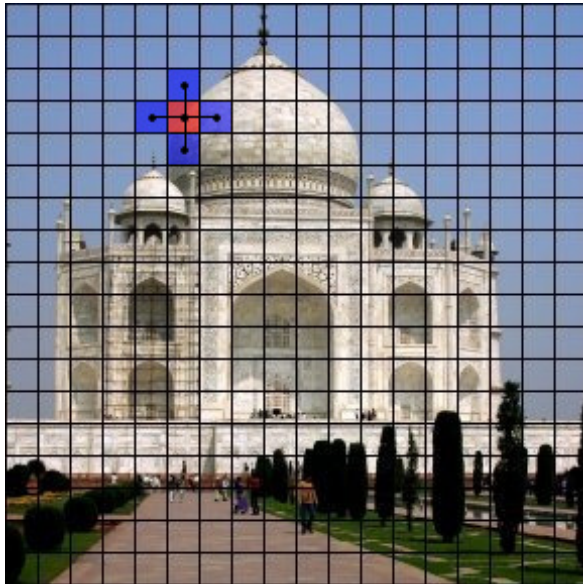
- ▶ Linear eigenvalue problems
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Extension to hypergraphs

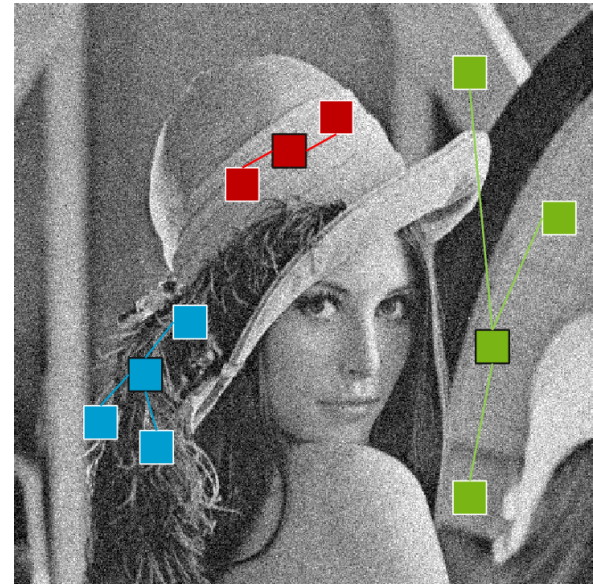
- ▶ Data modeling with hypergraphs
- ▶ Differential operators on hypergraphs
- ▶ Eigenvalue problems on hypergraphs

Discrete data modeling using weighted graphs

Question: How can we apply graphs for **image processing** ?



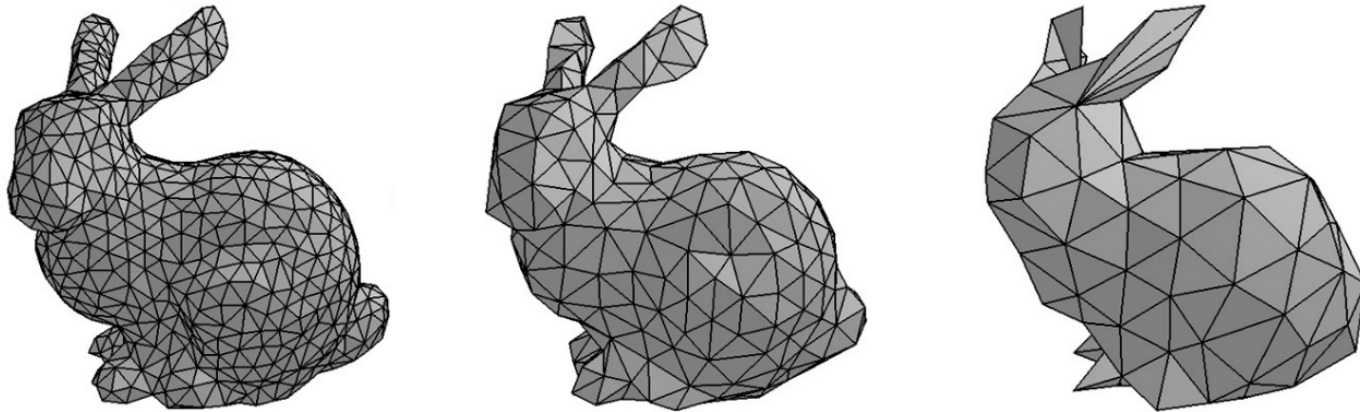
Local neighborhood of a pixel



Nonlocal neighborhood of a pixel

Discrete data modeling using weighted graphs

Question: How can we apply graphs for **polygon mesh processing** ?

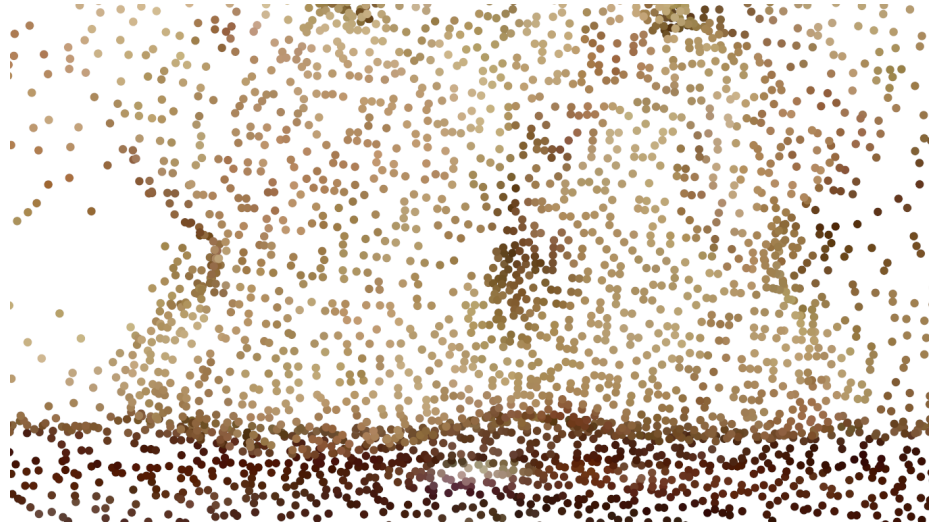


Polygon mesh approximation of a 3D surface.

