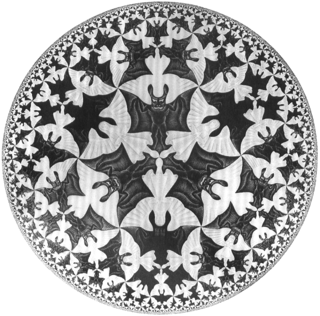
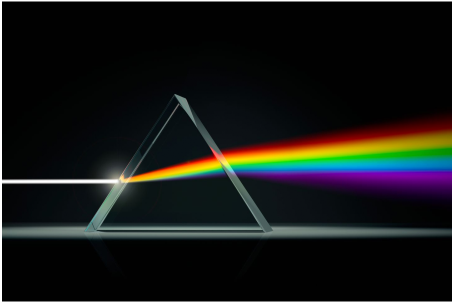
Manifold Learning and Spectral Methods



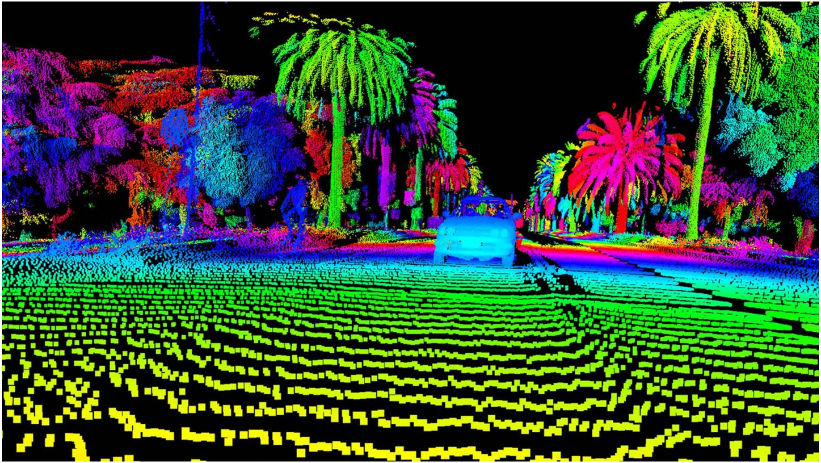


David Pfau

DeepMind

Buenos Aires MLSS, 28 June 2018

What this tutorial is about



Designing models for graph- or manifold-structured input

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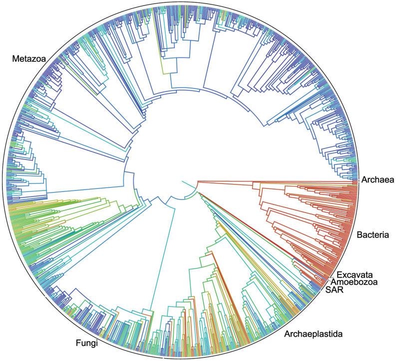
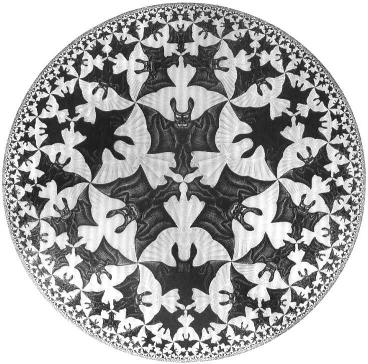
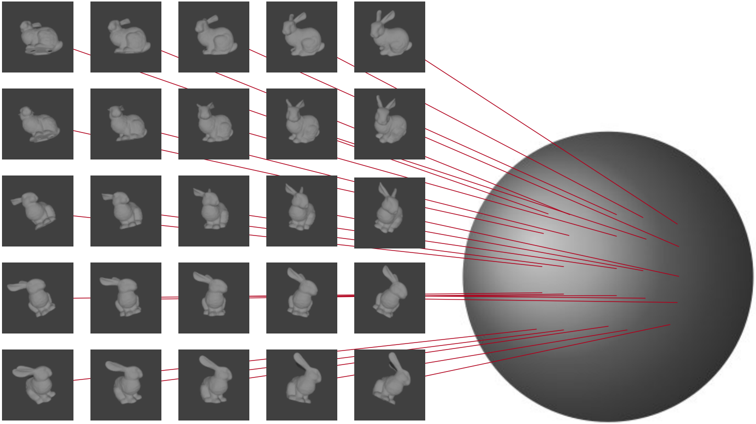




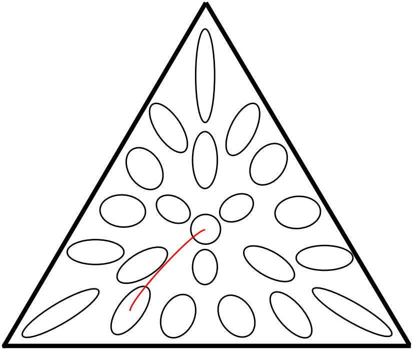
Designing models for data with latent graph- or manifold-structure

What this tutorial is about



Discovering latent manifold structure in data

What this tutorial is *not* about



$$\mathcal{F}(\theta) = \mathbb{E}_x \left[\nabla_\theta \mathrm{log} p(x|\theta) \nabla_\theta \mathrm{log} p(x|\theta)^T \right]$$

$$\theta_{t+1} \leftarrow \theta_t + \mathcal{F}^{-1} \nabla_\theta \mathrm{log} p(x_t|\theta_t)$$

Information geometry - the manifold structure of parameter space

Spectral Learning

Any learning algorithm where the usual tools (SGD, EM, MCMC...) are replaced with eigendecomposition or SVD

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Solves a nonconvex optimization exactly!

