Geometric deep learning: going beyond Euclidean data

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IEEE Signal Processing Magazine, 2017, 34(4):18-42.

Abstract

- Many scientific fields study data with an underlying structure that is a **non-Euclidean** space.
    - Graph and Manifold
    - Social networks, sensor networks, brain imaging
- Deep neural networks have recently proven to be powerful tools for a broad range of problems.
    - Data with an underlying Euclidean or grid-like structure
- **Geometric deep learning** is an umbrella term for emerging techniques attempting to generalize (structured) deep neural models to non-Euclidean domains

Introduction

- Deep learning
  - *Learning complicated concepts by building them from simpler ones in a hierarchical or multi-layer manner*
  - Neural networks are popular realizations of such deep multi-layer hierarchies

  - Qualitative breakthroughs
    - Speech recognition, machine translation…
    - The growing computational power and availability of large training datasets

Introduction

- **Why it's successful**
  - Ability to leverage statistical properties of the data
    - Stationarity and Compositionality (local statistics)
  - E.g., consider images as functions on the Euclidean space
    - **Stationarity** is owed to shift-invariance;
    - **Locality** is due to the local connectivity;
    - **Compositionality** stems from the multi-resolution structure of the grid.
- These properties are exploited by convolutional architectures
  - Extracting local features and reduces the number of parameters
  - Imposes some priors about the data

Introduction

- **Non-Euclidean geometric data**
  - In social networks, the characteristics of users can be modeled as **signals** on the vertices of the social graph
  - Sensor networks are graph models of distributed interconnected sensors, whose readings are modelled as time-dependent **signals** on the vertices
  - In genetics, gene expression data are modeled as **signals** defined on the regulatory network
- Non-Euclidean data implies no familiar properties
  - global parameterization, vector space structure, shift-invariance.
- The purpose of our paper is to show different methods of translating the key ingredients of successful deep learning methods such as convolutional neural networks to non-Euclidean data.

GEOMETRIC LEARNING PROBLEMS

- **Two classes of geometric learning problems**
  - 1. To characterize the structure of the data
  - 2. Analyzing functions defined on non-Euclidean domain
- First class: structure of the domain (embedding)
  - *Manifold learning* or *non-linear dimensionality reduction*
    - Data points with underlying lower dimensional structure embedded into a high-dimensional Euclidean space
    - Recovering the lower dimensional structure
  - Two steps of Manifold learning
    - Constructing a representation of local affinity of the data points
    - Data points are embedded into a low-dimensional space trying to preserve some criterion of the original affinity.

GEOMETRIC LEARNING PROBLEMS

- Second class: analyzing functions defined on a given non-Euclidean domain
  - Prediction: e.g., assume that we are given the geographic coordinates of the users of a social network, represented as **a time-dependent signal on the vertices** of the social graph. An important application in location-based social networks is **to predict the position of the user** given his or her past behavior, as well as that of his or her friends.

DEEP LEARNING ON EUCLIDEAN DOMAINS

- **Geometric priors**
  - 1. *Stationarity*
    - Translation operator

$$\mathcal{T}_v f(x) = f(x - v), \quad x, v \in \Omega,$$

    - The assumption is that the function y is either invariant or equivariant with respect to translations
  - $$y(\mathcal{T}_v f) = y(f)$$

DEEP LEARNING ON EUCLIDEAN DOMAINS

- **Geometric priors**
  - 2. *Local deformations and scale separation*
    - Deformation operator

$$\mathcal{L}_\tau f(x) = f(\underline{x - \tau(x)})$$

local translations, changes in point of view, rotations

$$|y(\mathcal{L}_\tau f) - y(f)| \approx \underline{\|\nabla \tau\|}$$

smoothness of a given deformation field

    - The quantity to be predicted does not change much if the input image is slightly deformed

DEEP LEARNING ON EUCLIDEAN DOMAINS

- **Geometric priors**
  - 2. *Local deformations and scale separation*
    - Long-range dependencies can be broken into Multi-scale local interaction terms

$$Y(x_1, x_2; v) = \mathrm{Prob}(f(u) = x_1 \ \text{and} \ f(u+v) = x_2)$$

      - *a*. this joint distribution will not be separable for any v
      - *b*. $Y(x_1, x_2; v) \approx Y(x_1, x_2; v(1+\epsilon))$ for small ϵ

