

Introduction to Graph Spectral Analysis

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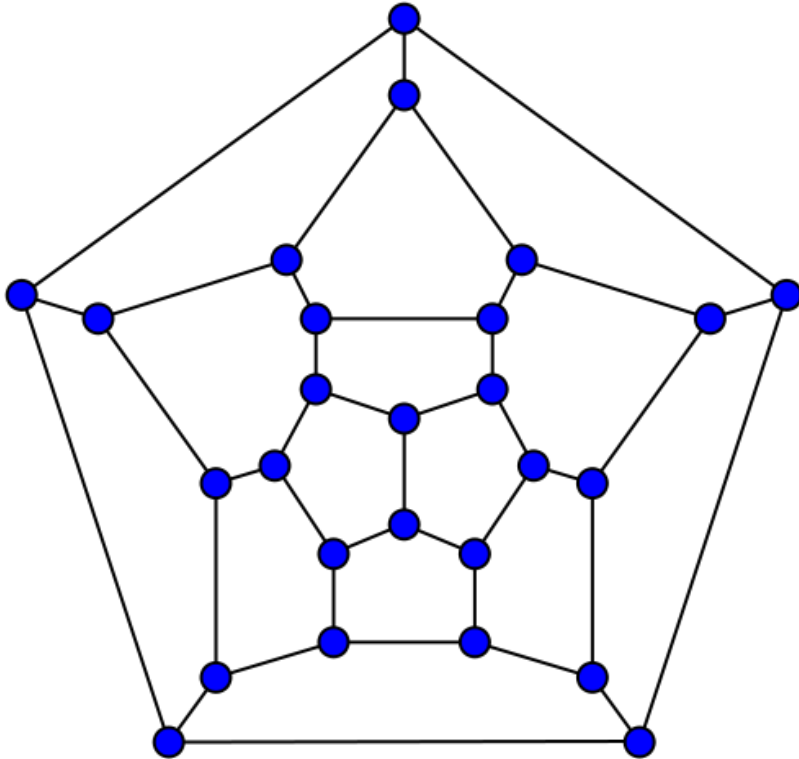


SAPIENZA
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Tuesday 28th July 2020
Verona, Italy

Context

Graphs



Eigenvalues & Eigenvectors



$$A \mathbf{v} = \lambda \mathbf{v}$$

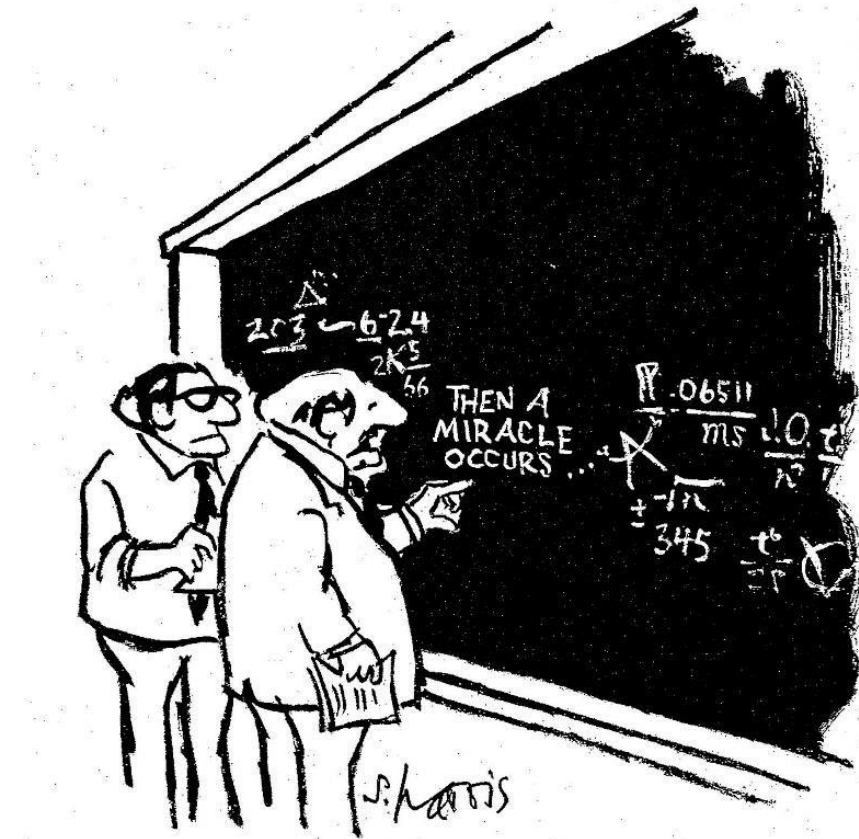
where $A \in \mathbb{R}^{m \times m}$ (Square Matrix)

eigenvectors $\rightarrow \mathbf{v} \in \mathbb{R}^{m \times 1}$ (Column Vector)

eigenvalues $\rightarrow \lambda \in \mathbb{R}^{m \times m}$ (Diagonal Matrix)

Index

- Basic concepts (linear algebra, function analysis)
- Dirichlet energy and smoothness
- Laplacian
- Graph Laplacian
- Eigen-decomposition of the Laplacian
- Spectral properties
- Applications (mincut, clustering, Fourier-like analysis)



"I THINK YOU SHOULD BE MORE EXPLICIT HERE IN STEP TWO."

Basis

Given a vector space \mathbf{V} , a subset \mathbf{B} is a *basis* iif:

- Its elements are linear independent
- And they span all the vectors in \mathbf{V}


The canonical base for $\mathbf{v} \in \mathbb{R}^3$

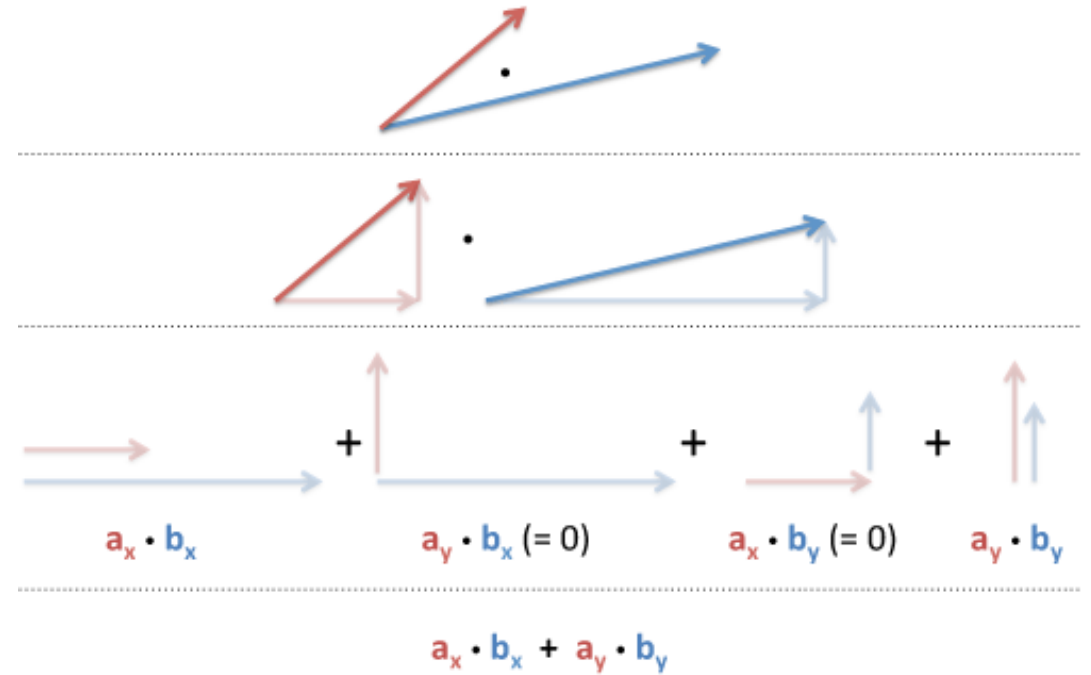
$$\alpha_1 \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} + \alpha_2 \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} + \alpha_3 \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} = \mathbf{v}$$

Every \mathbf{v} can be written as a weighted sum of the elements of the basis.

Basis - Properties

Defining an inner product:

$$\langle \mathbf{a}, \mathbf{b} \rangle = a_0 b_0 + a_1 b_1 + \cdots + a_n b_n = \sum_{i=0}^n a_i b_i$$




It is useful to see it as a projection operation

We say our basis $\mathbf{B} = \{\mathbf{b}_0, \mathbf{b}_1, \dots, \mathbf{b}_n\}$ is:

Orthogonal $\Rightarrow \forall i, j \in [0, n], \text{ if } i \neq j \text{ then } \langle \mathbf{b}_i, \mathbf{b}_j \rangle = 0 \Rightarrow$ Projection gives nothing

Normal $\Rightarrow \forall i, ||\mathbf{b}_i||_2 = \sqrt{\langle \mathbf{b}_i, \mathbf{b}_i \rangle} = 1 \Rightarrow$ Projection preserves length

Basis - Coefficients

$$\mathbf{v} = \mathbf{b}_1 c_1 + \mathbf{b}_2 c_2 + \mathbf{b}_3 c_3 + \dots$$

$$\mathbf{v} \cdot \mathbf{b}_2 = (\mathbf{b}_1 c_1 + \mathbf{b}_2 c_2 + \mathbf{b}_3 c_3 + \dots) \cdot \mathbf{b}_2$$

$$\frac{\mathbf{v} \cdot \mathbf{b}_2 - \mathbf{b}_2 \mathbf{b}_1 c_1 - \mathbf{b}_2 \mathbf{b}_3 c_3 - \dots}{\|\mathbf{b}_2\|_2} = c_2$$

If \mathbf{B} is orthonormal  $\begin{aligned} \langle \mathbf{b}_i, \mathbf{b}_j \rangle &= 0 \\ \|\mathbf{b}_2\|_2 &= 1 \end{aligned}$

$$\implies \mathbf{v} \cdot \mathbf{b}_2 = c_2$$

Each coefficient is independent and comes from a multiplication.

Basis - Functions

For functions:

$$f(x) = \alpha_1 g_1(x) + \alpha_2 g_2(x) + \alpha_3 g_3(x) + \dots$$

Weierstrass Theorem (of approximation):

Suppose f is a continuous real-valued function defined on the real interval $[a, b]$. For every $\epsilon > 0$, there exists a polynomial p such that for all x in $[a, b]$, we have $|f(x) - p(x)| < \epsilon$

i.e., Given a function, there exist a polynomial arbitrary close to it.