$$\mathbf{A} = \mathbf{\Phi}\mathbf{\Lambda}\mathbf{\Phi}^T$$

$$\min_{\substack{\mathbf{\Phi} \\ \mathbf{\Phi}^T\mathbf{\Phi}=\mathbf{I}}} \mathrm{Tr}(\mathbf{\Phi}^T\mathbf{A}\mathbf{\Phi})$$

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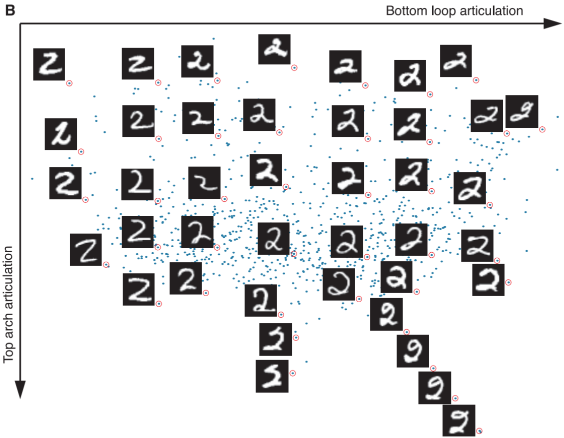
Functions on $\mathbb{R}^n$ can be decomposed with Fourier basis. Spectral analysis **generalizes Fourier analysis to manifolds and graphs**

What is this good for?



Tenenbaum, De Silva and Langford 2000

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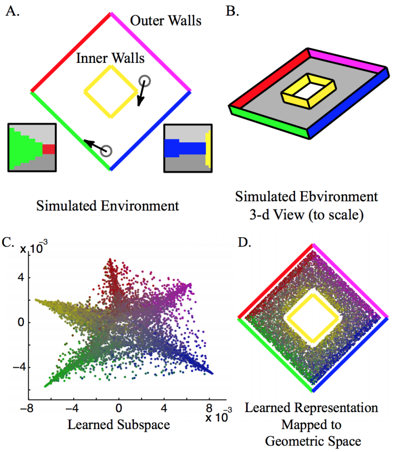

Boots, Siddiqi and Gordon 2011

Outline

Theory

Graphs

Manifolds and Differential Geometry

Spectral Theory

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The Geometry of Data

Classic Manifold Learning

Embedding Hierarchies in Hyperbolic Space

Analyzing the Geometry of Deep Generative Models

Outline

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- Graphs
- Manifolds and Differential Geometry
- Spectral Theory

The Geometry of Data

- Classic Manifold Learning
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- Analyzing the Geometry of Deep Generative Models

Spectral Deep Learning

- Convolutions on Graphs and Manifolds
- Spectral Graph Convolutional Neural Networks
- Inference in Spectral Learning with Deep Networks

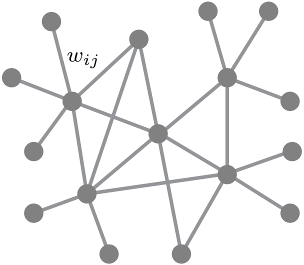
Part I

Theory

Graph Theory (in three slides)

Graphs

Weighted undirected graph $\mathcal{G}$ with vertices $\mathcal{V} = \{1, \ldots, n\}$, edges $\mathcal{E} \subseteq \mathcal{V} \times \mathcal{V}$ and edge weights $w_{ij} \geq 0$ for $(i, j) \in \mathcal{E}$



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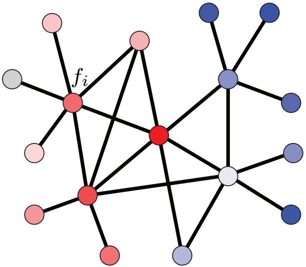
Functions over the vertices
$L^2(\mathcal{V}) = \{f : \mathcal{V} \to \mathbb{R}\}$



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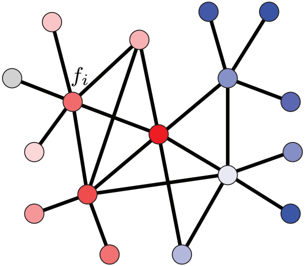

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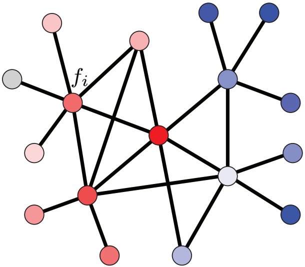

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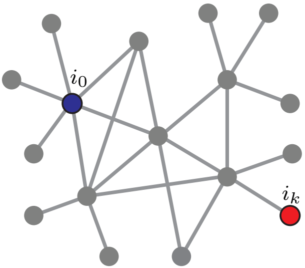
Inner product

$$\langle f, g \rangle_{L^2(\mathcal{V})} = \sum_{i \in \mathcal{V}} f_i \, g_i = \mathbf{f}^\top \mathbf{g}$$

Shortest paths on graphs

Dijkstra's Algorithm: Find sequence $i_0, \ldots, i_k \in \mathcal{V}$ from source i_0 to sink i_k that minimizes $\sum_t w_{i_t i_{t+1}}$



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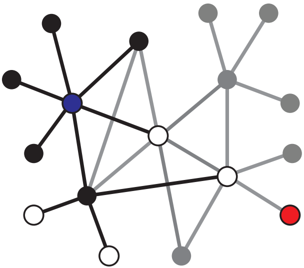
Create queue of active nodes and shortest-path tree, starting from source