    - long-range dependencies can be captured and down-sampled at different scales

DEEP LEARNING ON EUCLIDEAN DOMAINS

- **Convolutional neural networks**
  - Convolutional layers $\mathbf{g} = C_{\Gamma}(\mathbf{f})$

nonlinearity

Convolutional filter

$$g_l(x) = \xi\left(\sum_{l'=1}^{p}(f_{l'} \star \gamma_{l,l'})(x)\right)$$

q-dimensional output

p-dimensional input

DEEP LEARNING ON EUCLIDEAN DOMAINS

- **Convolutional neural networks**
  - Pooling layers

a neighborhood around x

$$g_l(x) = P(\{f_l(x') : x' \in \mathcal{N}(x)\}), \ \ l = 1, \ldots, q,$$

permutation-invariant function such as a L_p-norm (in the latter case, the choice of $p = 1, 2$ or ∞ results in *average-*, *energy-*, or *max-pooling*).

DEEP LEARNING ON EUCLIDEAN DOMAINS

- **Convolutional neural networks**
  - Generic hierarchical representation

$$U_\Theta(f) = (C_{\Gamma(K)} \cdots P \cdots \circ C_{\Gamma(2)} \circ C_{\Gamma(1)})(f)$$

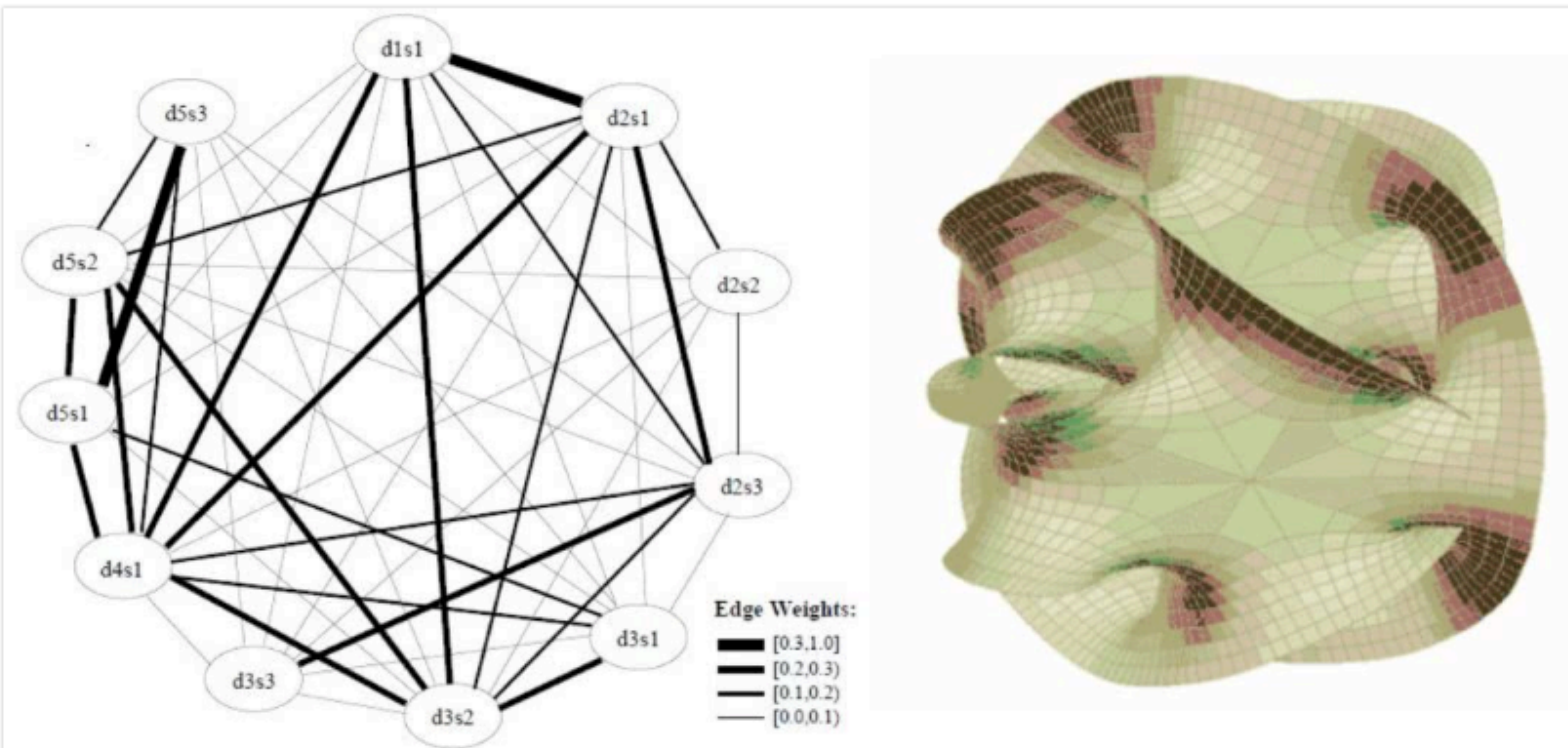
  - Supervised learning

$$\min_{\Theta} \sum_{i \in \mathcal{I}} L(U_\Theta(f_i), y_i),$$

  - A key advantage of CNNs explaining their success is that the **geometric priors** on which CNNs are based result in a learning complexity that avoids the curse of dimensionality.

THE GEOMETRY OF MANIFOLDS AND GRAPHS

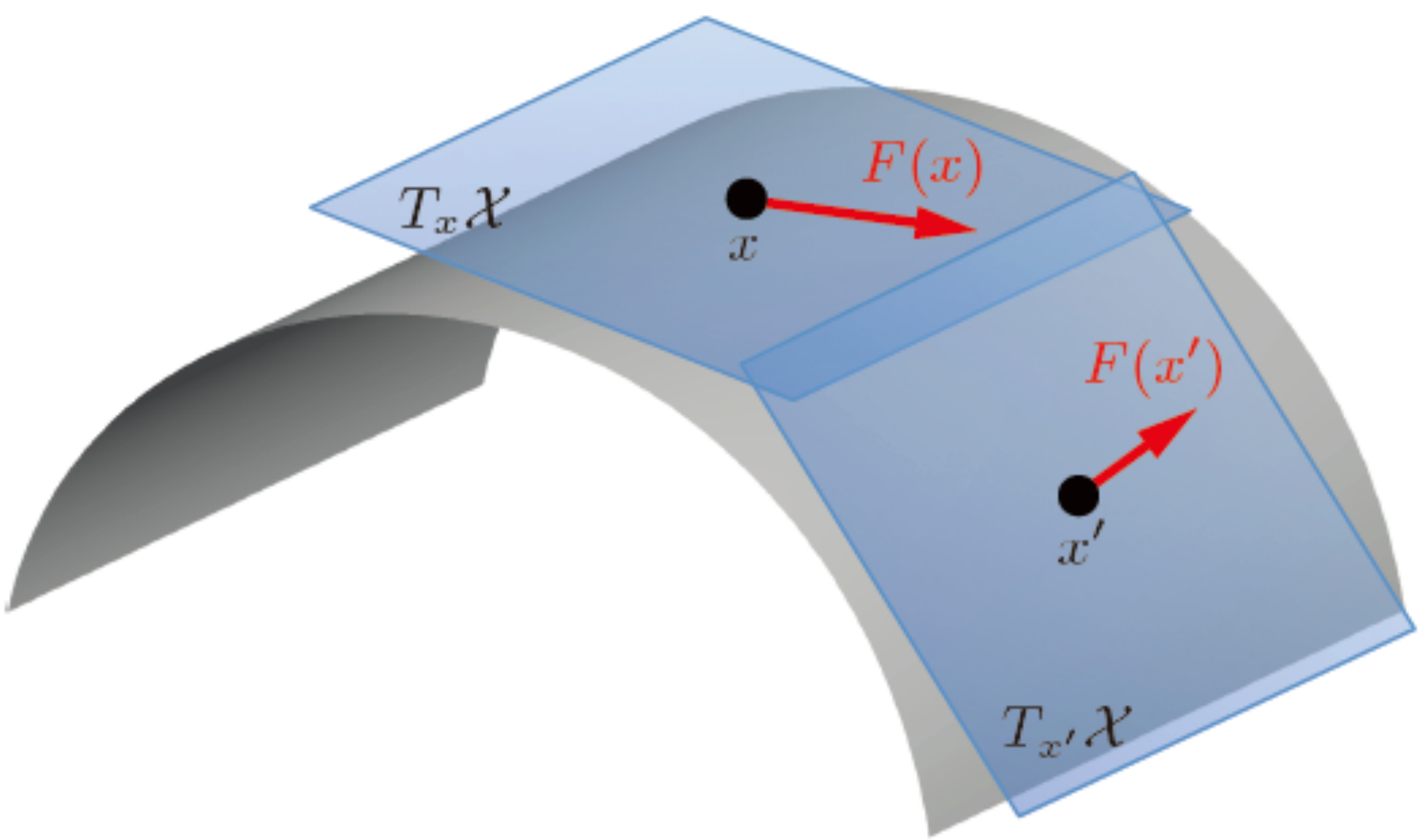
- Two prototypical structures**: manifolds and graphs**



THE GEOMETRY OF MANIFOLDS AND GRAPHS

- **Manifolds**
  - Roughly, a manifold is a space that is locally Euclidean.