Monomials are a basis for the functional space:

$$G(x) = \{g_i(x)\} = \{x^i\} = \{1, x, x^2, x^3, \dots\}$$

Basis – Coefficients for functions

$$G(x) = \{g_i(x)\} = \{x^i\} = \{1, x, x^2, x^3, \dots\}$$

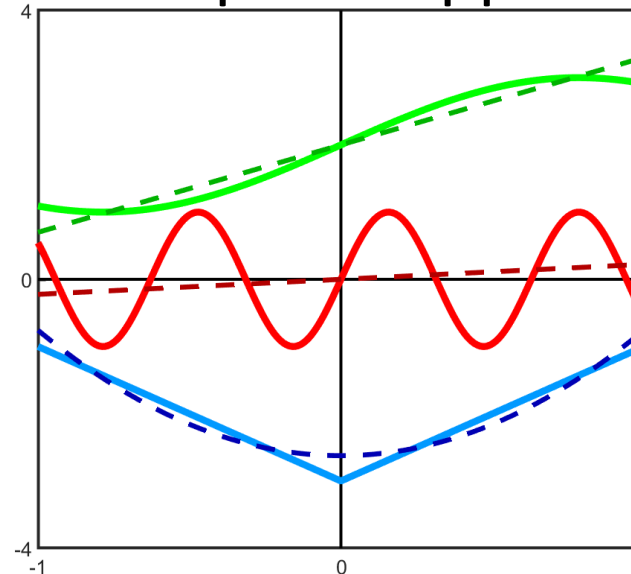
We use polynomial interpolation by sampling the function:

$$\begin{cases} y_1 = \alpha_1 g_1(x_1) + \alpha_2 g_2(x_1) + \alpha_3 g_3(x_1) + \dots \\ y_2 = \alpha_1 g_1(x_2) + \alpha_2 g_2(x_2) + \alpha_3 g_3(x_2) + \dots \\ y_3 = \alpha_1 g_1(x_3) + \alpha_2 g_2(x_3) + \alpha_3 g_3(x_3) + \dots \\ \dots \end{cases} \quad \Rightarrow \quad \begin{cases} y_1 = \alpha_1 \cdot 1 + \alpha_2 \cdot x_1 + \alpha_3 \cdot x_1^2 + \dots \\ y_2 = \alpha_1 \cdot 1 + \alpha_2 \cdot x_2 + \alpha_3 \cdot x_2^2 + \dots \\ y_3 = \alpha_1 \cdot 1 + \alpha_2 \cdot x_3 + \alpha_3 \cdot x_3^2 + \dots \\ \dots \end{cases}$$

$$\begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ \dots \end{bmatrix} = \begin{bmatrix} 1 & x_1 & x_1^2 & \dots \\ 1 & x_2 & x_2^2 & \dots \\ 1 & x_3 & x_3^2 & \dots \\ \dots & \dots & \dots & \dots \end{bmatrix} \cdot \begin{bmatrix} \alpha_1 \\ \alpha_2 \\ \alpha_3 \\ \dots \end{bmatrix}$$

$$\mathbf{y} = \mathbf{G}\mathbf{a} \quad \text{with } \mathbf{a} \text{ unknown} \quad \Rightarrow \quad \mathbf{G}^{-1}\mathbf{y} = \mathbf{a}$$

Example of approx



Coefficients are
informative on the
function behavior

Basis – Coefficients for functions (infinite sampling)

Considering
infinite sampling

$$\mathbf{x} = \begin{bmatrix} -1 \\ -1 + dx \\ -1 + 2dx \\ \dots \\ 1 - dx \\ 1 \end{bmatrix} \quad \mathbf{y} = \begin{bmatrix} f(-1) \\ f(-1 + dx) \\ f(-1 + 2dx) \\ \dots \\ f(1 - dx) \\ f(1) \end{bmatrix}$$

Defining an inner
product

$$\begin{aligned} \langle \mathbf{f}, \mathbf{g} \rangle &= \begin{bmatrix} f(-1) \\ f(-1 + dx) \\ f(-1 + 2dx) \\ \dots \\ f(1 - dx) \\ f(1) \end{bmatrix} \cdot \begin{bmatrix} g(-1) \\ g(-1 + dx) \\ g(-1 + 2dx) \\ \dots \\ g(1 - dx) \\ g(1) \end{bmatrix} \\ &= f(-1)g(-1) + f(-1 + dx)g(-1 + dx) + \dots + f(1)g(1) \\ &= \int_{-1}^1 f(x)g(x)dx \end{aligned}$$

Basis – Properties for functions

$$\langle \mathbf{f}, \mathbf{g} \rangle = \int_{-1}^1 f(x)g(x)dx$$

Orthogonality

Vectors

$$\langle v, w \rangle = 0$$

Functions

$$\langle f, g \rangle = \int_{-1}^1 f(x)g(x)dx = 0$$

$$\langle 1, x \rangle = \int_{-1}^1 1 \cdot x dx = \left. \frac{x^2}{2} \right|_{-1}^1 = \frac{1}{2} - \frac{1}{2} = 0$$

$$\langle x, x^2 \rangle = \int_{-1}^1 x \cdot x^2 dx = \left. \frac{x^4}{4} \right|_{-1}^1 = \frac{1}{4} - \frac{1}{4} = 0$$

$$\langle 1, x^2 \rangle = \int_{-1}^1 1 \cdot x^2 dx = \left. \frac{x^3}{3} \right|_{-1}^1 = \frac{1}{3} + \frac{1}{3} = \frac{2}{3}$$

Normality

$$\langle v, v \rangle = 1$$

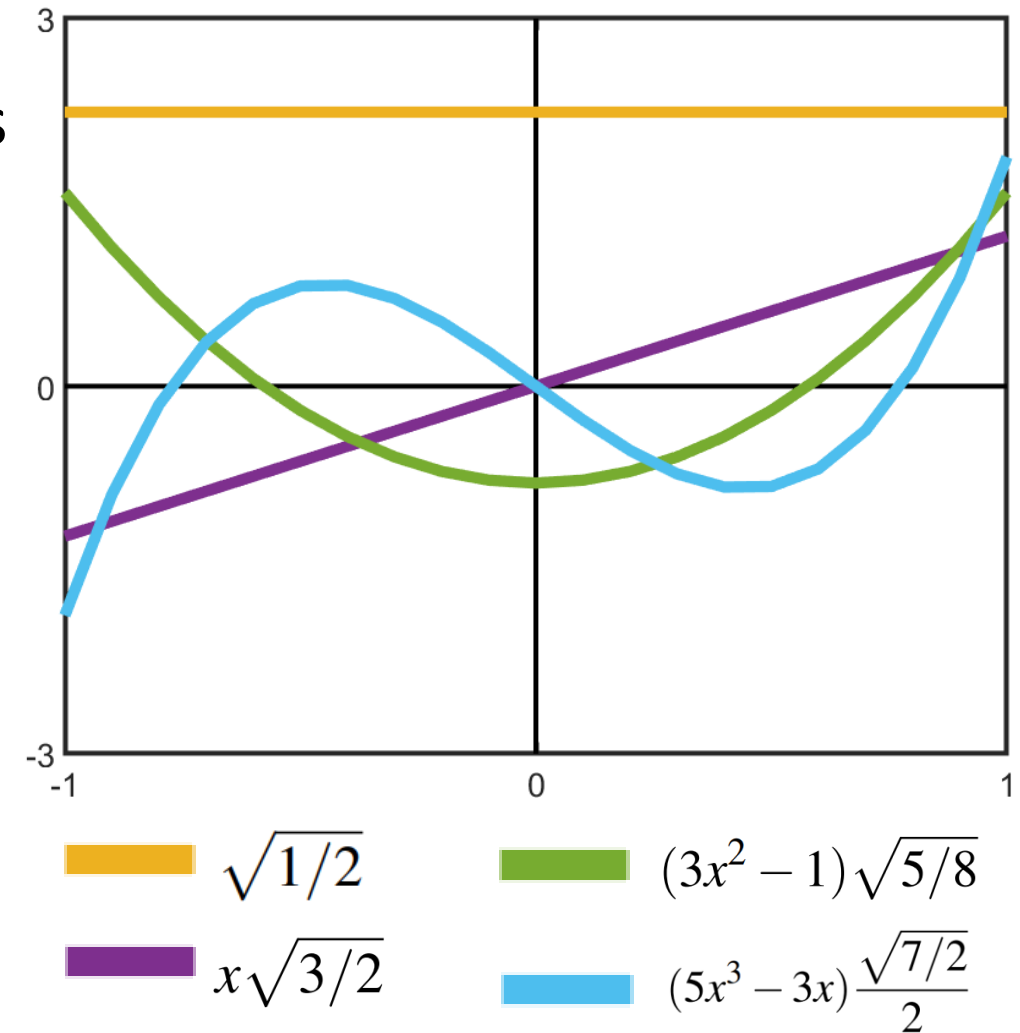
$$\langle f, f \rangle = \int_{-1}^1 f(x)^2 dx = 1$$

$$\langle 1, 1 \rangle = \int_{-1}^1 1 dx = \left. x \right|_{-1}^1 = 1 + 1 = 2$$

Basis – Orthonormalization for functions

Gram-Schmidt process over the monomial basis produces the **Legendre Polynomials**, that are orthonormals.

There are other useful properties for functional basis?

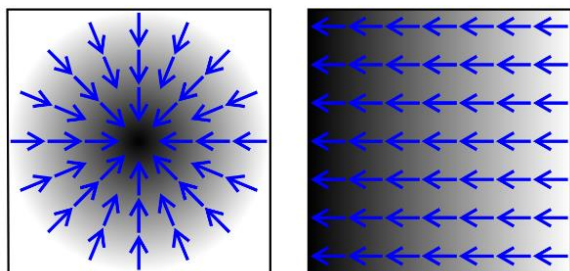


Gradient, Divergence, Laplacian

Important tools from analysis:

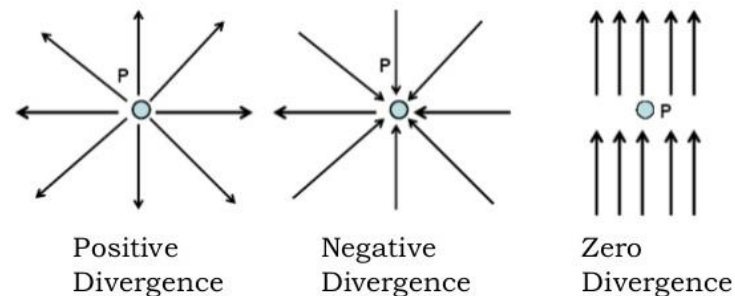
The gradient

$$\nabla: \left(\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z}, \dots \right)$$



The divergence

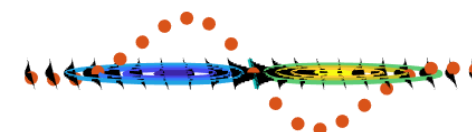
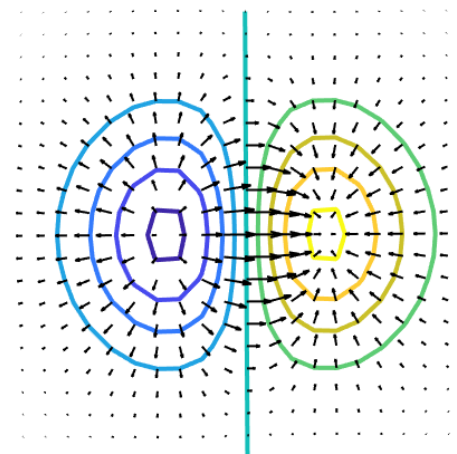
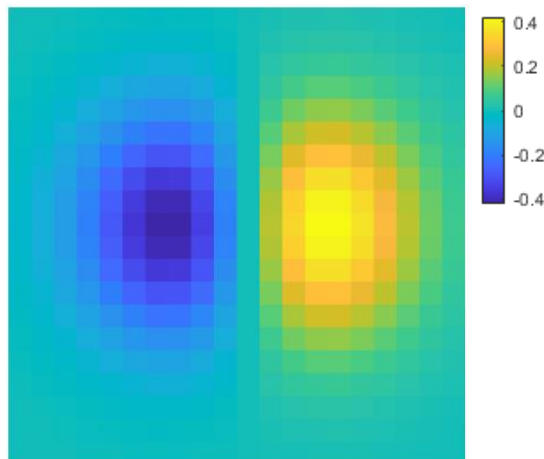
$$\text{div}: \frac{\partial}{\partial x} + \frac{\partial}{\partial y} + \frac{\partial}{\partial z} + \dots$$



The Laplacian

$$\Delta: \text{div } \nabla = \frac{\partial^2}{\partial^2 x} + \frac{\partial^2}{\partial^2 y} + \frac{\partial^2}{\partial^2 z} + \dots$$

The change of a rate of change



Note: in 1D, the Laplacian is equal to the second order derivative.