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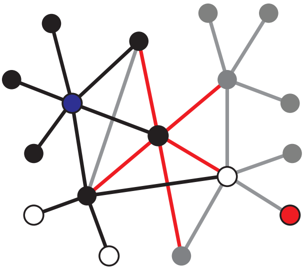

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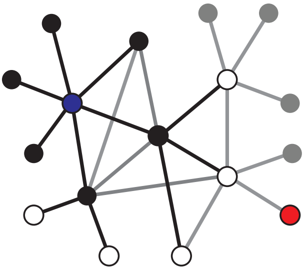

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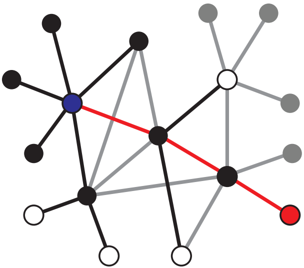

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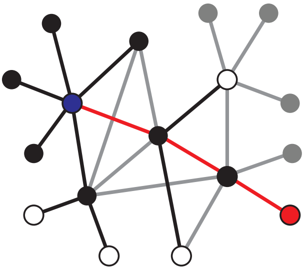

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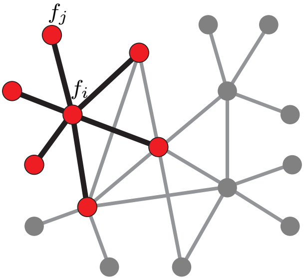
Complexity: $\mathcal{O}(|\mathcal{E}| + |\mathcal{V}| \log |\mathcal{V}|)$

Graph Laplacian

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

$$(\Delta f)_i = \sum_{j:(i,j)\in\mathcal{E}} w_{ij}(f_i - f_j)$$



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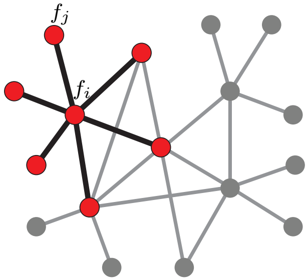
$$
\begin{aligned}
(\Delta f)_i &= \sum_{j:(i,j)\in\mathcal{E}} w_{ij}(f_i - f_j) \\
&= f_i \sum_{j:(i,j)\in\mathcal{E}} w_{ij} - \sum_{j:(i,j)\in\mathcal{E}} w_{ij} f_j
\end{aligned}
$$

(up to scale) difference between f and its local average



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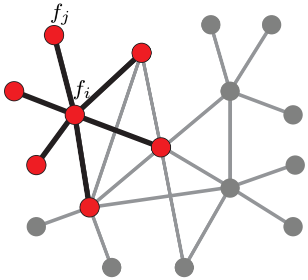
(up to scale) difference between f and its local average

Represented as a positive semi-definite $n \times n$ matrix $\mathbf{\Delta} = \mathbf{D} - \mathbf{W}$ where $\mathbf{W} = (w_{ij})$ and $\mathbf{D} = \mathrm{diag}(\sum_{j\neq i} w_{ij})$



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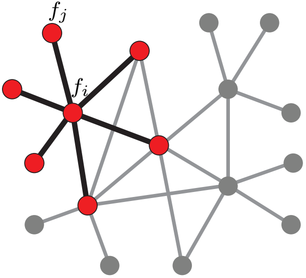


Dirichlet energy of f

$$\|f\|^2_{\mathcal{G}} = \frac{1}{2}\sum_{ij=1}^{n} w_{ij}(f_i - f_j)^2 = \mathbf{f}^\top \mathbf{\Delta} \mathbf{f}$$

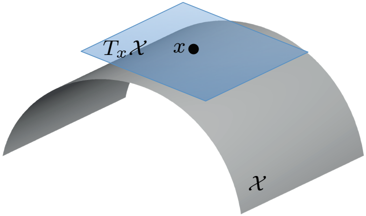
measures the smoothness of f (how fast it changes locally)

Manifolds and Differential Geometry

Riemannian manifolds

Manifold $\mathcal{X}$ = locally flat space (no non-differentiable corners)

Tangent plane $T_x\mathcal{X}$ = local Euclidean representation of manifold $\mathcal{X}$ around x



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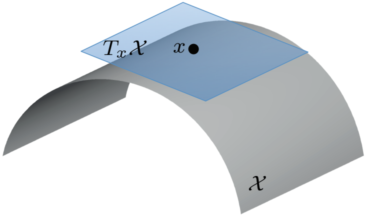
Riemannian metric describes the local intrinsic structure at x

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



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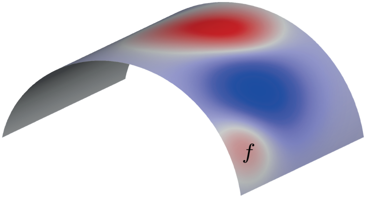

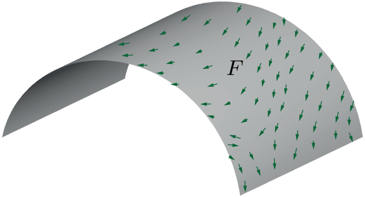

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Inner products

$$\langle f, g \rangle_{L^2(\mathcal{X})} = \int_{\mathcal{X}} f(x) g(x) dx$$

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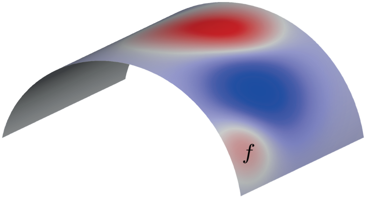
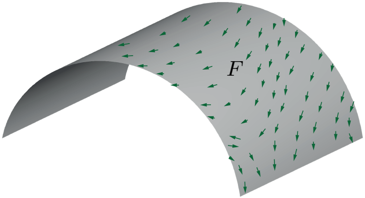
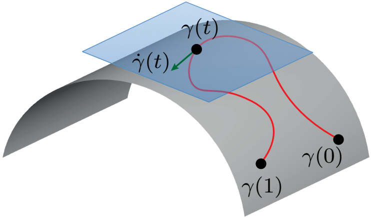