Formally speaking, a (differentiable) *d-dimensional manifold* $\mathcal{X}$ is a topological space where each point x has a neighborhood that is topologically equivalent (homeomorphic) to a d-dimensional Euclidean space, called the *tangent space* and denoted by $T_x\mathcal{X}$ (see Figure 1, top).



On each tangent space, we define an inner product

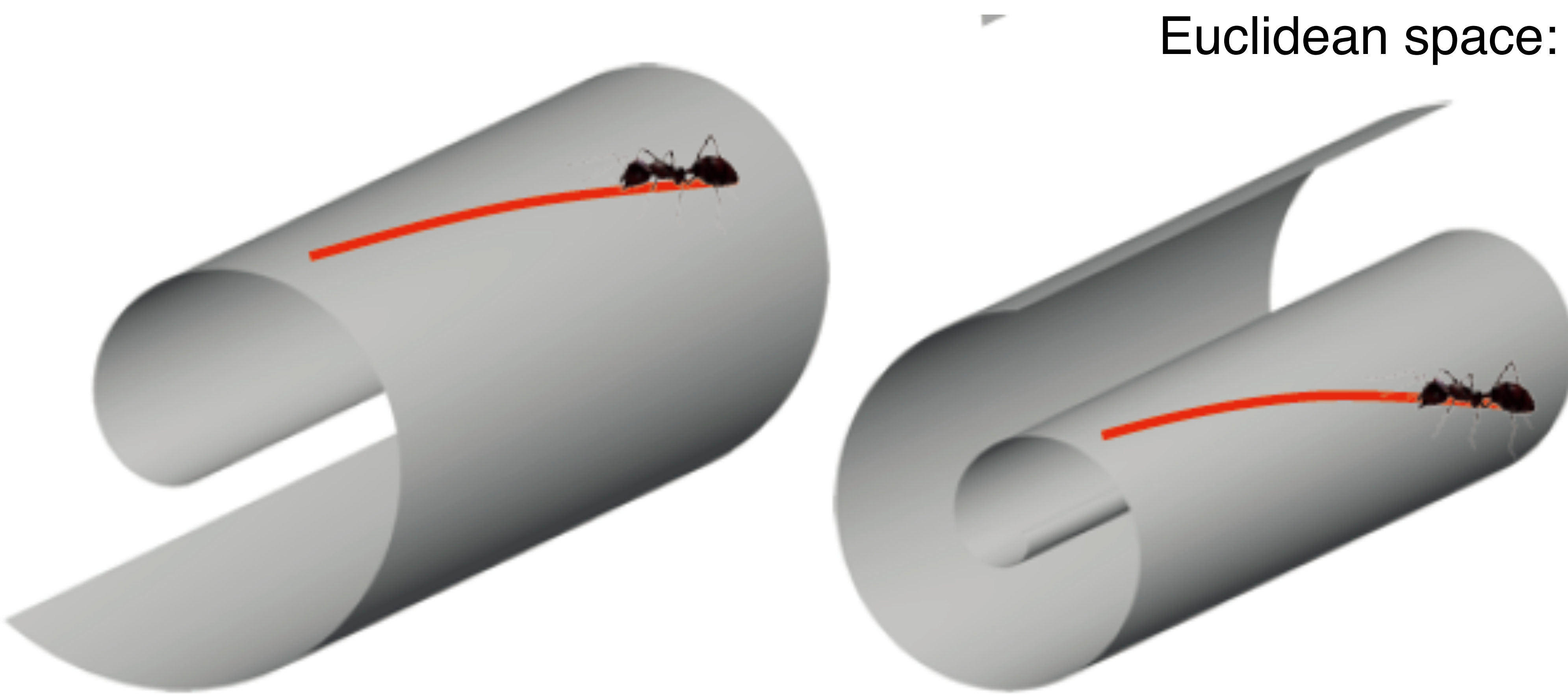
$$\langle \cdot, \cdot \rangle_{T_x\mathcal{X}} : T_x\mathcal{X} \times T_x\mathcal{X} \to \mathbb{R},$$