Smoothness – Dirichlet Energy


Dirichlet Energy:

$$E(f) = \int_X ||\nabla f(x)||^2 dx$$

It measures the variability of the function.

First Green Identity:

A miracle occurs


$$E(f) = \int_X ||\nabla f(x)||^2 dx = \cdots = \int_X f(x) \Delta f(x) dx$$

We want the orthonormal basis that minimizes this energy.

Smoothness – (Discrete) Dirichlet Energy

$$E(f) = \int_X f(x) \Delta f(x) dx$$

$$E(\phi_i) = \int_X \phi_i(x) \Delta \phi_i(x) dx = \langle \phi_i, \Delta \phi_i \rangle$$

$$\mathbf{\Phi}_k = [\phi_0 \quad \phi_1 \quad \phi_2 \quad \dots \quad \phi_k]$$

$$\mathbf{\Phi}_k \in \mathbb{R}^{n \times k}$$

$$\min_{\phi_0} E(\phi_0) \quad \text{s.t.} \quad \|\phi_0\| = 1$$

$$\min_{\phi_i} E(\phi_i) \quad \text{s.t.} \quad \|\phi_i\| = 1, \quad \phi_i \perp \text{span}\{\phi_0, \dots, \phi_{i-1}\}$$

$$\boxed{\min_{\mathbf{\Phi}_k} \text{trace}(\mathbf{\Phi}_k^T \Delta \mathbf{\Phi}_k) \quad \text{s.t.} \quad \mathbf{\Phi}_k^T \mathbf{\Phi}_k = \mathbf{I}}$$

Smoothness – (Discrete) Dirichlet Energy

$$\min_{\Phi_k} \text{trace}(\Phi_k^T \Delta \Phi_k) \quad \text{s.t.} \quad \Phi_k^T \Phi_k = \mathbf{I}$$

$$\Delta \Phi_k = \Phi_k \Lambda_k$$

The set of eigenvectors (also called *eigenfunctions*) of the Laplacian is an orthonormal basis, optimal for the smoothness.

In the 1D case they are the standard Fourier basis:

$$\Delta \sin(n\theta) = -|n|^2 \sin(n\theta)$$

$$\Delta e^{n2\pi i\theta} = -|n|^2 4\pi^2 e^{n2\pi i\theta}$$

First part summary

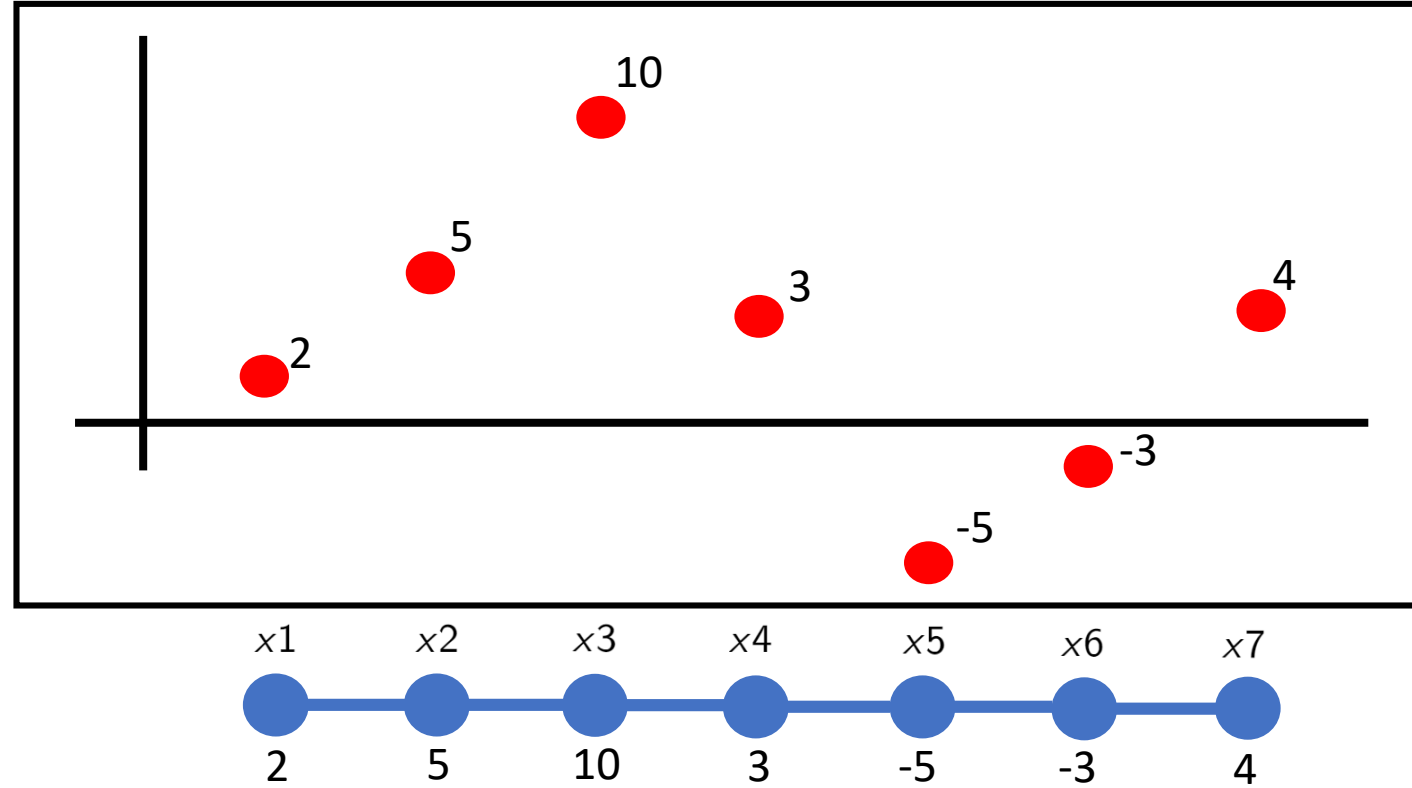
We have seen so far:

- The concept of basis
- The properties of basis (Orthogonality and Normality)
- How to extend these to the functions
- Some main tools: gradient, divergence, Laplacian
- The Dirichlet Energy to add a new property (Smoothness)
- The link with Fourier Basis

Key idea: given a domain, we need a Laplacian.



Discrete Setting



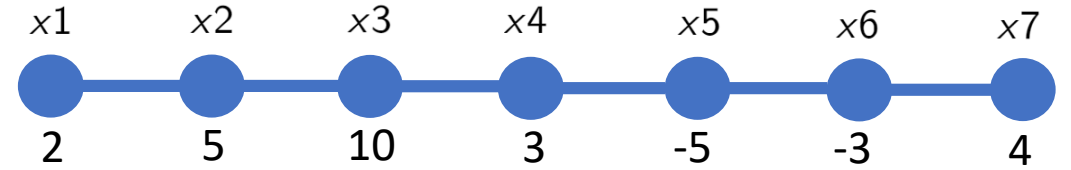
Vertices $\{x_1, x_2, x_3, x_4, x_5, x_6, x_7\}$

Edges connect consecutive points

The y-value is a function on the graph $F : V \rightarrow \mathbb{R}$

Discrete Setting

$$f(x) = \begin{bmatrix} 2 & 5 & 10 & 3 & -5 & -3 & 4 \end{bmatrix}$$



$$f'(x_i) = \frac{f(x_{i+1}) - f(x_i)}{h}$$

$$f'(x) = \begin{bmatrix} 3 & 5 & -7 & -8 & 2 & 7 & \dots \end{bmatrix}$$

$$f''(x_i) = \frac{f'(x_i) - f'(x_i - 1)}{h} = \dots = \frac{f(x_{i+1}) + f(x_{i-1}) - 2f(x_i)}{h^2}$$

assuming $h = 1$:

$$f''(x_i) = f(x_{i+1}) + f(x_{i-1}) - 2f(x_i)$$

$$f''(x) = \begin{bmatrix} \dots & 2 & -12 & -1 & 10 & 5 & \dots \end{bmatrix}$$

Encode distance of a point from the mean of the neighbor values.

1D Discrete Laplacian

$$f(x) = \begin{bmatrix} 2 & 5 & 10 & 3 & -5 & -3 & 4 \end{bmatrix}$$

$$f''(x_i) = f(x_{i+1}) + f(x_{i-1}) - 2f(x_i)$$

$$f''(x_i) = Lf = \begin{bmatrix} -1 & 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & -2 & 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & -2 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & -2 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & -2 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 & -2 & 1 \\ 0 & 0 & 0 & 0 & 0 & 1 & -1 \end{bmatrix} \begin{bmatrix} 2 \\ 5 \\ 10 \\ 3 \\ -5 \\ -3 \\ 4 \end{bmatrix} = \begin{bmatrix} \dots \\ 2 \\ -12 \\ -1 \\ 10 \\ 5 \\ \dots \end{bmatrix}$$

$$L_{ij} = \begin{cases} 1 & \text{if } i \neq j, i \sim j \\ -d_{ij} & \text{if } i = j \\ 0 & \text{otherwise} \end{cases} \quad \text{or more generally} \quad \begin{cases} w_{ij} & \text{if } i \neq j, i \sim j \\ -\sum_{j \neq i, j \sim i} w_{ij} & \text{if } i = j \\ 0 & \text{otherwise} \end{cases}$$

$L = W - D$, where D is the diagonal matrix of the degrees, and W is the weighted adjacency matrix.