Shortest paths on manifolds

Curve $\gamma(\cdot) : [0, 1] \to \mathcal{X}$ = smooth path along manifold



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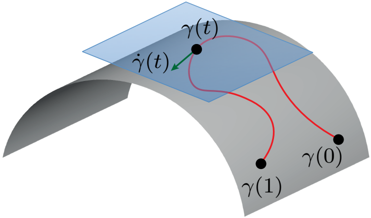

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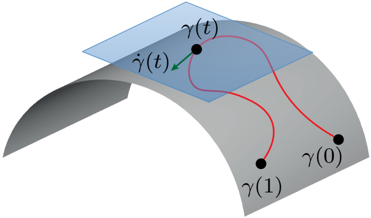

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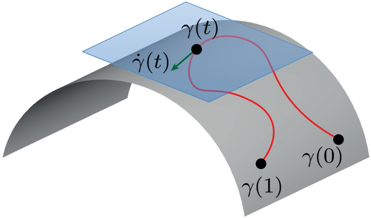

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Geodesic shortest curve between points

$$\gamma^* = \min_{\substack{\gamma \\ \gamma(0)=x_0 \\ \gamma(1)=x_1}} \mathcal{S}[\gamma]$$

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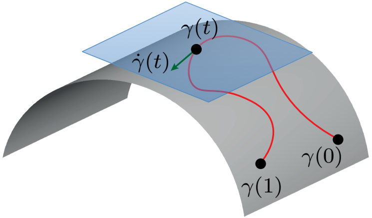
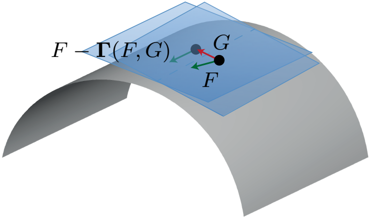


Geodesic is a path such that the velocities are locally parallel

Parallel Transport

Connection $\mathbf{\Gamma}_x(F, G)$: infinitesimal change to vector $F \in T_x\mathcal{X}$ that keeps it locally parallel when moved in the direction $G \in T_x\mathcal{X}$.



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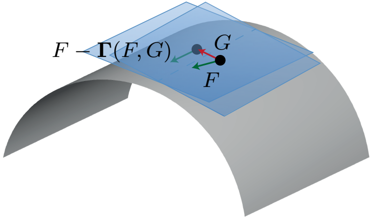
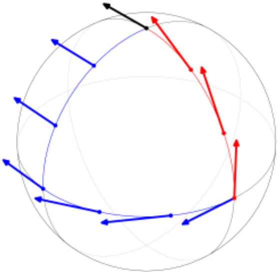
Parallel transport Sequence of vectors $F(t) \in T_{\gamma(t)}\mathcal{X}$ along curve γ that are all locally parallel.





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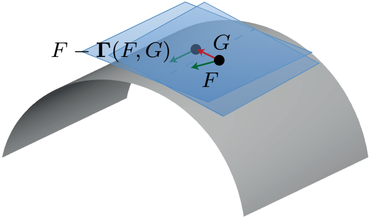

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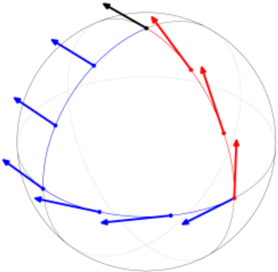
$$\dot{F}(t) + \mathbf{\Gamma}_{\gamma(t)}(F(t), \dot{\gamma}(t)) = 0$$



Geodesic equation

Parallel transport:

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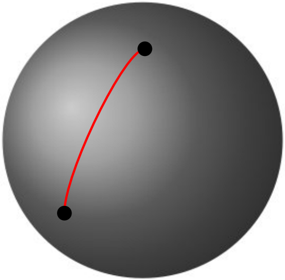
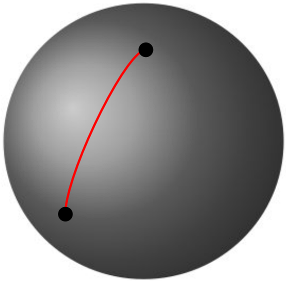


Geodesic equation



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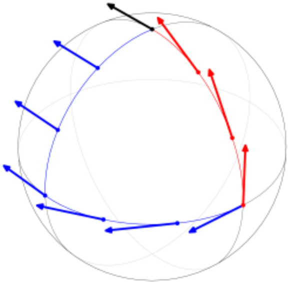

A geodesic is a curve such that if you parallel transport its velocity at a point along itself, the vector always remains tangent to the curve

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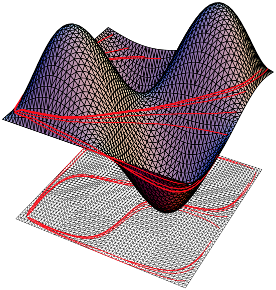

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Solve numerically on meshes with fast marching method