¹Image: Gabriel Peyré

Discrete data modeling using weighted graphs

Question: How can we apply graphs for **point cloud processing**?

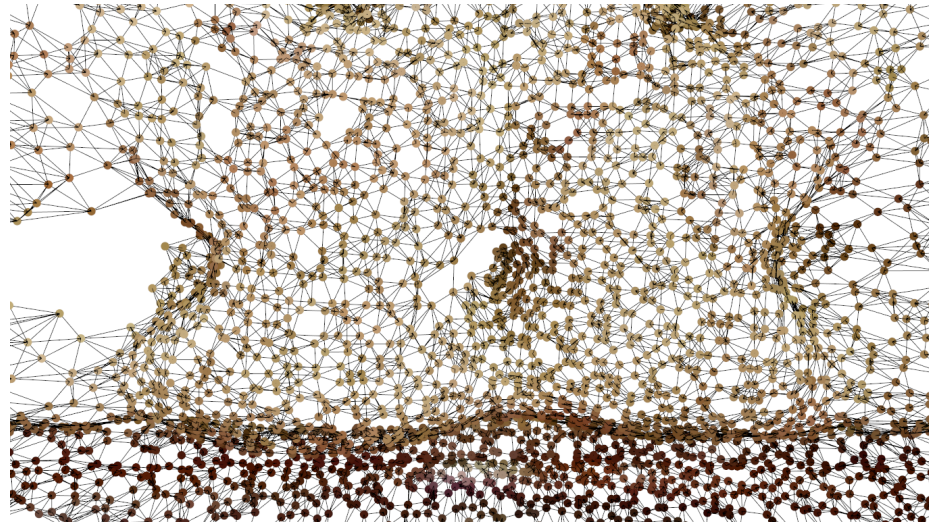


Colored 3D point cloud data of a scanned chair

¹Image: Abderrahim Elmoataz

Discrete data modeling using weighted graphs

Question: How can we apply graphs for **point cloud processing**?

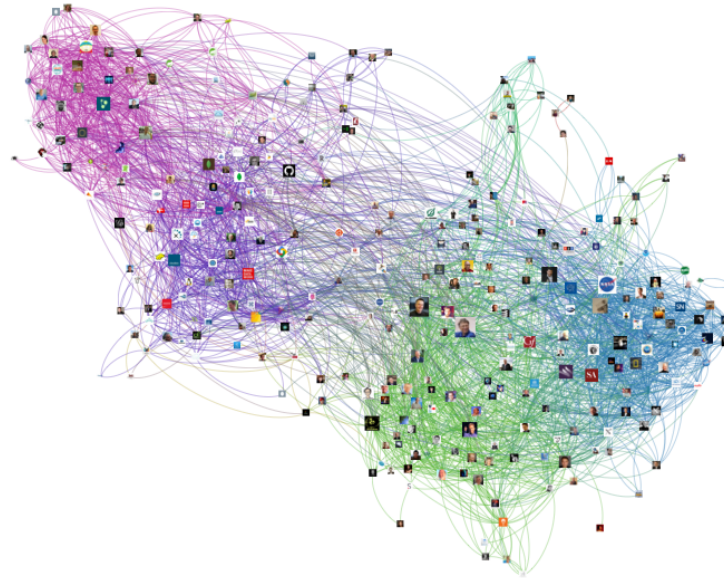


Graph construction on a 3D point cloud

¹Image: Abderrahim Elmoataz

Discrete data modeling using weighted graphs

Question: How can we apply graphs for **social network analysis**?



¹Image: Caleb Jones

Discrete data modeling using weighted graphs

Question: How can we apply graphs for machine learning?

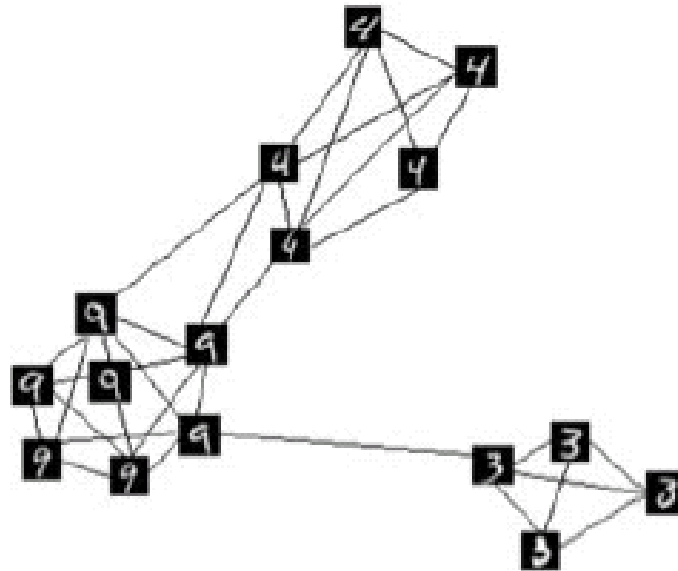


Subset of handwritten digits from MNIST database² Graph construction using suitable similarity features

²Y. LeCun, C. Cortes, C. Burges: *The MNIST database of handwritten digits*

Discrete data modeling using weighted graphs

Question: How can we apply graphs for machine learning?