Laplacian Eigenvectors

$$E(f) = \int_X \|\nabla f(x)\|^2 dx = \int_X f(x) \Delta f(x) dx$$

$$E(f) = \sum \langle \nabla f, \nabla f \rangle = \sum_i f_i (\Delta f)_i$$

$$\sum_{(i,j) \in E} (f_i - f_j)^2 = f^T L f$$

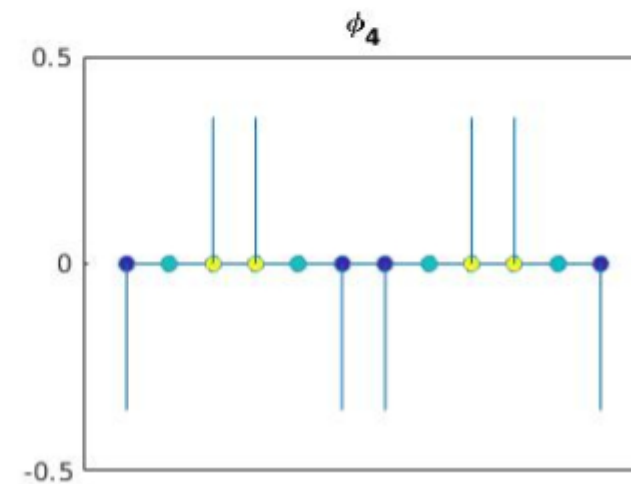
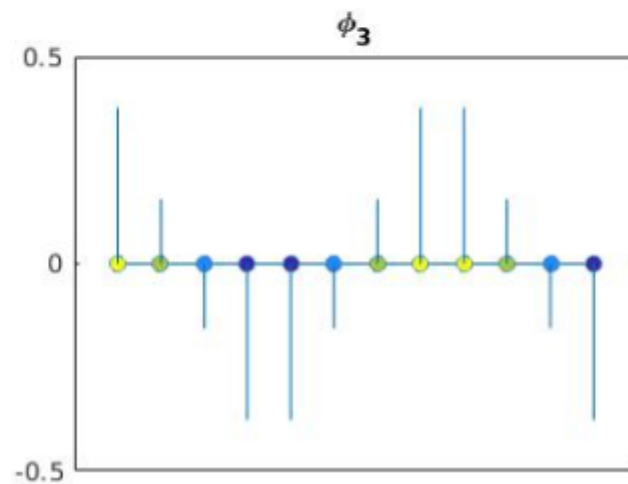
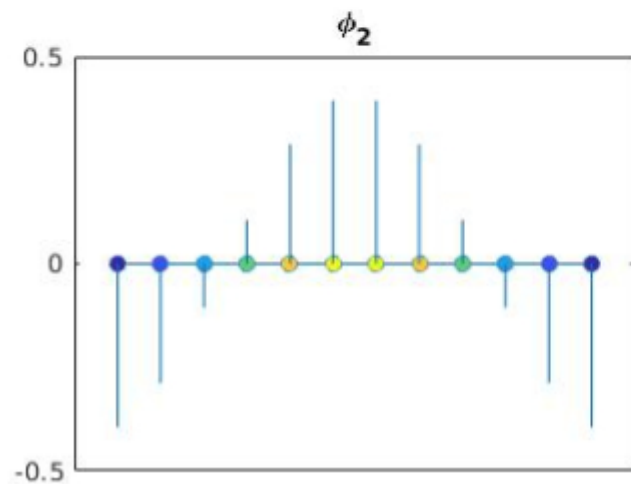
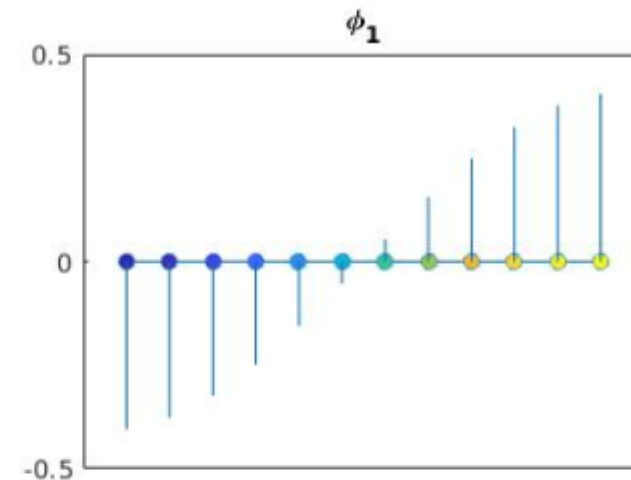
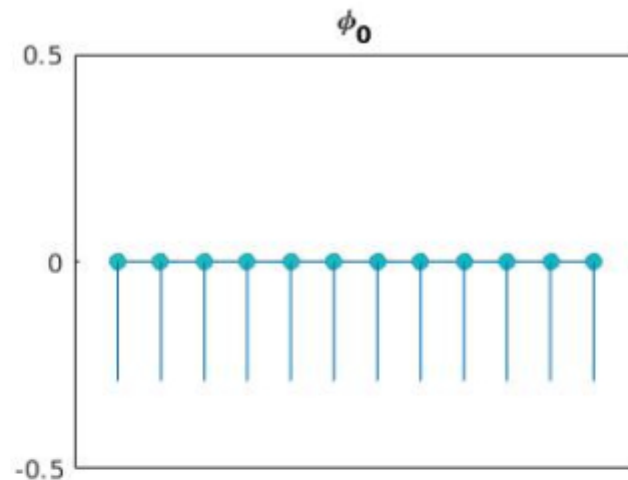
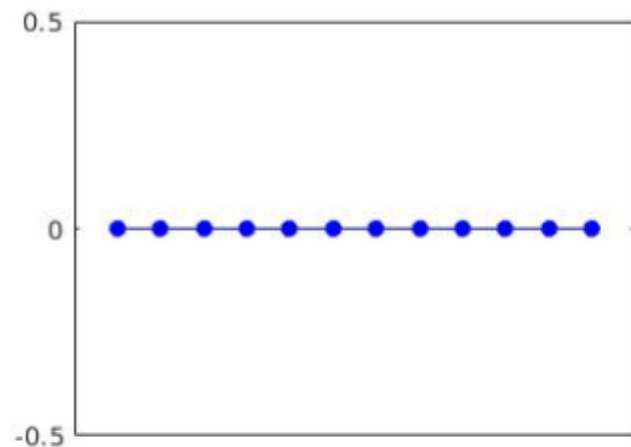
$$\lambda = f^T L f$$

$$\lambda f = L f$$

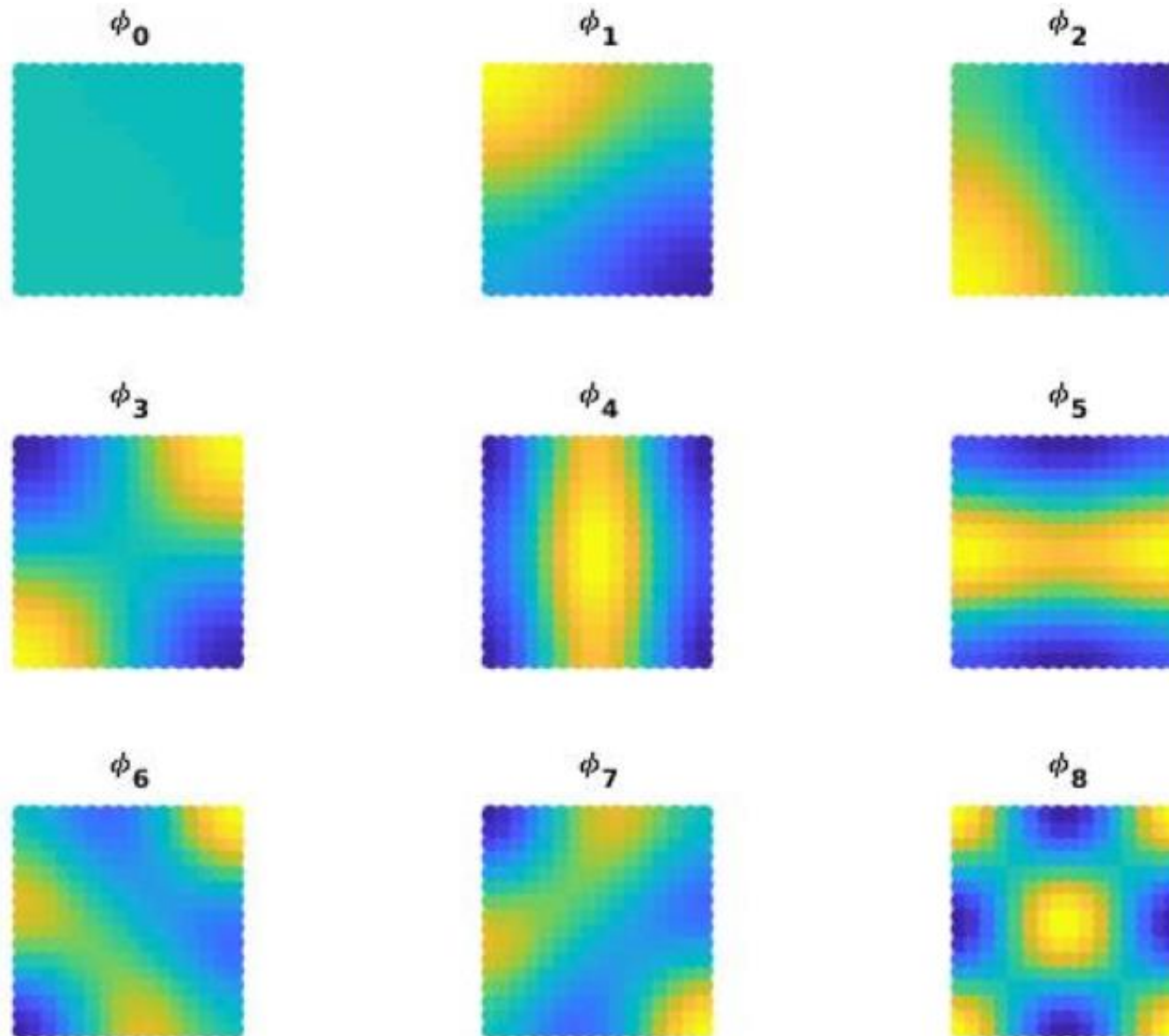
L is symmetric  its eigenvalues are real and non-negative

$$\lambda_i = \phi_i^T L \phi_i \geq 0$$

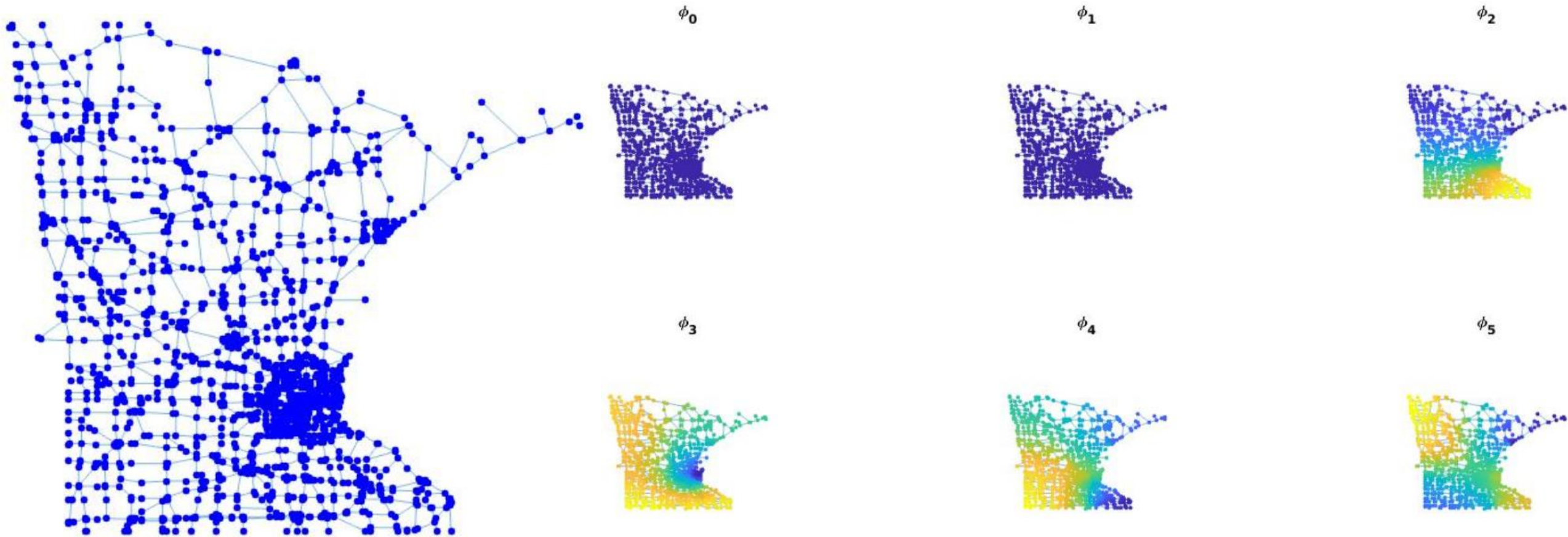
Laplacian Eigenvectors – 1D



Laplacian Eigenvectors – 2D



Laplacian Eigenvectors – Generic Graph



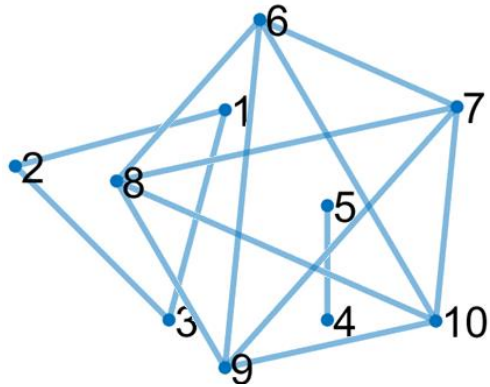
Disconnected components

Consider the eigenvalues 0 on a connected graph:

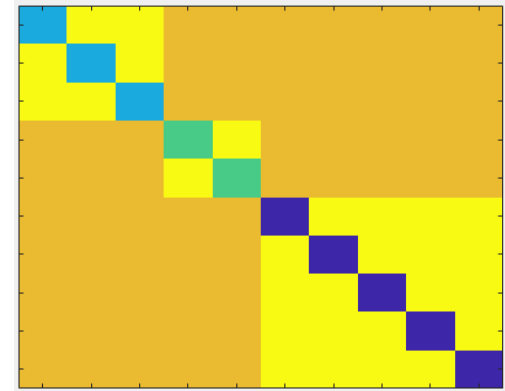
$$\sum_{(i,j) \in E} (\phi_i - \phi_j)^2 = \phi^T L \phi = 0 \implies (\phi_i - \phi_j)^2 = 0, \forall (i,j) \implies \phi_i = \phi_j$$

ϕ_0 is the constant function.

Consider the adjacency matrix on a disconnected graph \implies Block matrix

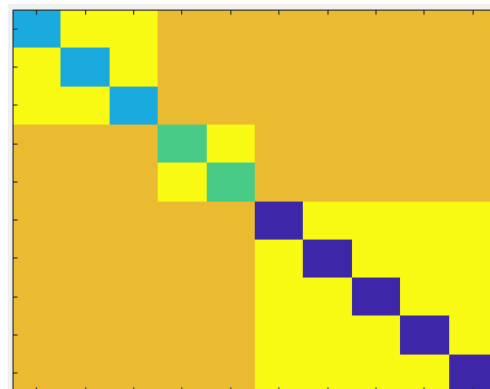
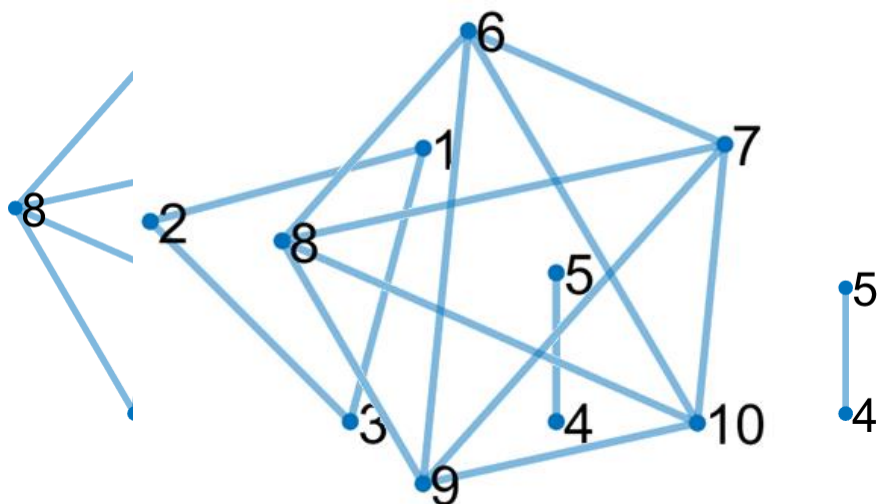


$$W = \begin{bmatrix} A_1 & & \\ & A_2 & \\ & & \dots \\ & & & A_k \end{bmatrix} \quad L = \begin{bmatrix} L_1 & & \\ & L_2 & \\ & & \dots \\ & & & L_k \end{bmatrix}$$



The eigenfunctions of a block matrix are the union of the eigenfunctions of the blocks \implies 0s eigenvalues as many as connected components.

Disconnected components



$$\lambda_0 = 0$$

$$\lambda_1 = 0$$

$$\lambda_2 = 0$$

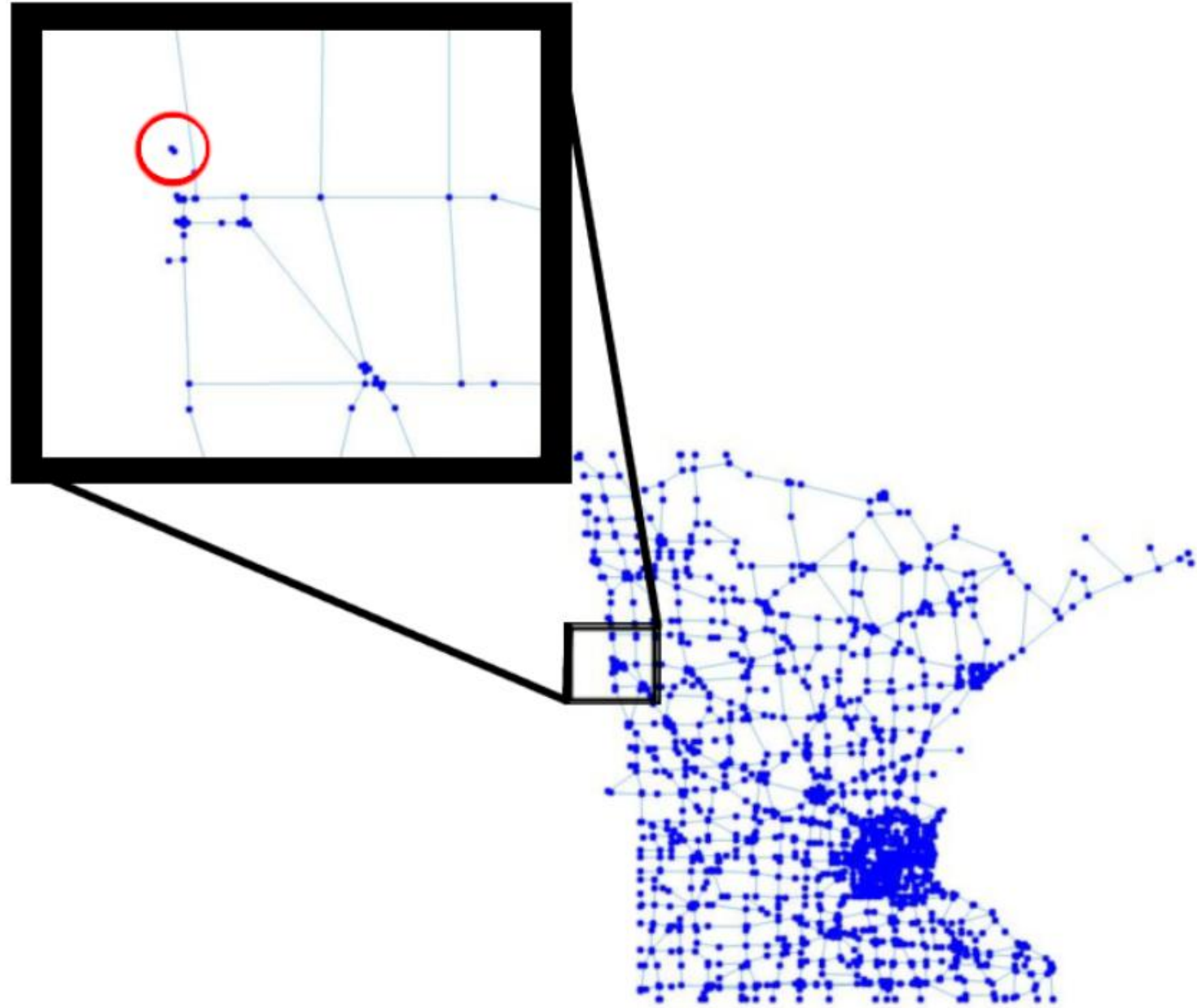
$$\lambda_3 = 2$$

$$\lambda_4 = 3$$

...

$$\phi_0 = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0.4472 \\ 0.4472 \\ 0.4472 \\ 0.4472 \\ 0.4472 \end{bmatrix} \quad \phi_1 = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0.7071 \\ 0.7071 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} \quad \phi_2 = \begin{bmatrix} 0.5774 \\ 0.5774 \\ 0.5774 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} \quad \phi_3 = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0.7071 \\ -0.7071 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} \quad \dots$$

Disconnected components



Min-cut

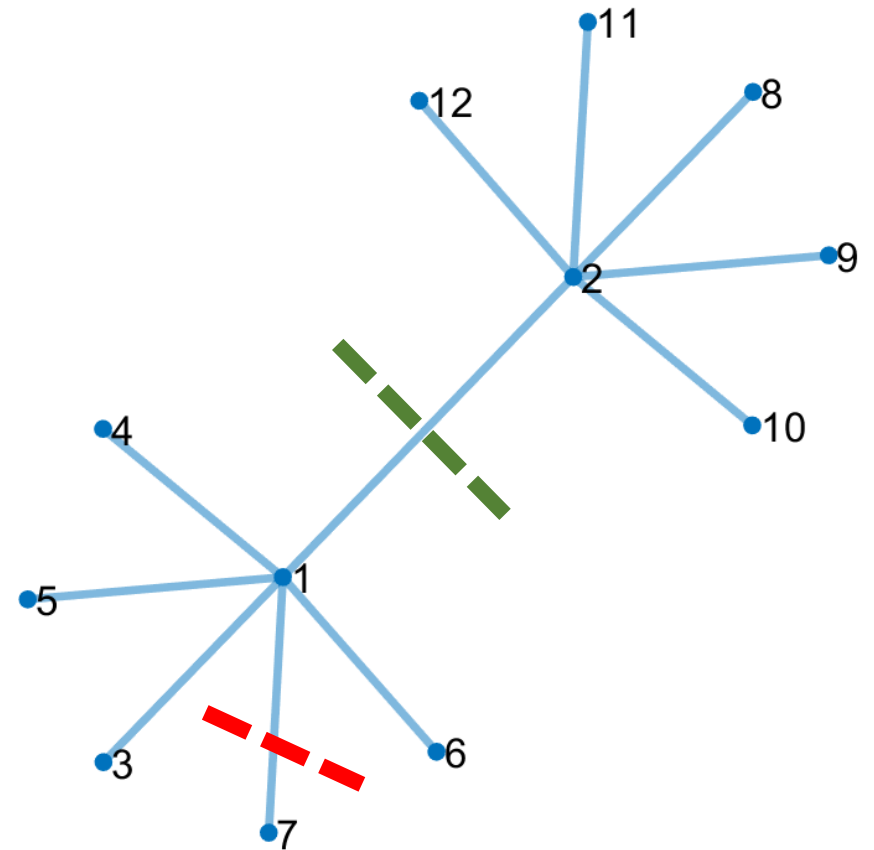
Minimum number of edges to remove to disconnect the graph.