Riemannian metric in differential geometry

THE GEOMETRY OF MANIFOLDS AND GRAPHS

- **Manifolds**
  - A manifold equipped with a metric is called a **Riemannian manifold**
  - **Nash Embedding Theorem**: any sufficiently smooth Riemannian manifold can be realized in a Euclidean space of sufficiently high dimension

Riemannian metric: intrinsic
Euclidean space: extrinsic



THE GEOMETRY OF MANIFOLDS AND GRAPHS

- **Graphs and discrete differential operators**

weighted undirected graphs, formally defined as a pair $(\mathcal{V}, \mathcal{E})$, where $\mathcal{V} = \{1, \ldots, n\}$ is the set of n vertices, and $\mathcal{E} \subseteq \mathcal{V} \times \mathcal{V}$ is the set of edges, where the graph being undirected implies that $(i, j) \in \mathcal{E}$ iff $(j, i) \in \mathcal{E}$. Furthermore, we associate a weight $a_i > 0$ with each vertex $i \in \mathcal{V}$, and a weight $w_{ij} \geq 0$ with each edge $(i, j) \in \mathcal{E}$.

THE GEOMETRY OF MANIFOLDS AND GRAPHS

- **Graphs and discrete differential operators**

Real functions $f : \mathcal{V} \rightarrow \mathbb{R}$ and $F : \mathcal{E} \rightarrow \mathbb{R}$ on the vertices and edges of the graph, respectively, are roughly the discrete analogy of continuous scalar and tangent vector fields in differential geometry.[4] We can define Hilbert spaces $L^2(\mathcal{V})$ and $L^2(\mathcal{E})$ of such functions by specifying the respective inner products,

$$\langle f, g \rangle_{L^2(\mathcal{V})} = \sum_{i \in \mathcal{V}} a_i f_i g_i; \tag{20}$$

$$\langle F, G \rangle_{L^2(\mathcal{E})} = \sum_{i \in \mathcal{E}} w_{ij} F_{ij} G_{ij}. \tag{21}$$

THE GEOMETRY OF MANIFOLDS AND GRAPHS

- **Graphs and discrete differential operators**
  - Graph gradient: mapping functions defined on vertices to functions defined on edges

$$\nabla : L^2(\mathcal{V}) \to L^2(\mathcal{E})$$

$$(\nabla f)_{ij} \quad = \quad f_i - f_j$$

  - Graph divergence

$$L^2(\mathcal{E}) \to L^2(\mathcal{V})$$

$$(\mathrm{div} F)_i \quad = \quad \frac{1}{a_i} \sum_{j:(i,j)\in\mathcal{E}} w_{ij} F_{ij}$$

THE GEOMETRY OF MANIFOLDS AND GRAPHS

- **Graphs and discrete differential operators**
  - Graph Laplacian $\Delta = -\mathrm{div}\nabla.$

$$\Delta : L^2(\mathcal{V}) \to L^2(\mathcal{V})$$

$$(\Delta f)_i \quad = \quad \frac{1}{a_i} \sum_{(i,j)\in\mathcal{E}} w_{ij}(f_i - f_j).$$

  - **Intuitive geometric interpretation**: the difference between the local average of a function around a point and the value of the function at the point itself.

$$\mathbf{\Delta f} \quad = \quad \mathbf{A}^{-1}(\mathbf{D} - \mathbf{W})\mathbf{f}.$$

THE GEOMETRY OF MANIFOLDS AND GRAPHS

- **Fourier analysis on non-Euclidean domains**
  - The Laplacian operator is a self-adjoint positive-semidefinite operator

$$\Delta\phi_i = \lambda_i\phi_i, \quad i = 0, 1, \ldots$$

orthonormal eigenfunctions

eigenvalues

  - The eigenfunctions are the smoothest functions in the sense of the Dirichlet energy and can be interpreted as a generalization of the standard **Fourier basis** to a non-Euclidean domain.