Kimmel and Sethian 1998

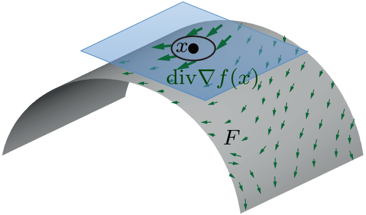
Manifold Laplacian

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

$$\Delta f(x) = -\mathrm{div}\,\nabla f(x)$$

where gradient $\nabla : L^2(\mathcal{X}) \to L^2(T\mathcal{X})$
and divergence $\mathrm{div} : L^2(T\mathcal{X}) \to L^2(\mathcal{X})$
are adjoint operators

$$\langle F, \nabla f \rangle_{L^2(T\mathcal{X})} = \langle -\mathrm{div} F, f \rangle_{L^2(\mathcal{X})}$$



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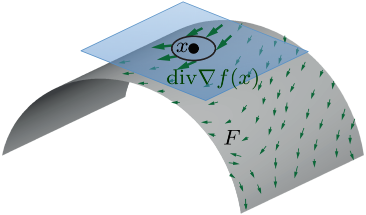

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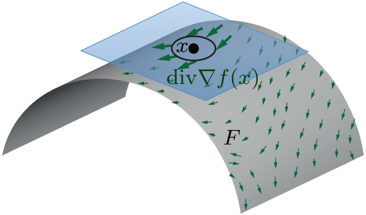

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Continuous limit of graph Laplacian
under some conditions

Dirichlet energy of f

$$\langle \nabla f, \nabla f \rangle_{L^2(T\mathcal{X})} = \int_{\mathcal{X}} f(x) \Delta f(x) dx$$

measures the smoothness of f (how fast it changes locally)

Spectral Theory for Graphs and Manifolds

Orthogonal bases on graphs

Find the smoothest orthogonal basis $\{\phi_1, \ldots, \phi_n\} \subseteq L^2(\mathcal{V})$

$$
\begin{aligned}
&\min_{\phi_1} \; E_{\mathrm{Dir}}(\psi_1) \quad \text{s.t.} \quad \|\phi_1\| = 1 \\
&\min_{\phi_k} \; E_{\mathrm{Dir}}(\psi_k) \quad \text{s.t.} \quad \|\phi_k\| = 1, \quad k = 2, 3, \ldots n \\
&\qquad\qquad\qquad\qquad\qquad\;\; \phi_k \perp \mathrm{span}\{\phi_1, \ldots, \phi_{k-1}\}
\end{aligned}
$$

Orthogonal bases on graphs

Find the smoothest orthogonal basis $\{\phi_1, \ldots, \phi_n\} \subseteq L^2(\mathcal{V})$

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

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Solution: $\mathbf{\Phi} =$ Laplacian eigenvectors

Laplacian eigenvectors and eigenvalues

Eigendecomposition of a graph Laplacian

$$\mathbf{\Delta} = \mathbf{\Phi}\mathbf{\Lambda}\mathbf{\Phi}^\top$$

where $\mathbf{\Phi} = (\boldsymbol{\phi}_1, \ldots, \boldsymbol{\phi}_n)$ are orthogonal eigenvectors $(\mathbf{\Phi}^\top\mathbf{\Phi} = \mathbf{I})$ and $\mathbf{\Lambda} = \mathrm{diag}(\lambda_1, \ldots, \lambda_n)$ the corresponding non-negative eigenvalues

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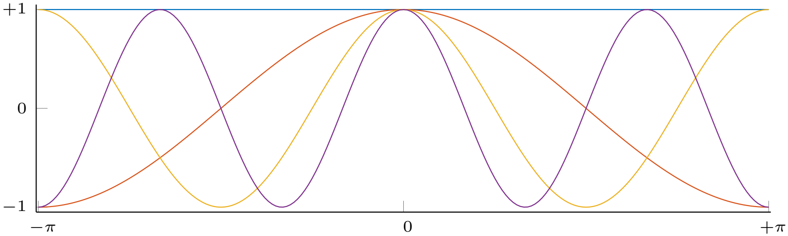

First eigenfunctions of 1D Euclidean Laplacian

Laplacian eigenvectors and eigenvalues

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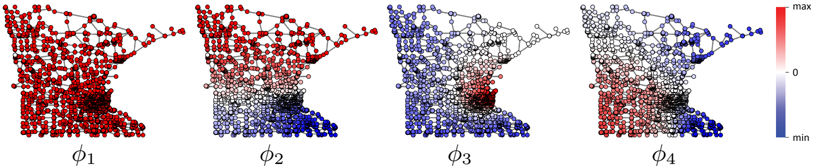

First eigenfunctions of a graph Laplacian

Laplacian eigenvectors and eigenvalues

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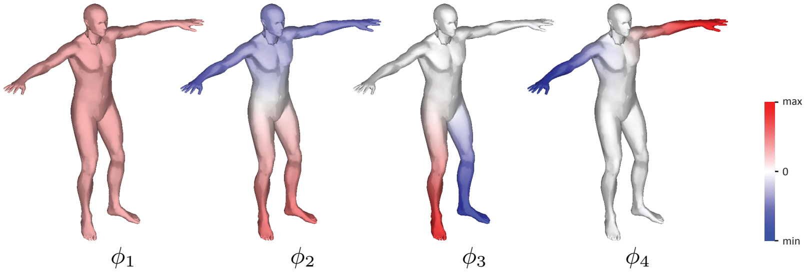

First eigenfunctions of a manifold Laplacian

Fourier analysis on Euclidean spaces

A function $f : [-\pi, \pi] \to \mathbb{R}$ can be written as a Fourier series

$$f(x) = \sum_{k \geq 0} \frac{1}{2\pi} \int_{-\pi}^{\pi} f(x') e^{-ikx'} dx' e^{ikx}$$