Given a Graph (V, E) , find the minimum cut
s.t. the two disjoint sets $A, B \subset V$

$$\text{min cut}(A, B) = \sum_{i \in A, j \in B} w_{ij}$$

Green and red cuts have the same cost.
In general we prefer a *balanced* cut.

$$|A_1| = |\bar{A}_1| = 0.5$$



Ratiocut

Approximation of a balanced cut

$$\min \text{Ratiocut}(A_1, \dots, A_k) = \sum_{i=1}^k \frac{\text{cut}(A_i, \bar{A}_i)}{|A_i|}$$

Case of split in two

$$\min \text{Ratiocut}(A_1, \bar{A}_1) = \frac{\text{cut}(A_1, \bar{A}_1)}{|A_1|} + \frac{\text{cut}(\bar{A}_1, A_1)}{|\bar{A}_1|} = \epsilon$$

$$|\bar{A}_1| \text{cut} + |A_1| \text{cut} = \epsilon |A_1| |\bar{A}_1|$$

$$\frac{\text{cut}}{|A_1| |\bar{A}_1|} = \frac{\epsilon}{|V|}$$

$$\min \text{Ratiocut}(A_1, \bar{A}_1) = \frac{\text{cut}}{|A_1| |\bar{A}_1|}$$

$$\text{maximize } |A_1| |\bar{A}_1| \implies |A_1| = |\bar{A}_1| = 0.5$$

$$\text{minimize } \text{cut} \implies \text{few «bridge» edges}$$

Ratiocut

$$\sum_{(i,j) \in E} (\phi_{1_i} - \phi_{1_j})^2 = \lambda_1 \quad \text{Minimize Dirichlet Energy}$$

$$\phi_0 \perp \phi_1 \implies \langle \phi_0, \phi_1 \rangle = 0 \implies \sum_i \phi_{0_i} \phi_{1_i} = 0 \implies \phi_{1_1} + \phi_{1_2} + \dots = 0$$



First eigenfunction is constant

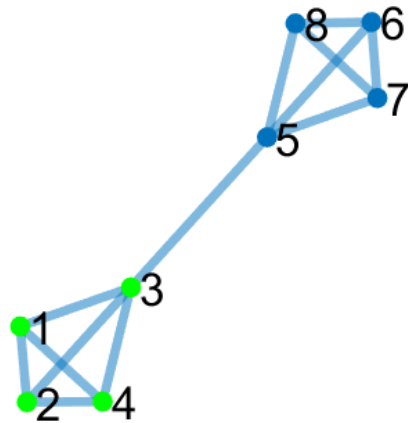
Also:

$\|\phi_1\| = 1$ \longrightarrow Split the graph evenly by sign \longrightarrow Relaxed version of RatioCut

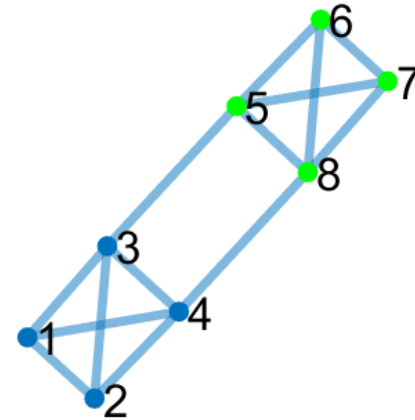
$\phi_{1_1} + \phi_{1_2} + \dots = 0$

Fiedler value

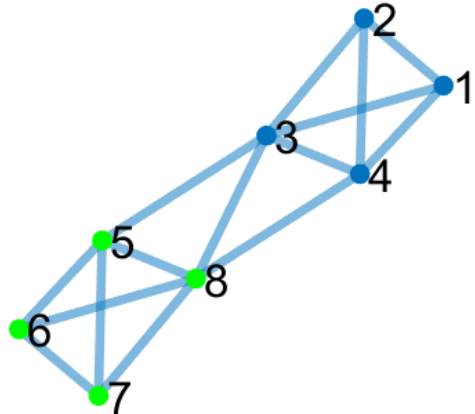
$$\lambda_1 = 0.35425$$



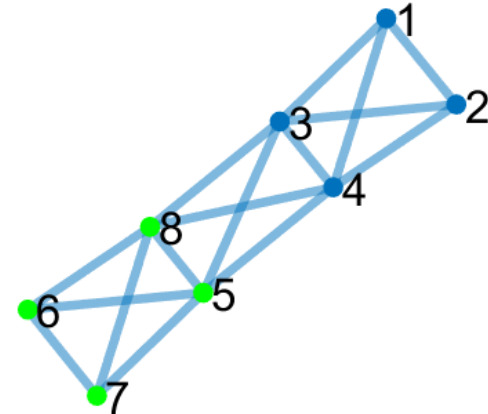
$$\lambda_1 = 0.76393$$



$$\lambda_1 = 0.94863$$



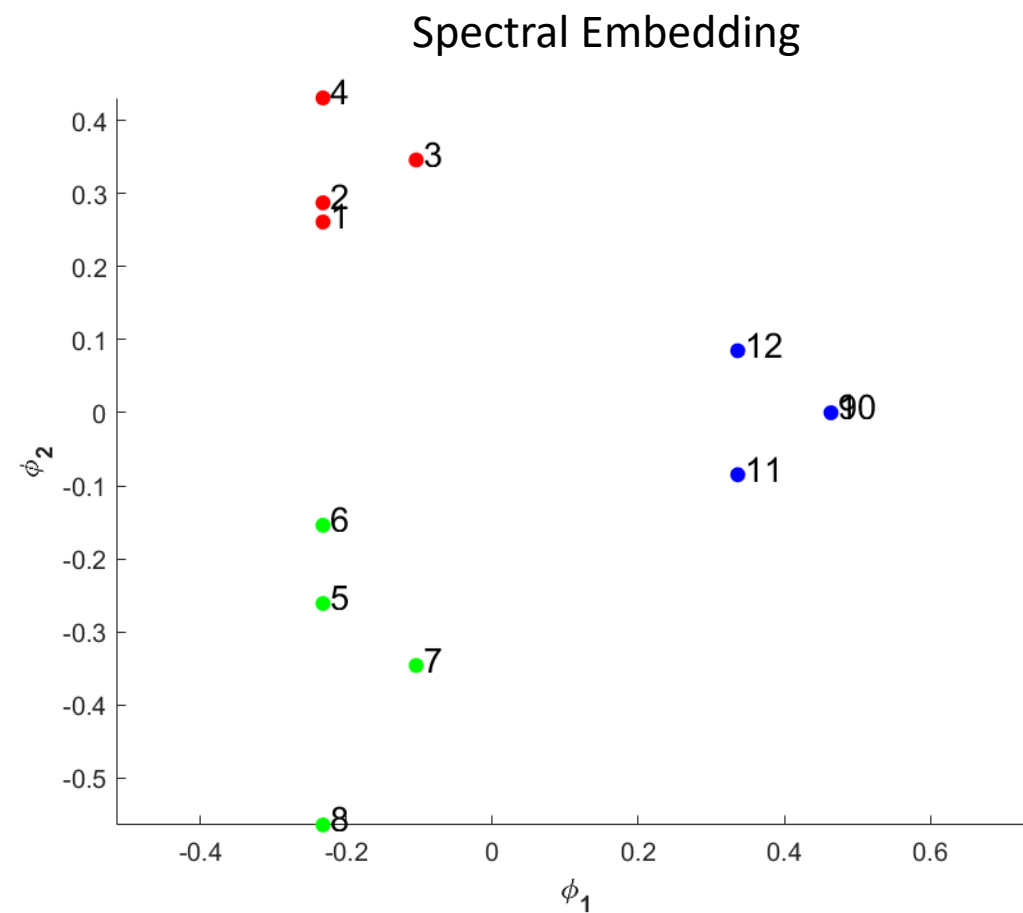
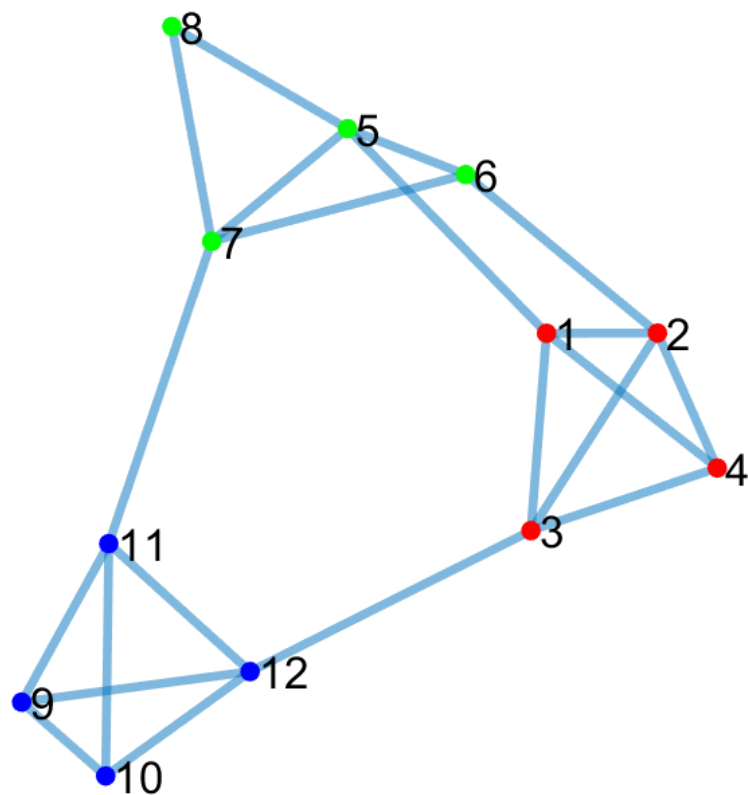
$$\lambda_1 = 1.1716$$