[IN3] Physical interpretation of Laplacian eigenfunctions: Given a function f on the domain $\mathcal{X}$, the *Dirichlet energy*

$$\mathcal{E}_{\text{Dir}}(f) = \int_{\mathcal{X}} \|\nabla f(x)\|^2_{T_x\mathcal{X}} dx = \int_{\mathcal{X}} f(x)\Delta f(x)dx, \quad (27)$$

measures how smooth it is (the last identity in (27) stems from (19)). We are looking for an orthonormal basis on $\mathcal{X}$, containing k smoothest possible functions (FIGS3), by solving the optimization problem

$$\begin{aligned}
&\min_{\phi_0} \mathcal{E}_{\text{Dir}}(\phi_0) \quad \text{s.t.} \quad \|\phi_0\| = 1 && (28)\\
&\min_{\phi_i} \mathcal{E}_{\text{Dir}}(\phi_i) \quad \text{s.t.} \quad \|\phi_i\| = 1, \quad i = 1, 2, \dots k-1\\
&\qquad\qquad\qquad\qquad\quad\; \phi_i \perp \text{span}\{\phi_0, \dots, \phi_{i-1}\}.
\end{aligned}$$

In the discrete setting, when the domain is sampled at n points, problem (28) can be rewritten as

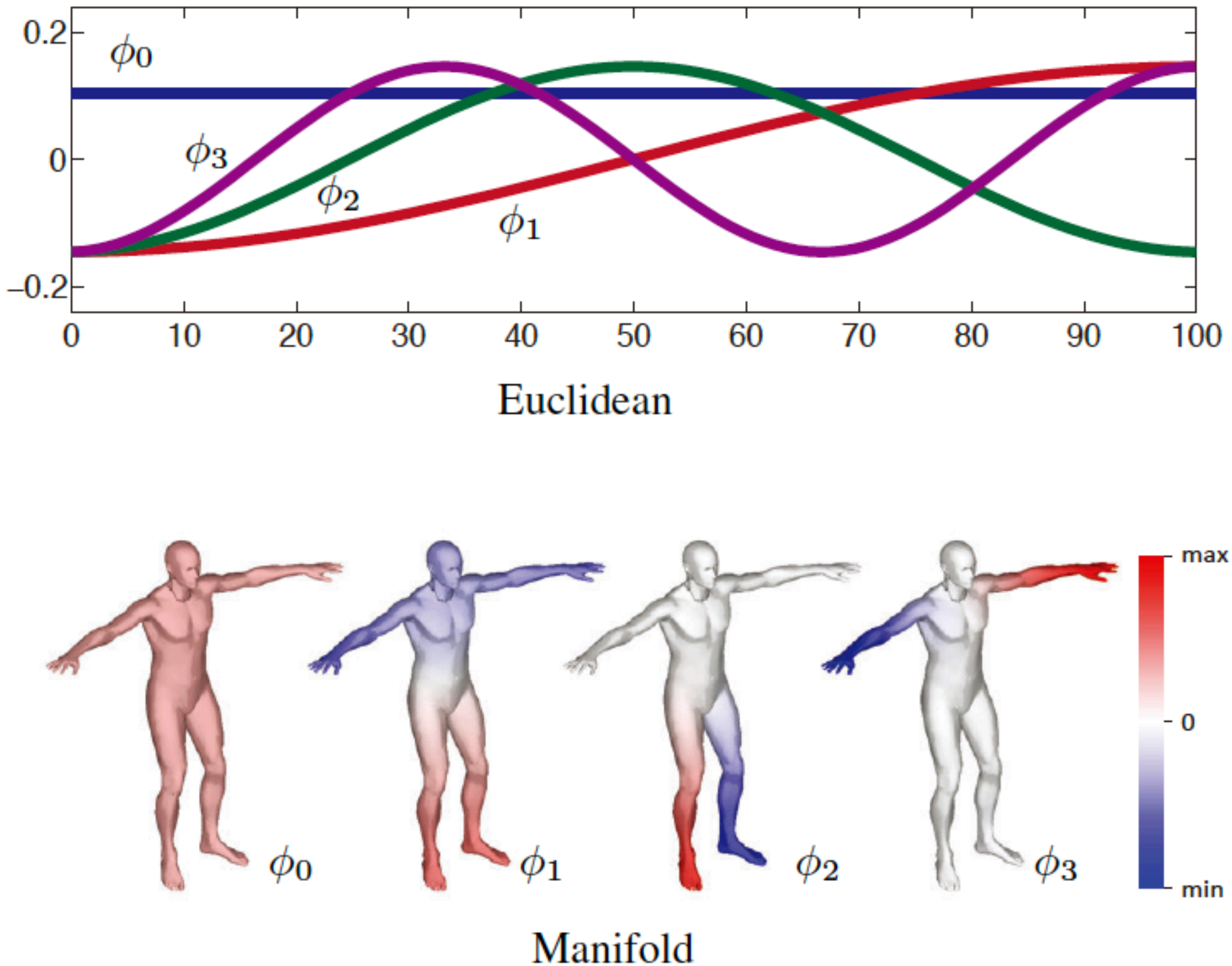
$$\min_{\mathbf{\Phi}_k \in \mathbb{R}^{n\times k}} \text{trace}(\mathbf{\Phi}_k^\top \mathbf{\Delta} \mathbf{\Phi}_k) \quad \text{s.t.} \quad \mathbf{\Phi}_k^\top \mathbf{\Phi}_k = \mathbf{I}, \quad (29)$$