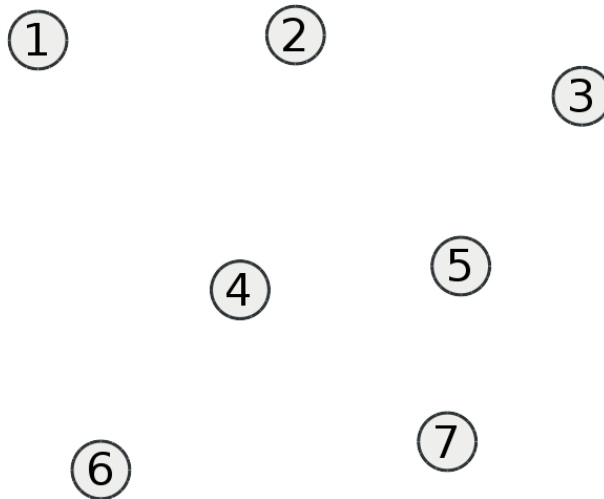
Finite weighted graphs

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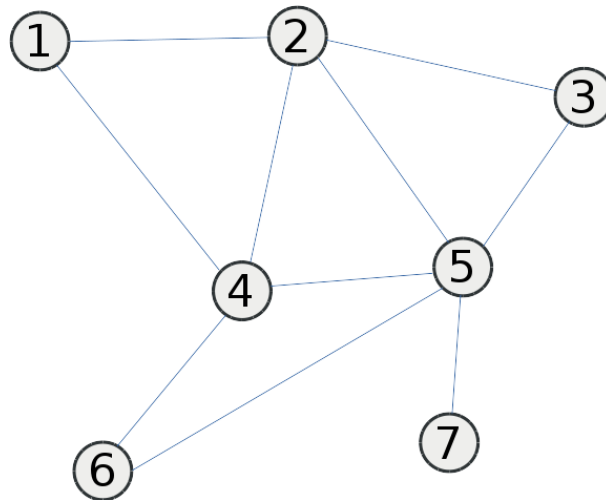
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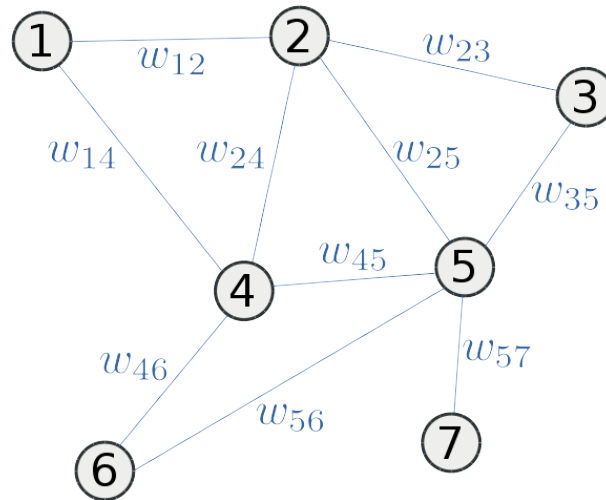
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- ▶ a **weight function** $w: E \rightarrow [0, 1]$ **with:** $w(u, v) > 0 \Leftrightarrow (u, v) \in E$



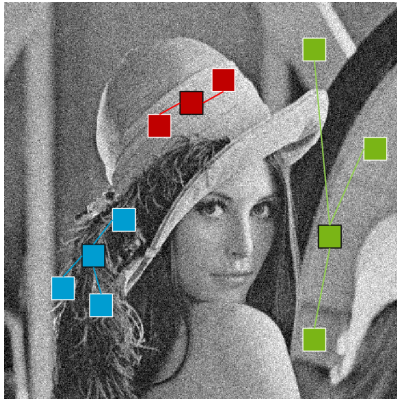
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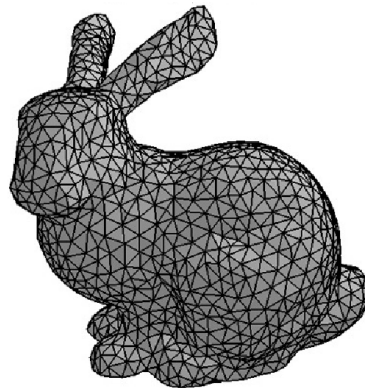
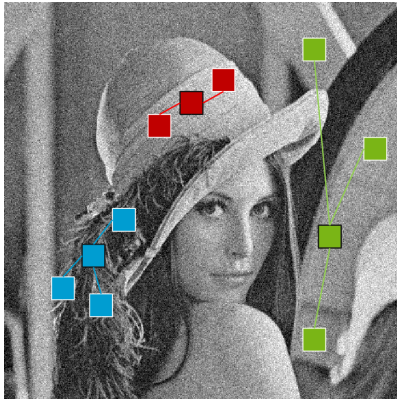
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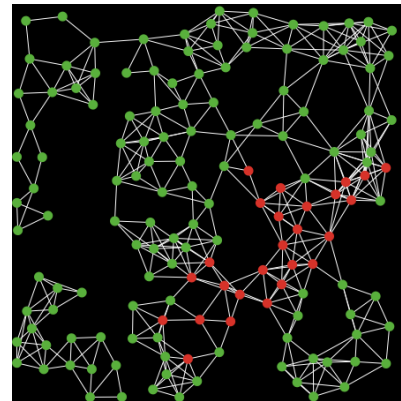
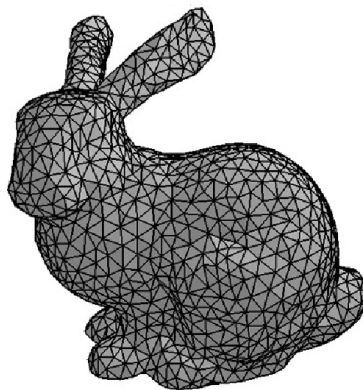
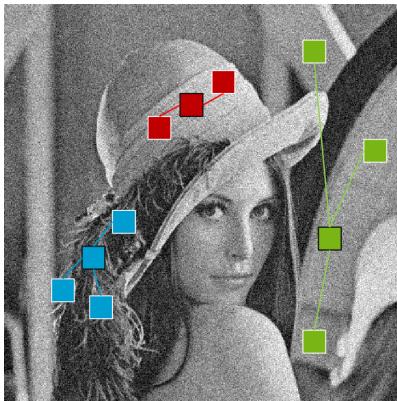
- ▶ Grayscale values or RGB colors
- ▶ 3D coordinates