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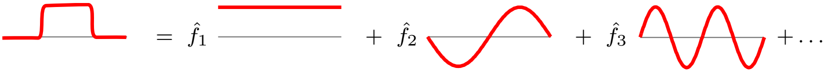

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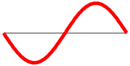
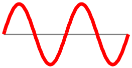
$$f(x) = \sum_{k \geq 0} \underbrace{\langle f, e^{ikx} \rangle_{L^2([-\pi,\pi])}}_{\hat{f}_k \text{ Fourier coefficient}} e^{ikx}$$

 $= \hat{f}_1$  $+ \; \hat{f}_2$  $+ \; \hat{f}_3$  $+ \ldots$

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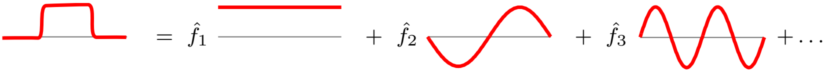

Fourier basis = Laplacian eigenfunctions: $-\frac{d^2}{dx^2} e^{ikx} = k^2 e^{ikx}$

Fourier analysis on graphs and manifolds

A function $f : \mathcal{V} \to \mathbb{R}$ can be written as Fourier series

$$f = \sum_{k=1}^{n} \underbrace{\langle f, \phi_k \rangle_{L^2(\mathcal{V})}}_{\hat{f}_k} \phi_k$$

Fourier basis = Laplacian eigenfunctions: $\Delta \phi_k = \lambda_k \phi_k$

Fourier analysis on graphs and manifolds

A function $f : \mathcal{V} \to \mathbb{R}$ can be written as Fourier series

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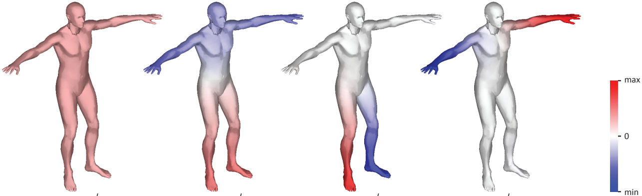
Fourier basis = Laplacian eigenfunctions: $\Delta \phi_k = \lambda_k \phi_k$

λ_k = frequency



ϕ_1 ϕ_2 ϕ_3 ϕ_4

First Fourier basis elements of a manifold.

Summary

Manifolds and graphs are natural extensions of vector spaces

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Lines can be generalized to shortest paths and geodesics

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Lines can be generalized to shortest paths and geodesics

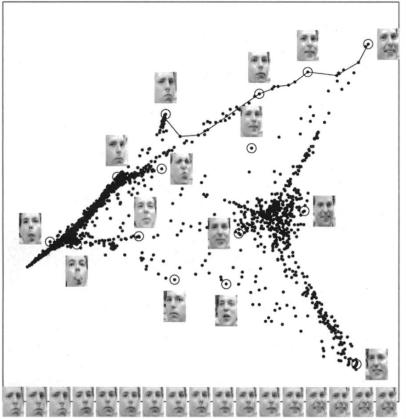
The Laplacian operator defines smoothness of a function

Spectral decompositions generalize Fourier analysis

The Geometry of Data

Classic Manifold Learning: A Time Before Deep Learning

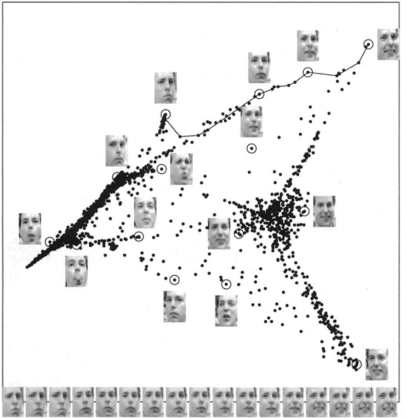
Manifold Learning



Learn nonlinear embedding of data into low dimensional space that preserves distances locally

Roweis and Saul 2000

Manifold Learning

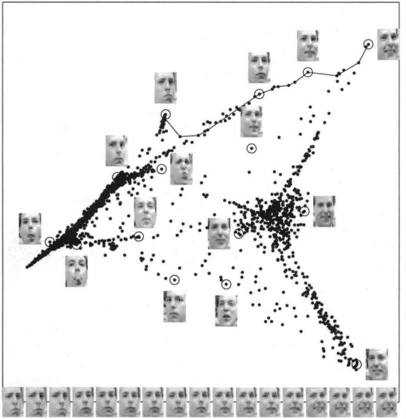


Learn nonlinear embedding of data into low dimensional space that preserves distances locally

The data itself does not have to be manifold structured

Roweis and Saul 2000

Manifold Learning



Learn nonlinear embedding of data into low dimensional space that preserves distances locally

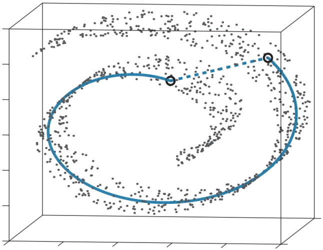
The data itself does not have to be manifold structured

The dataset has some latent manifold structure

Roweis and Saul 2000

IsoMap

Compute nearest neighbors graph of dataset



Tenenbaum, de Silva and Langford 2000

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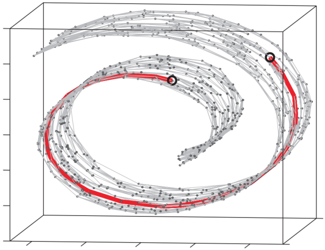
Compute nearest neighbors graph of dataset

Construct matrix $\mathbf{D} \in \mathbb{R}^{n \times n}$ of geodesic distances between pairs of data by Dijkstra's algorithm