where $\mathbf{\Phi}_k = (\phi_0, \dots \phi_{k-1})$. The solution of (29) is given by the first k eigenvectors of $\mathbf{\Delta}$ satisfying

$$\mathbf{\Delta}\mathbf{\Phi}_k = \mathbf{\Phi}_k \mathbf{\Lambda}_k, \tag{30}$$

where $\mathbf{\Lambda}_k = \mathrm{diag}(\lambda_0, \dots, \lambda_{k-1})$ is the diagonal matrix of corresponding eigenvalues. The eigenvalues $0 = \lambda_0 \leq \lambda_1 \leq \dots \lambda_{k-1}$ are non-negative due to the positive-semidefiniteness of the Laplacian and can be interpreted as 'frequencies', where $\phi_0 = \mathrm{const}$ with the corresponding eigenvalue $\lambda_0 = 0$ play the role of the DC.

The Laplacian eigendecomposition can be carried out in two ways. First, equation (30) can be rewritten as a generalized eigenproblem $(\mathbf{D} - \mathbf{W})\mathbf{\Phi}_k = \mathbf{A}\mathbf{\Phi}_k\mathbf{\Lambda}_k$, resulting in $\mathbf{A}$-orthogonal eigenvectors, $\mathbf{\Phi}_k^\top \mathbf{A}\mathbf{\Phi}_k = \mathbf{I}$. Alternatively, introducing a change of variables $\mathbf{\Psi}_k = \mathbf{A}^{1/2}\mathbf{\Phi}_k$, we can obtain a standard eigendecomposition problem $\mathbf{A}^{-1/2}(\mathbf{D} - \mathbf{W})\mathbf{A}^{-1/2}\mathbf{\Psi}_k = \mathbf{\Psi}_k\mathbf{\Lambda}_k$ with orthogonal eigenvectors $\mathbf{\Psi}_k^\top\mathbf{\Psi}_k = \mathbf{I}$. When $\mathbf{A} = \mathbf{D}$ is used, the matrix $\mathbf{\Delta} = \mathbf{A}^{-1/2}(\mathbf{D} - \mathbf{W})\mathbf{A}^{-1/2}$ is referred to as the *normalized symmetric Laplacian.*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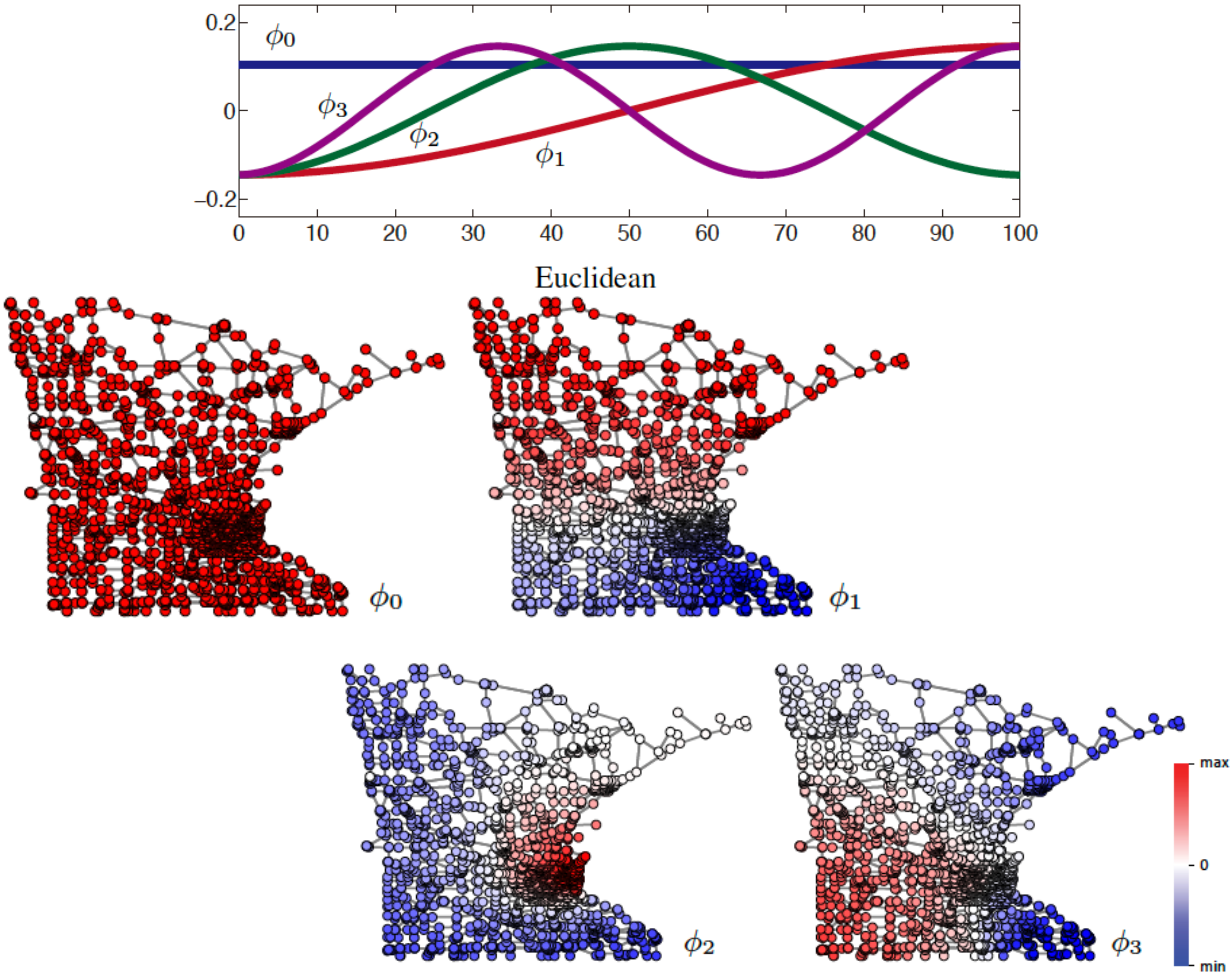