Finite weighted graphs

Application data can be represented by a **vertex function** $f: V \rightarrow \mathbb{R}^m$, e.g.,

- ▶ Grayscale values or RGB colors
- ▶ 3D coordinates
- ▶ Labels
- ▶ ...



Weighted gradient and divergence operator

Let (V, E, w) be a graph, $f \in H(V)$ a vertex function and $G \in H(E)$ an edge function.

Weighted gradient and divergence operator

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The **gradient** $\nabla: H(V) \rightarrow H(E)$ of $f \in H(V)$ along an edge $(u, v) \in E$ is given as:

$$\nabla f(u, v) = \sqrt{w(u, v)}(f(v) - f(u)) \quad (1)$$

¹A. Elmoataz, O. Lézoray, S. Boughleux: *Nonlocal Discrete Regularization on Weighted Graphs*. IEEE TIP 17 (2008)

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One can deduce the **adjoint operator** $\nabla^*: H(E) \rightarrow H(V)$ of ∇ by the property:

$$\langle \nabla f, G \rangle_{H(E)} = \langle f, \nabla^* G \rangle_{H(V)} \quad (2)$$

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Then the **divergence** $\text{div}: H(E) \rightarrow H(V)$ of G in a vertex $u \in V$ is given as:

$$\text{div } G(u) = -\nabla^* G(u) = \sum_{v \sim u} \sqrt{w(u, v)}(G(u, v) - G(v, u)) \quad (3)$$

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Translating variational problems to graphs

Example: A general **variational data denoising model**

Translating variational problems to graphs

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Find a **minimizer** $f: V \rightarrow \mathbb{R}^m$ of the energy functional

$$E(f) = \lambda \|f - f_0\|^2 + \|\nabla f\|_{p,q}^p, \quad \lambda > 0$$

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with $\|\nabla f\|_{p,q} = \left(\frac{1}{p} \sum_{u \in V} \left(\sum_{v \sim u} \|\nabla f(u, v)\|^q \right)^{\frac{p}{q}} \right)^{\frac{1}{p}}, \quad 1 \leq p, q < \infty.$

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Special cases:

$p=q=1$: (Anisotropic) total variation regularization

$p=q=2$: Generalized Tikhonov regularization

Graph p-Laplace operators

Observation:

Optimality conditions for the p-Dirichlet energy lead to the **graph p-Laplace operator**:

$$\Delta_p f(u) = \operatorname{div} (|\nabla f|^{p-2} \nabla f) (u) = \sum_{v \sim u} (w(u, v))^{p/2} |f(v) - f(u)|^{p-2} (f(v) - f(u))$$

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Special case for $p = 2$:

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The graph Laplace operator is **linear** and can be expressed as matrix $L \in \mathbb{R}^{n \times n}$ via

$$L = D - W, \tag{4}$$

where D is the **degree matrix** and W is the **weight matrix** of the weighted graph.

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Principal component analysis

Aim:

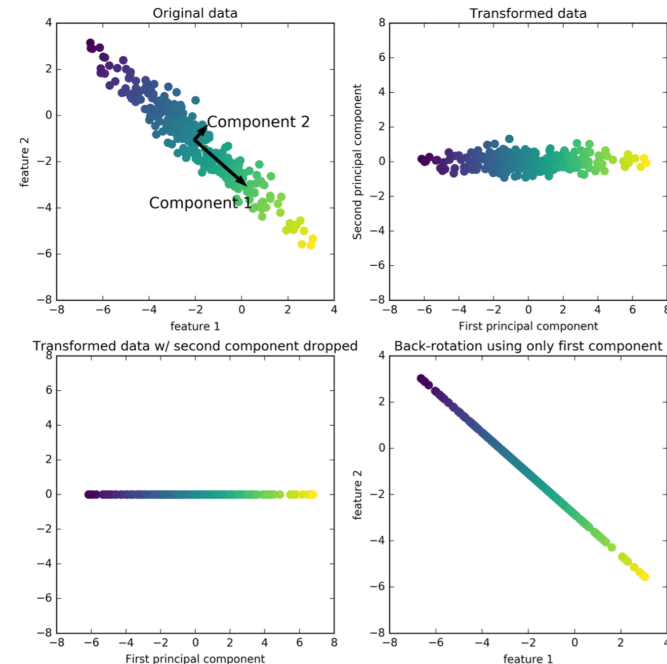
Dimension reduction / data simplification

Eigenvalue problem:

Compute the **biggest eigenvalues** and corresponding eigenvectors via

$$\Sigma x = \lambda x,$$

for which $\Sigma = \mathbb{E}[XX^T]$ is the **covariance matrix** of the given (centralized) data X .