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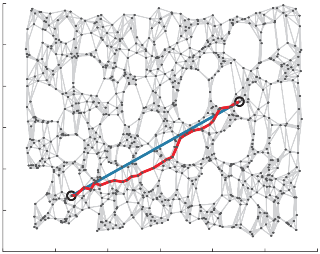
Embed data in low dimensional space with multidimensional scaling (MDS):



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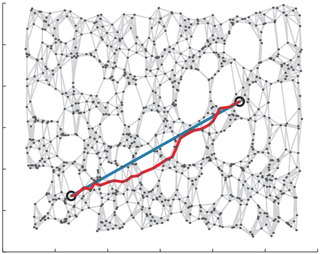

$$\mathbf{B} = -\frac{1}{2}\left(\mathbf{I} - \frac{1}{n}\mathbf{1}\mathbf{1}^T\right)\mathbf{D}\left(\mathbf{I} - \frac{1}{n}\mathbf{1}\mathbf{1}^T\right)$$

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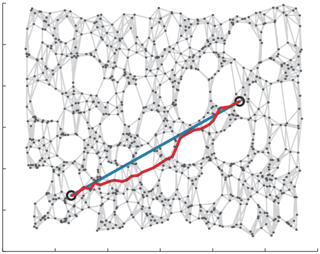

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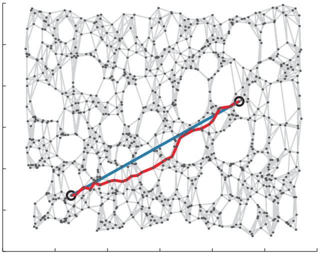
Embedding: $\left(\sqrt{\lambda_1}\phi_1, \ldots, \sqrt{\lambda_k}\phi_k\right)$



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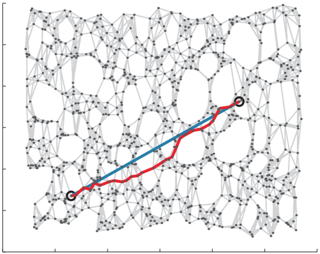

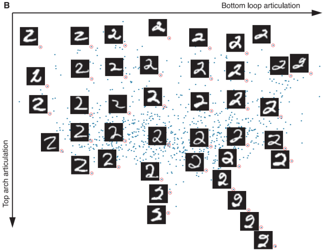

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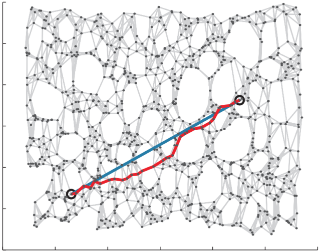
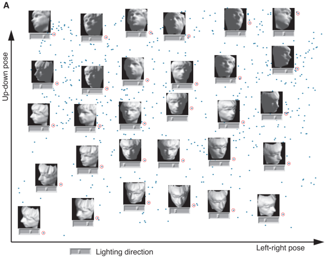
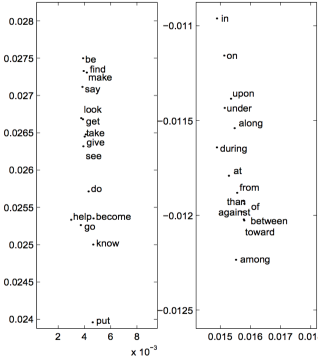




Tenenbaum, de Silva and Langford 2000

Laplacian eigenmaps

Compute weighted nearest neighbors graph of dataset



Belkin and Niyogi 2002

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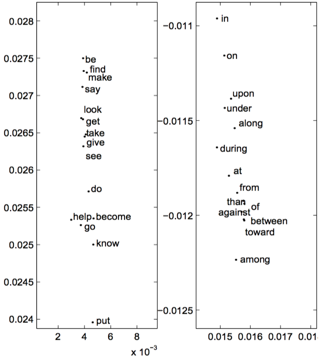
Compute weighted nearest neighbors graph of dataset

Construct graph Laplacian matrix $\mathbf{\Delta} = \mathbf{D} - \mathbf{W}$



Belkin and Niyogi 2002

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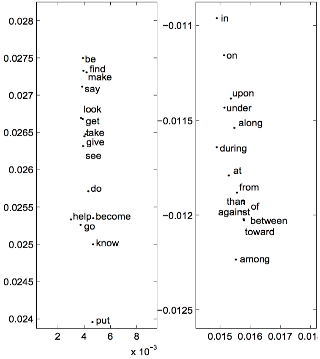

Belkin and Niyogi 2002

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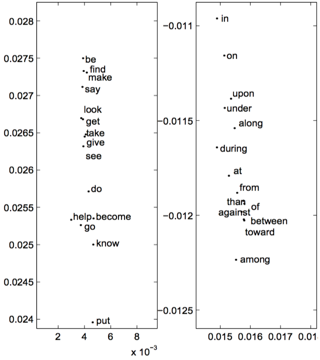
Embedding: $(\phi_2, \ldots, \phi_k)$



Belkin and Niyogi 2002

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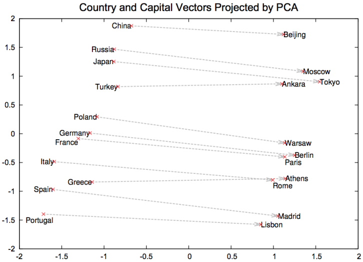
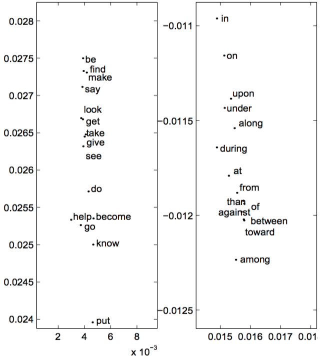
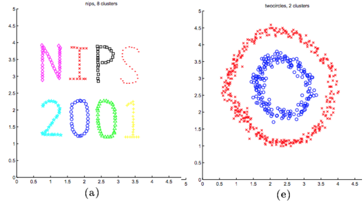