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THE GEOMETRY OF MANIFOLDS AND GRAPHS

A square-integrable function f on $\mathcal{X}$ can be decomposed into *Fourier series* as

$$f(x) \;=\; \sum_{i \geq 0} \underbrace{\langle f, \phi_i \rangle_{L^2(\mathcal{X})}}_{\hat{f}_i} \phi_i(x), \tag{32}$$

analysis stage

synthesis stage

SPECTRAL METHODS

- **Spectral CNN (SCNN)**

$$\mathbf{g}_l = \xi \left(\sum_{l'=1}^{q} \mathbf{\Phi}_k \mathbf{\Gamma}_{l,l'} \mathbf{\Phi}_k^\top \mathbf{f}_{l'} \right)$$

$\mathbf{\Gamma}_{l,l'}$ is a $k \times k$ diagonal matrix of spectral multipliers

- Using only the first *k* eigenvectors in sets a cutoff frequency which depends on the intrinsic regularity of the graph and also the sample size.

SPECTRAL METHODS

- **Spectral CNN (SCNN)**
  - A fundamental limitation of the spectral construction is its limitation to a single domain
    - Basis dependent

Domain	$\mathcal{X}$	$\mathcal{X}$	$\mathcal{Y}$
Basis	$\mathbf{\Phi}$	$\mathbf{\Phi}$	$\mathbf{\Psi}$
Signal	$\mathbf{f}$	$\mathbf{\Phi W \Phi}^\top \mathbf{f}$	$\mathbf{\Psi W \Psi}^\top \mathbf{f}$

SPECTRAL METHODS

- **Spectral CNN (SCNN)**
  - A fundamental limitation of the spectral construction is its limitation to a single domain
    - Basis dependent
    - It is possible to construct compatible orthogonal bases **across different domains** resorting to a joint diagonalization procedure
      - Social graph
      - Computer graphics
  - Another limitation: too many parameters

$$pqk = O(n)$$

    - On Euclidean domains, this is achieved by learning convolutional kernels with small spatial support, which enables the model to learn a number of parameters independent of the input size.