Spectral Clustering

$$\phi_1, \phi_2, \dots, \phi_d$$

$$\{\phi_1(v), \phi_2(v), \dots, \phi_d(v)\}$$

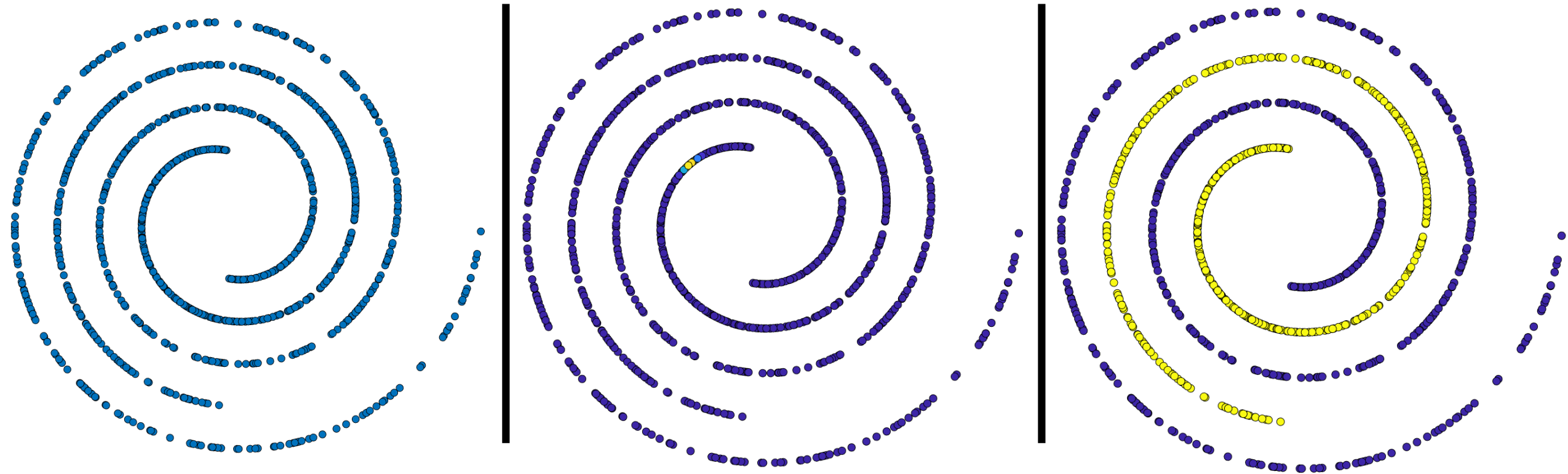


Spectral Clustering – 2D

We can build a fully-connected adjacency matrix setting the weight as:

$$d(x_i, x_j) = e^{\frac{-|x_i - x_j|}{2\sigma^2}}$$

Other strategies are possible (e.g. K-NN).



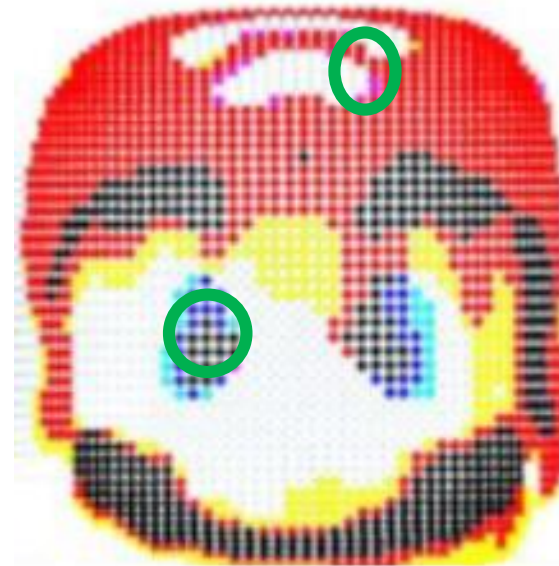
Graph Signal Processing



original f



graph f



$$\Phi(f^T \Phi)^T$$



synth f

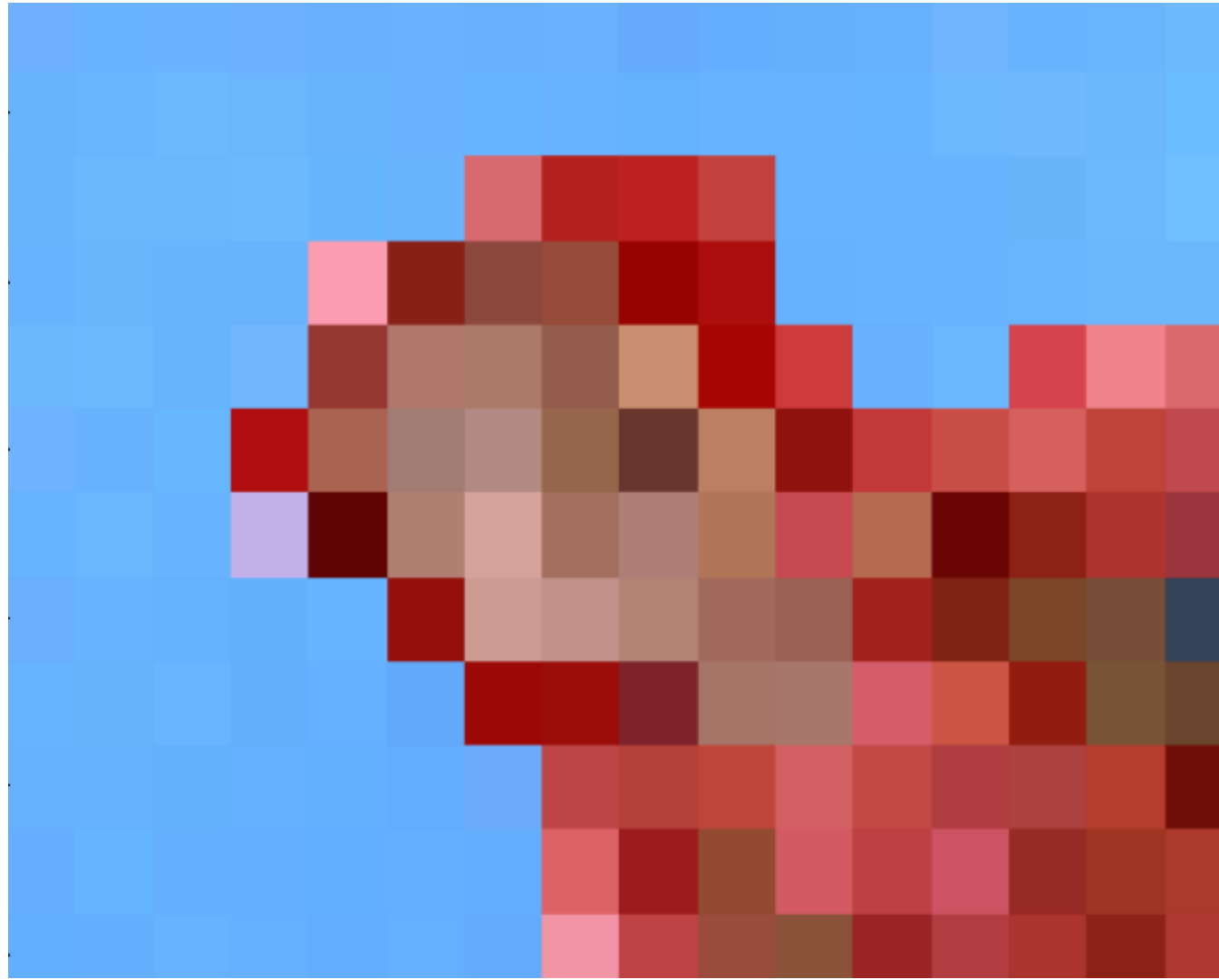
Denoising and compression

This image is $64 \times 64 = 4096$ nodes, for the 3 RGB channels: 12288 values.
We have represented 3 signals with the first 500 eigenfunctions \Rightarrow 1500 values.

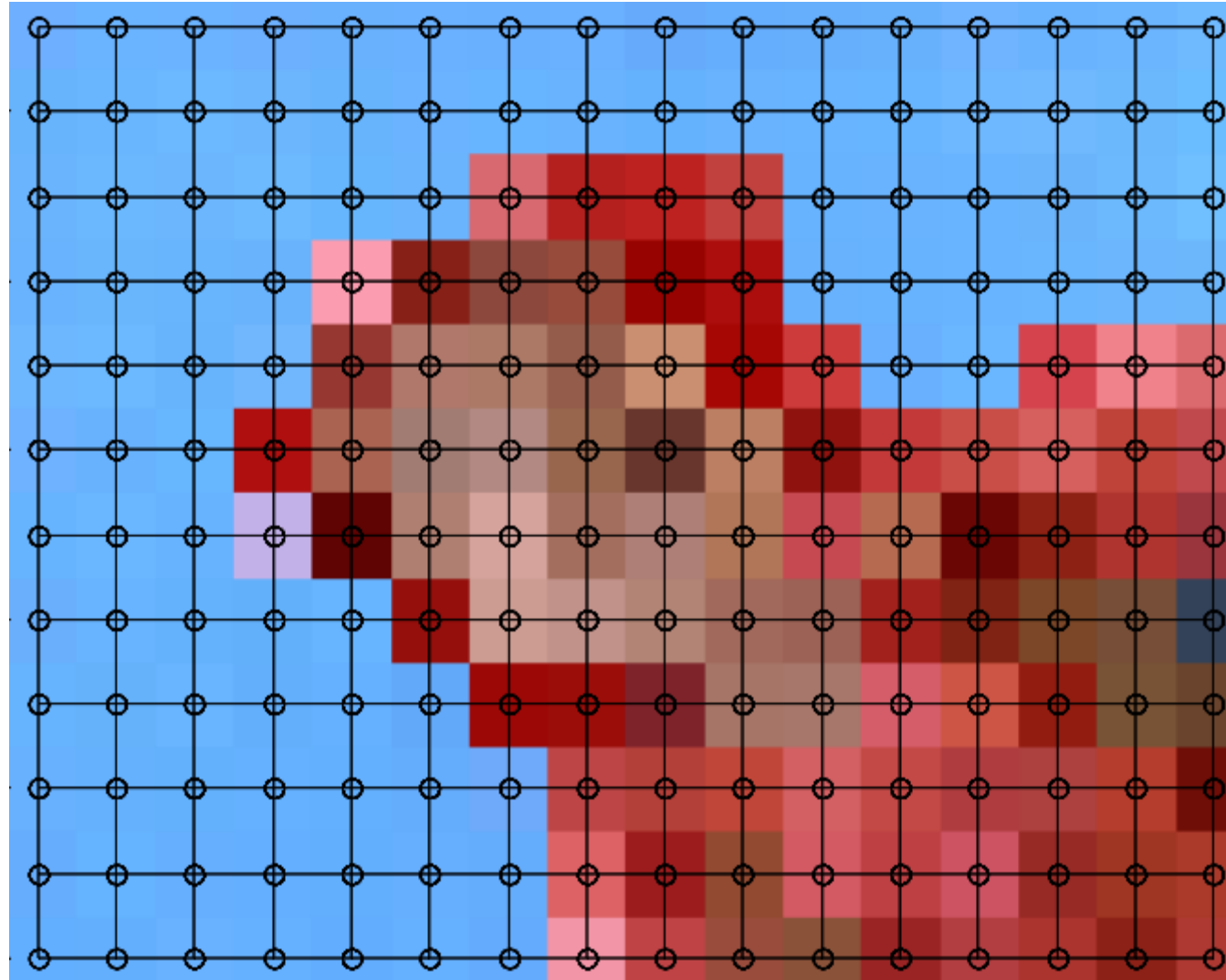
Segmentation (Shi-Malik '00)