³Image courtesy: Ashwin N

PageRank algorithm⁵

Aim:

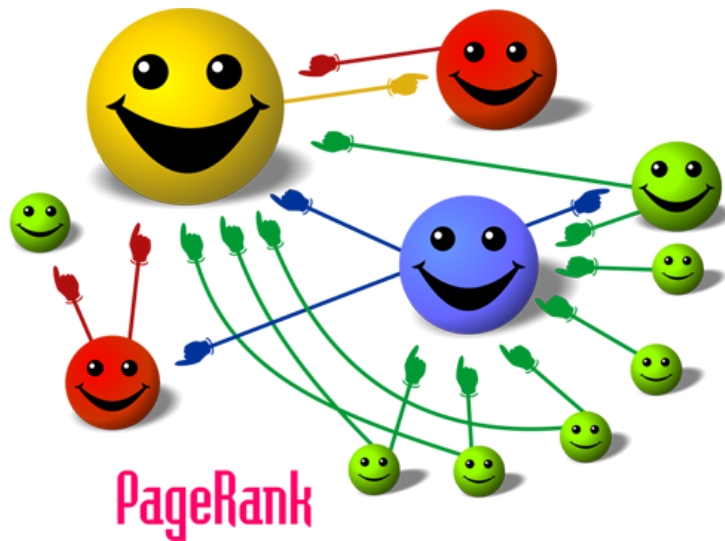
Recommendation system for websites based on HTML links

Eigenvalue problem:

Compute the **biggest eigenvalue** and corresponding eigenvector via

$$Gx = \lambda x,$$

for which $G = \beta M + \frac{(1-\beta)}{n} \mathbb{1}$ is the **Google matrix**.



⁴Image courtesy: Wikimedia – Felipe Micaroni Lalli

⁵L. Page, S. Brin, R. Motwani, T. Winograd: *The PageRank Citation Ranking: Bringing Order to the Web*. Technical Report (1999)

Spectral clustering⁷

Aim:

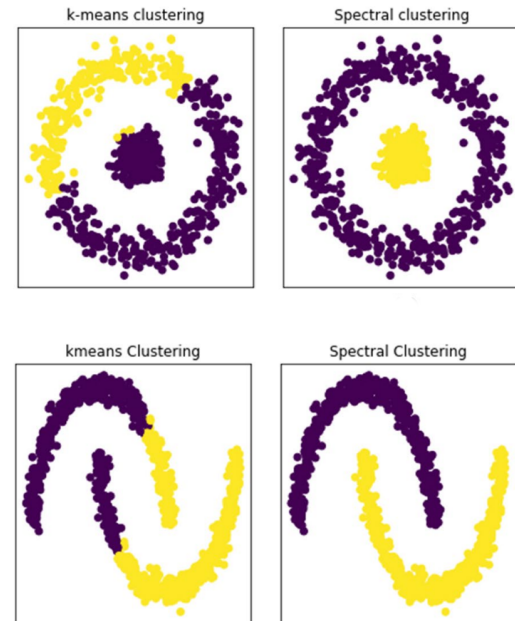
Unsupervised data clustering

Eigenvalue problem:

Compute the **second smallest eigenvalue** and corresponding eigenvector via

$$Lx = \lambda x,$$

for which $L = D - W$ is the **graph Laplacian matrix** of the given graph.



⁶Image: M. El Hamri, Y. Bennani, I. Falih: *Hierarchical optimal transport for unsupervised domain adaptation*. Machine Learning 111:4159–4182 (2022)

⁷U. von Luxburg: *A Tutorial on Spectral Clustering*. arXiv:0711.0189 (2007)

What is a nonlinear eigenvalue problem?

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Aim:

Find an element u of a suitable space X and a scalar $\lambda \in \mathbb{R}$ s.t. for two (possibly) **nonlinear functionals** $T, S: X \rightarrow \mathbb{R}$ the following equation is fulfilled:

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Interesting case:⁸

- ▶ X is reflexive Banach space
- ▶ $T(u) := \partial J(u) \in X^*$ with J as proper, l.s.c., convex functional
- ▶ $S(u) := \partial H(u) \in X^*$ with H as proper, l.s.c., convex, abs. p -homogeneous functional

⁸L. Bungert, M. Burger: *Gradient Flows and Nonlinear Power Methods for the Computation of Nonlinear Eigenfunctions*, Handbook of Numerical Analysis (2021)

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Example:

For $p > 1$, $X := W_0^{1,p}(\Omega)$, $J(u) := \frac{1}{p} \int_{\Omega} \|\nabla u(x)\|^p dx$ and $H(u) := \frac{1}{p} \|u\|_{L^p(\Omega)}^p$ we get:

$$-\Delta_p u(x) = \lambda |u(x)|^{p-2} u(x) \quad (6)$$

⁸L. Bungert, M. Burger: *Gradient Flows and Nonlinear Power Methods for the Computation of Nonlinear Eigenfunctions*, Handbook of Numerical Analysis (2021)

How to compute nonlinear eigenfunctions?

Flow-based approaches:

$$u'(t) = -\nabla J(u(t))$$

- ▶ R. Hynd, E. Lindgren: *Approximation of the least Rayleigh quotient for degree p homogeneous functionals*. Journal of Functional Analysis 272 (2017)
- ▶ G. Gilboa: *Iterative Methods for Computing Eigenvectors of Nonlinear Operators*. Handbook of Mathematical Models and Algorithms in Computer Vision and Imaging (2021)
- ▶ L. Bungert, M. Burger, D. Tenbrinck: *Computing Nonlinear Eigenfunctions via Gradient Flow Extinction*

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Inverse power methods:

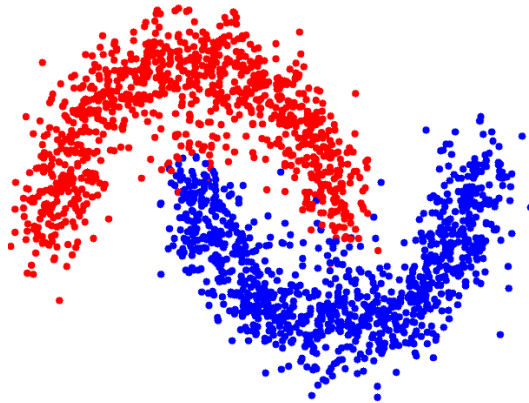
$$u^{k+1} = \frac{(\nabla J(u^k))^{-1}}{\|(\nabla J(u^k))^{-1}\|}$$