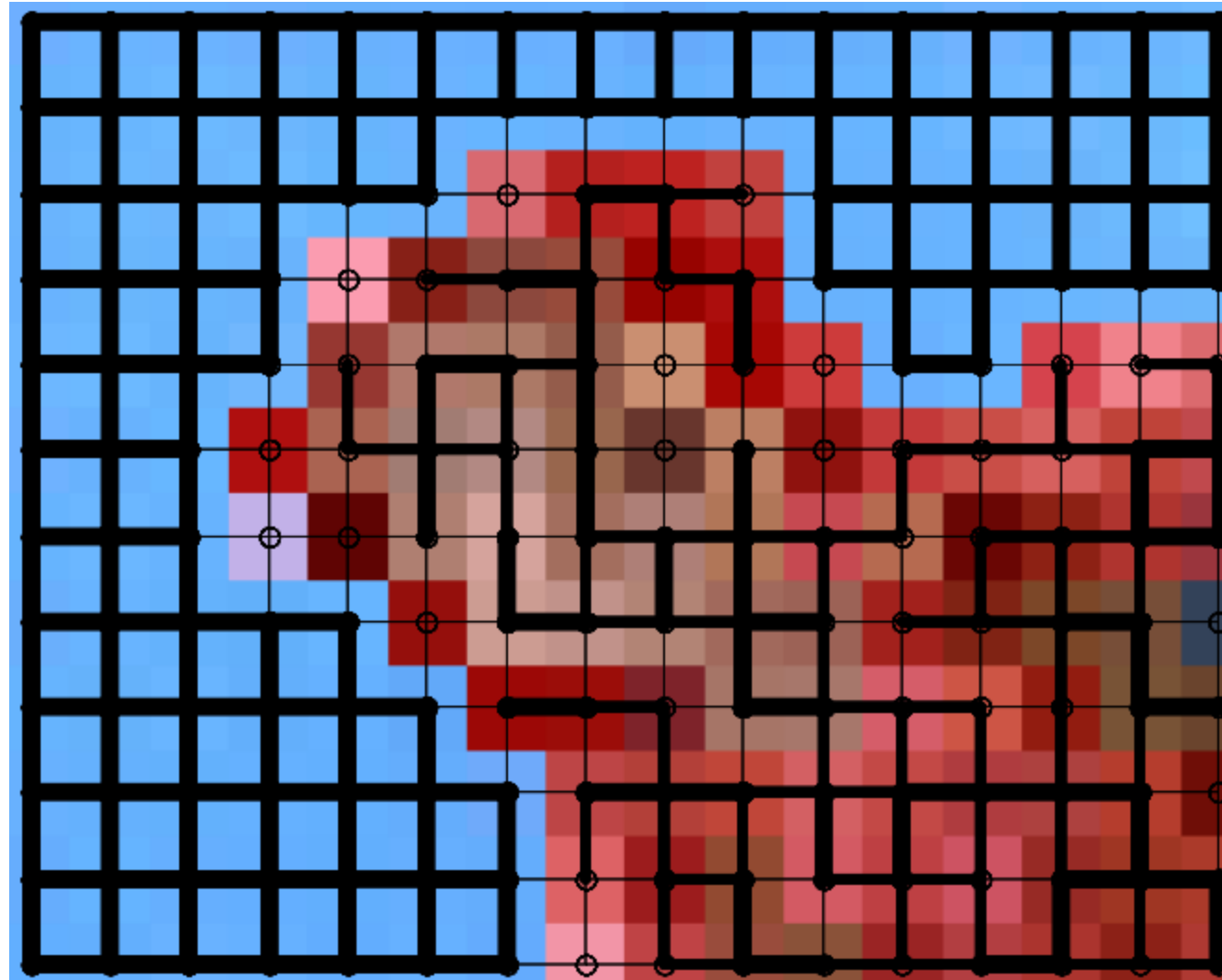
Segmentation (Shi-Malik '00)



Segmentation (Shi-Malik '00)



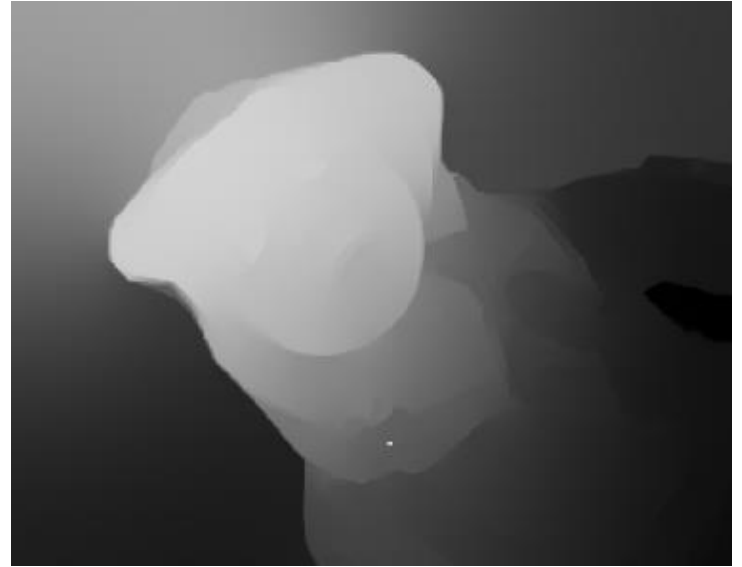
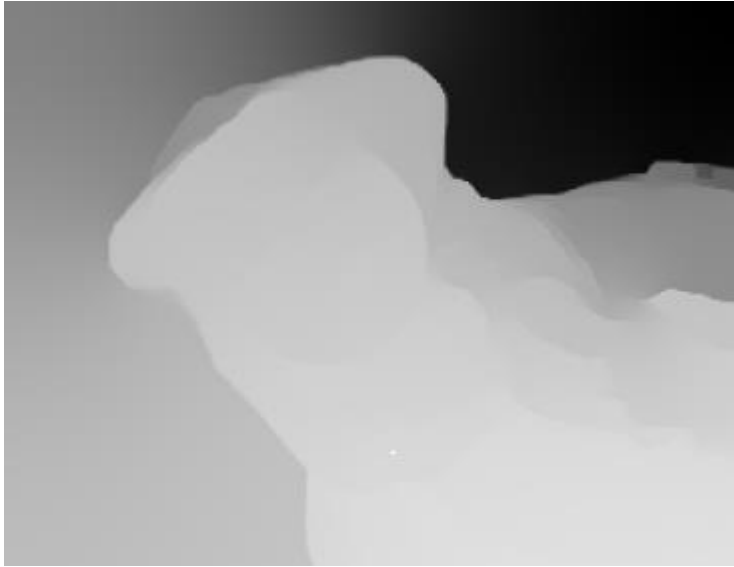
Segmentation (Shi-Malik '00)



edge weight $e^{-\text{diff}(\text{pixel } i, \text{pixel } j)^2 / t^2}$

Segmentation (Shi-Malik '00)

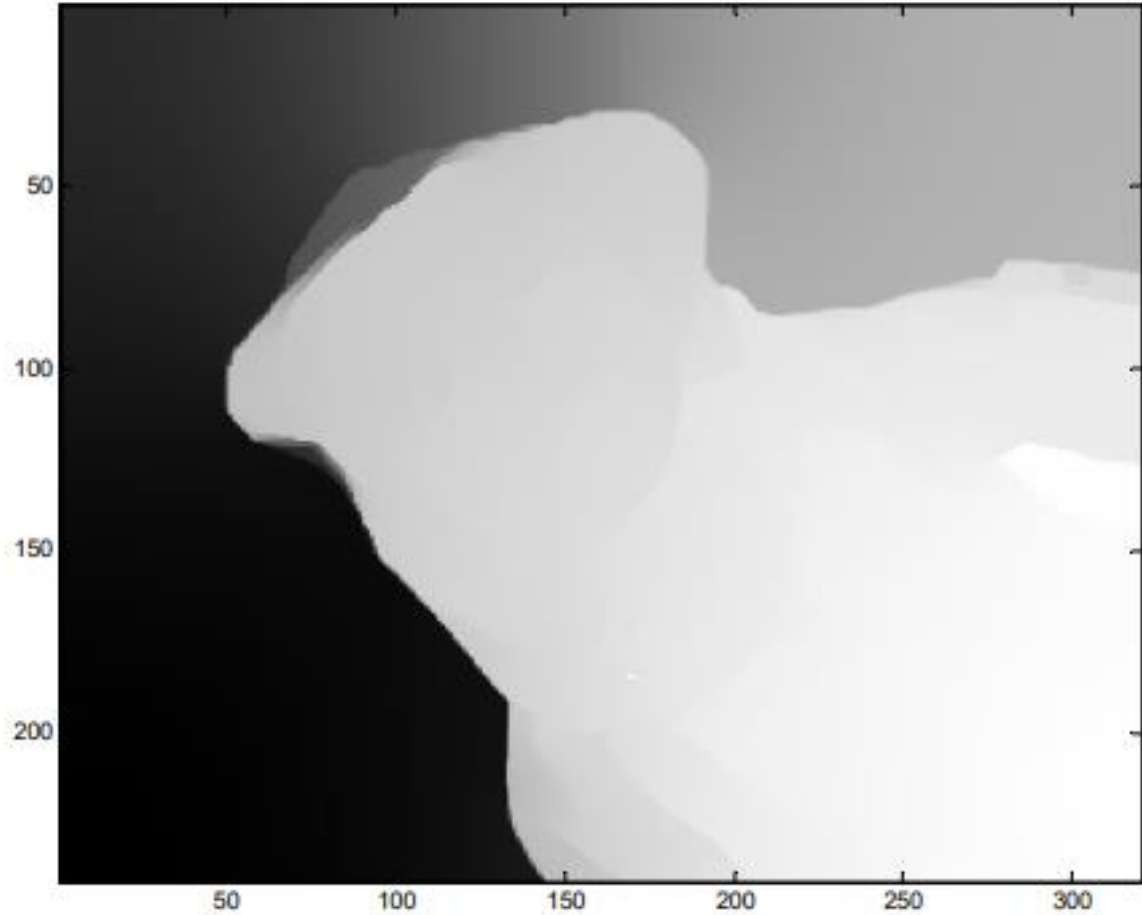
Eigen



Segm.



Segmentation (Miller and Tolliver '06)



For a graph $G = (V, E, w^0)$ prescribe the number of partitions k that the edge cut is to yield. Given a valid **reweighting scheme**, iteration of the SR-Step produces a sequence of N weightings $\{w^{(N)}\}$ such that the graph $G^N = (V, E, w^N)$ is disconnected into k components by the weighting w^N .

Segmentation (Neto and Felzenszwalb '20)



Both graphs are defined over the same set of vertices, corresponding to the pixels in an image.

1. The graph G_{grid} is a grid over the image pixels, where each pixel is connected to the four neighboring pixels with an edge of weight 1. This graph encourages neighboring pixels to be grouped together, independent of their appearance.
2. The graph G_{data} is a fully connected graph that encourages pixels with similar appearance to be grouped together, independent of their location. The weights in G_{data} are based on appearance similarity of pixels, and do not depend on pixel locations,

$$w(i, j) = \exp \left(-\frac{\|I(i) - I(j)\|^2}{2\sigma^2} \right). \quad (6)$$

In our experiments, we use a Lanczos Process to compute the second **largest** eigenvector of P .

Summary

We have learned:

- How to extend Laplacian to non-euclidean domain
- Why their eigenfunctions are so important
- How this operator and its eigendecomposition touch the connectivity
- Several applications of its eigendecomposition

! Exercises !

<https://github.com/riccardomarin/SpectralShapeAnalysis>

It could take some time to configure the environment

Lunch it in advance