- ▶ M. Hein, T. Bühler: *An Inverse Power Method for Nonlinear Eigenproblems with Applications in 1-Spectral Clustering and Sparse PCA*. Advances in Neural Information Processing Systems 23 (2010)
- ▶ F. Bozorgnia: *Convergence of Inverse Power Method for First Eigenvalue of p -Laplace Operator*. Numerical Functional Analysis and Optimization 37 (2016)
- ▶ J. Laubmann, D. Tenbrinck, M. Friedrich: *Duality of Nonlinear Eigenproblems*. soon on ArXiv (2025)

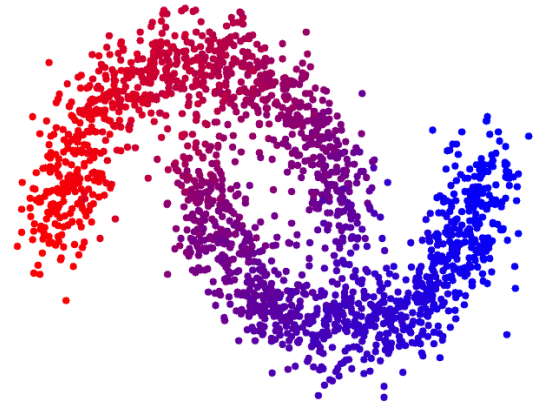
Nonlinear spectral clustering

In this setting one solves the following eigenvalue problem via **inverse power iterations**:

$$0 \in \Delta_1 u - \lambda \operatorname{sign}(u)$$



Eigenvector of 1-Laplacian



Eigenvector of 2-Laplacian

⁹Image: M. Hein, T. Bühler: *An Inverse Power Method for Nonlinear Eigenproblems with Applications in 1-Spectral Clustering and Sparse PCA*. Advances in Neural Information Processing Systems 23 (2010)

Nonlinear spectral image fusion

In this setting one has $J(u) = TV(u) = \int_{\Omega} ||\nabla u(x)|| dx$ and solves the eigenvalue problem via **gradient flow**:

$$\lambda u \in \partial J(u)$$



¹⁰Image: M. Benning, M. Möller, R. Nossek, M. Burger, D. Cremers, G. Gilboa, C. Schönlieb: *Nonlinear Spectral Image Fusion*. SSVM (2017)

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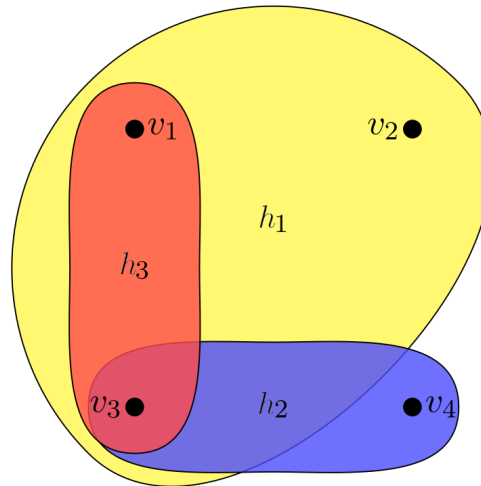
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Discrete data modeling using weighted hypergraphs

Idea:

Directly extend (traditional) weighted graphs by allowing **more vertices in edges** instead of only pairs of vertices.



¹¹X. Ouvrard: *Hypergraphs: an introduction and review*. arXiv (2020)

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Applications fields:

► Molecular chemistry

J. Jost, R. Mulas: *Hypergraph Laplace operators for chemical reaction networks*. Advances in Mathematics 351 (2019)

► Social network analysis

A. Fazeney, D. Tenbrinck, M. Burger: *Hypergraph p -Laplacians, Scale Spaces, and Information Flow in Networks*. SSVM (2023)

► Machine Learning

Y. Feng, H. You, Z. Zhang, R. Ji, Y. Gao: *Hypergraph Neural Networks*. AAAI Conference (2019)

¹¹X. Ouvrard: *Hypergraphs: an introduction and review*. arXiv (2020)

Hypergraphs for modeling co-authorship in papers

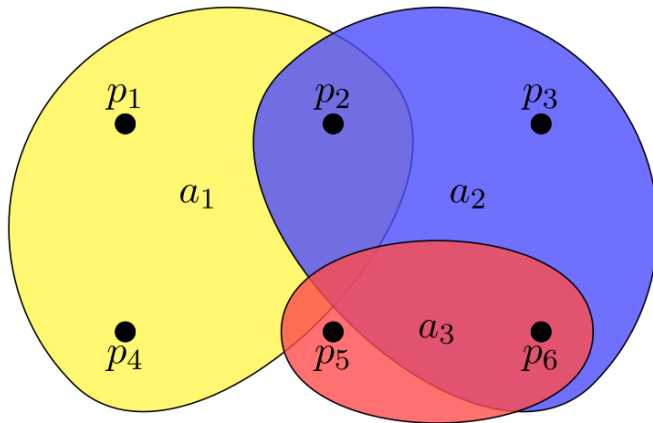
Example:

Set of **scientific papers** $P := \{p_1, \dots, p_6\}$ and set of **authors** $A := \{a_1, a_2, a_3\}$. Possible modeling with hypergraphs:

Hypergraphs for modeling co-authorship in papers

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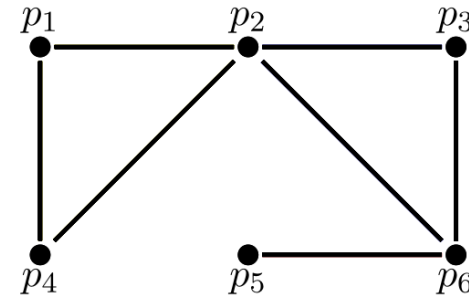
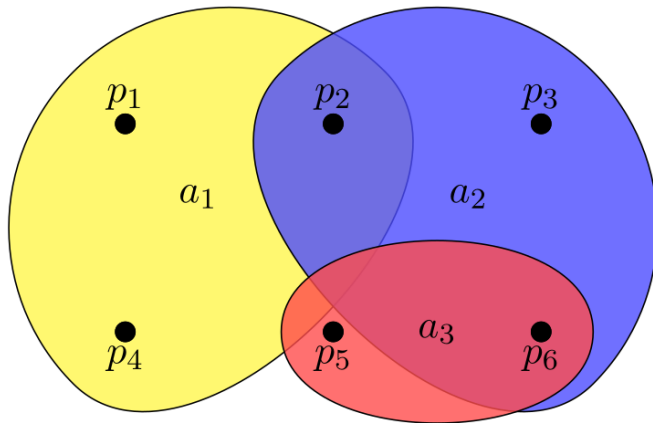
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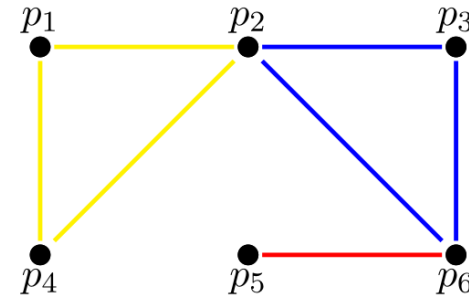
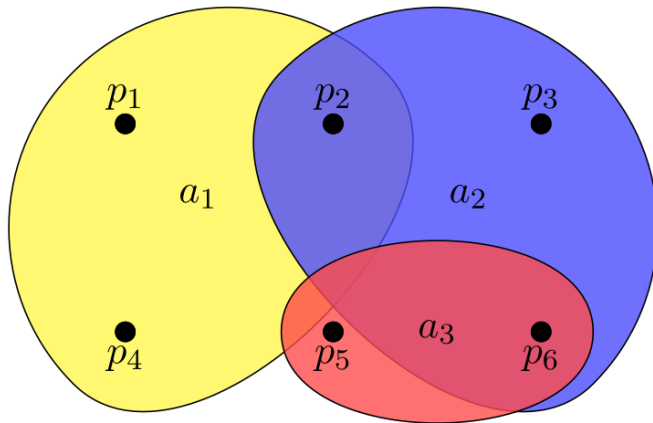
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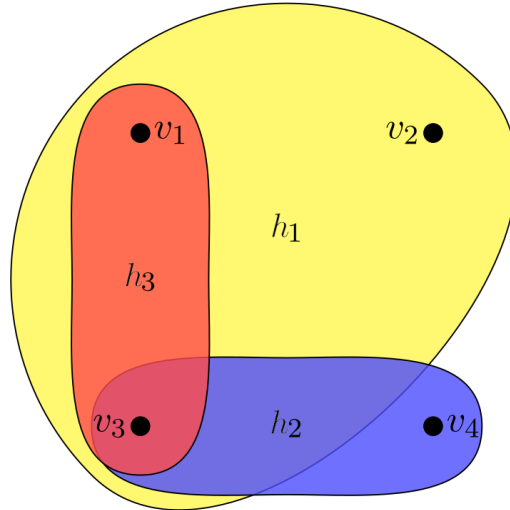
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Finite weighted hypergraphs

A finite weighted **hypergraph** $HG = (V, H, w)$ consists of:

- ▶ a finite set of **vertices** $V = (v_1, \dots, v_n)$
- ▶ a finite set of **hyperedges** $H \subset \mathcal{P}(V) \setminus \emptyset$
- ▶ a **weight function** $w: H \rightarrow [0, 1]$ with: $w(h) > 0 \Leftrightarrow h \in H$



¹²Image: C. Schiller: *The PageRank Algorithm on Graphs and Hypergraphs*. Bachelor's thesis at FAU (2024)

Differential operators on hypergraphs

Observation:

There are **several possibilities** to generalize the weighted graph gradient operator, e.g., sum, min/max, mean, random, ...

¹³A. Fazeney, D. Tenbrinck, K. Lukin, M. Burger: Hypergraph p -Laplacians and Scale Spaces. JMIV 66. p. 529-549 (2024)

¹⁴J. Jost, R. Mulas, D. Zhang: p -Laplace Operators for Oriented Hypergraphs. Vietnam Journal of Mathematics Oct (2021)

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Let $h \in H$ be a hyperedge and $u \in h$ be a **chosen vertex** within h . Then the **hypergraph gradient operator** is defined as:

$$\nabla^u f(h) = \nabla f(u; h) := \sqrt{w(h)} \sum_{v_i \in h} (f(v_i) - f(u)) \quad (7)$$

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Analogously to weighted graphs, we deduce the **hypergraph p -Laplace operator**¹⁴ as:

$$\Delta_p f(u) = \operatorname{div} (|\nabla^u f|^{p-2} \nabla^u f) (u) \quad (8)$$

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Eigenvalue problems on hypergraphs

Aim:

Formulate eigenvalue problems on hypergraphs, e.g., the **linear case** of $p = 2$:

Find a vertex function $f: V \rightarrow \mathbb{R}$ such that for all $u \in V$ we have:

$$\lambda f(u) = \Delta f(u) \tag{9}$$

Eigenvalue problems on hypergraphs

Aim:

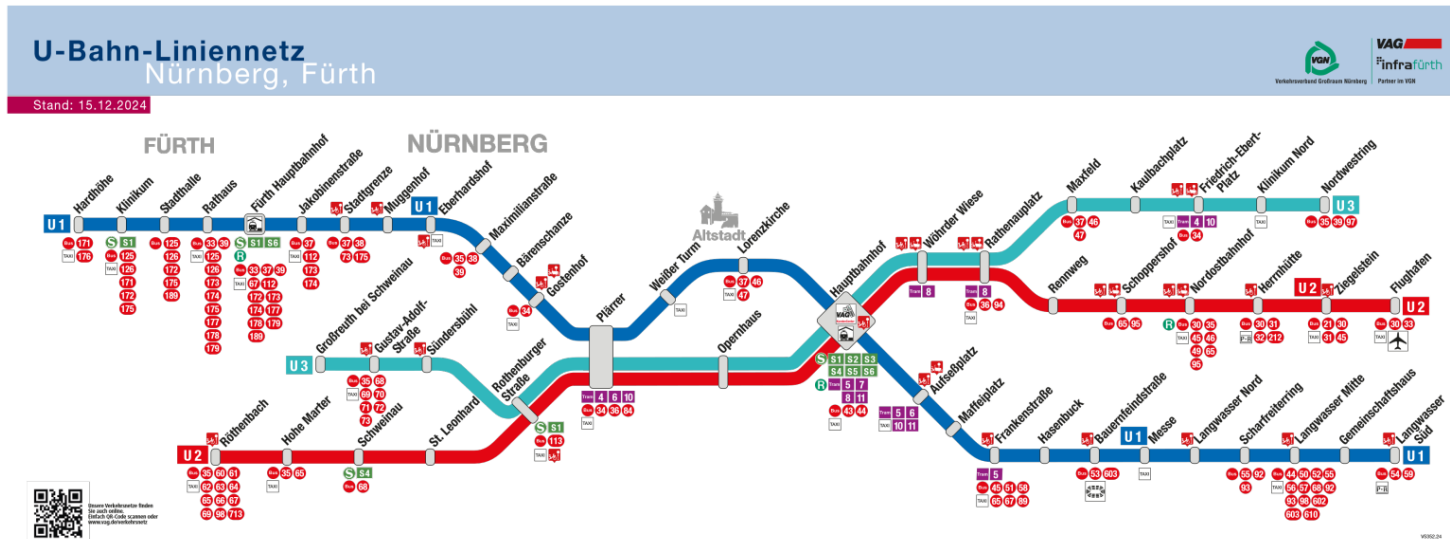
Formulate eigenvalue problems on hypergraphs, e.g., the **linear case** of $p = 2$:

Find a vertex function $f: V \rightarrow \mathbb{R}$ such that for all $u \in V$ we have:

$$\lambda f(u) = \Delta f(u) = \operatorname{div}(\nabla^u f)(u) = \sum_{\substack{h \in H \\ u \in h}} w(h) \sum_{v_i \in h} (f(v_i) - f(u)) \quad (9)$$

Eigenvalue problems on hypergraphs

Example: PageRank¹⁵ on subway stations in Nürnberg

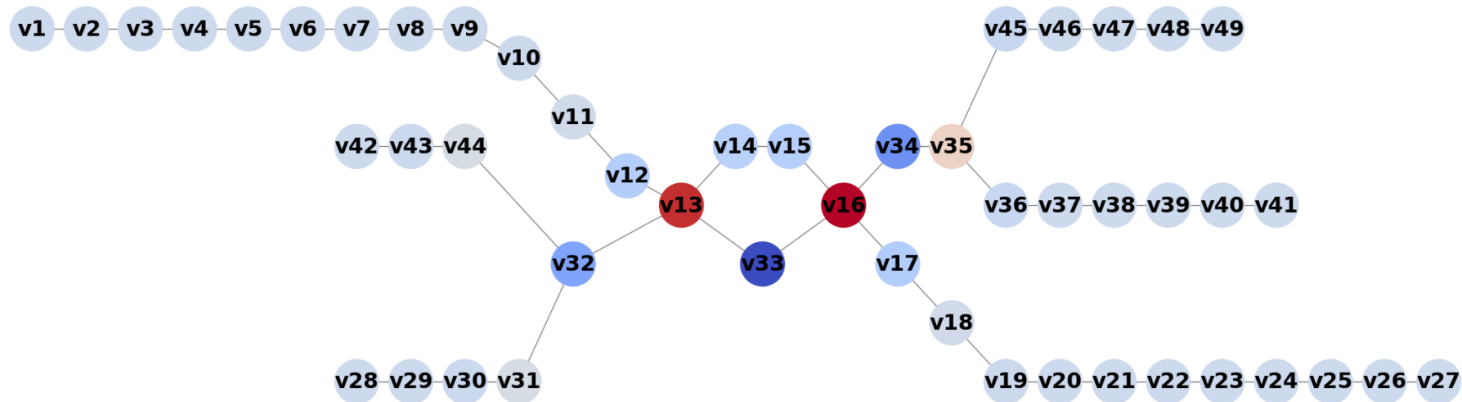


¹⁵Y. Takai, A. Miyauchi, M. Ikeda, Y. Yoshida: *Hypergraph clustering based on PageRank*. Proceedings of KDD. p.1970-1978 (2020)

¹⁶T. Strauß: The eigenvalue problem on hypergraphs. Bachelor's thesis at FAU (2025)

Eigenvalue problems on hypergraphs

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Conclusion

Take-away message:

- ▶ Weighted graphs are a **universal tool** for data modeling
- ▶ Hypergraphs extend graphs and allow for **additional information**
- ▶ **(Nonlinear) eigenvalue problems** are used for various applications in machine learning and data science
- ▶ **Next goal:** Investigate nonlinear eigenvalue problems on hypergraphs

Thank you for your attention!

Kudos to my collaborators:



M. Burger



A. Fazen



L. Bungert



M. Friedrich



J. Laubmann

Any questions?