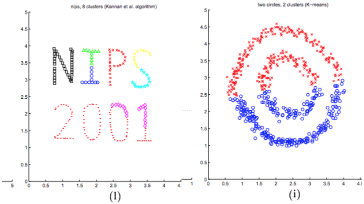


Spectral clustering

Same embedding as Laplacian eigenmaps, but use embedding vectors for clustering instead of visualization



Spectral Clustering



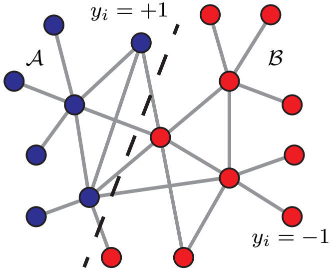
Other

Ng, Jordan and Weiss 2002

Normalized cuts

Minimum (normalized) cut problem:
partition vertices into sets $\mathcal{A}, \mathcal{B} \subset \mathcal{V}$

$$\mathrm{NCut}(\mathbf{y}) = \frac{\sum_{i \in \mathcal{A}, j \in \mathcal{B}} w_{ij}}{\sum_{i \in \mathcal{A}, j \in \mathcal{V}} w_{ij}} + \frac{\sum_{i \in \mathcal{B}, j \in \mathcal{A}} w_{ij}}{\sum_{i \in \mathcal{B}, j \in \mathcal{V}} w_{ij}}$$



Shi and Malik 2000

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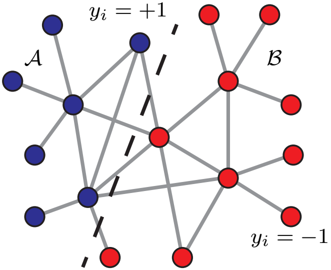

$$\begin{aligned} \mathrm{NCut}(\mathbf{y}) &= \frac{\sum_{i \in \mathcal{A}, j \in \mathcal{B}} w_{ij}}{\sum_{i \in \mathcal{A}, j \in \mathcal{V}} w_{ij}} + \frac{\sum_{i \in \mathcal{B}, j \in \mathcal{A}} w_{ij}}{\sum_{i \in \mathcal{B}, j \in \mathcal{V}} w_{ij}} \\ &= \frac{\mathbf{y}^T(\mathbf{D} - \mathbf{W})\mathbf{y}}{\mathbf{y}^T\mathbf{y}} \end{aligned}$$

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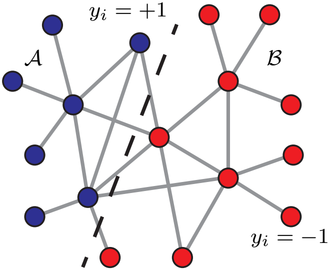

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Shi and Malik 2000

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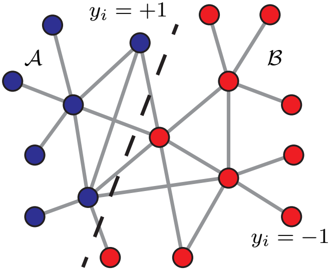

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Relax optimization from binary vectors to continuous vectors. Solution is bottom eigenfunctions of graph Laplacian.

Shi and Malik 2000

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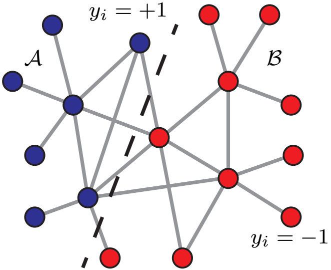

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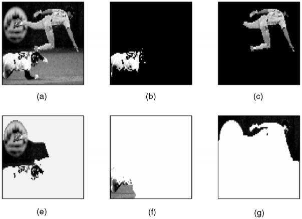

Used in image segmentation where each vertex is a pixel

Shi and Malik 2000

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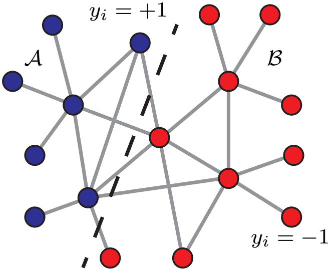
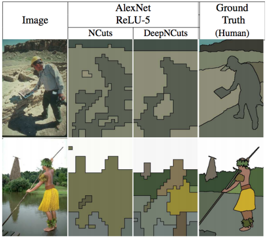


Relax optimization from binary vectors to continuous vectors. Solution is bottom eigenfunctions of graph Laplacian.

Can be incorporated as layer inside a deep network by backpropagating through eigendecomposition



Shi and Malik 2000; Ionescu, Vantzos and Sminchisescu 2015

Inference on held-out data

A common pattern:

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Construct Gram matrix from kernel $k(\mathbf{x}, \mathbf{x}')$

$$\mathbf{M} = \begin{bmatrix} k(\mathbf{x}_1, \mathbf{x}_1) & k(\mathbf{x}_1, \mathbf{x}_2) & \dots & k(\mathbf{x}_1, \mathbf{x}_n) \\ k(\mathbf{x}_2, \mathbf{x}_1) & k(\mathbf{x}_2, \mathbf{x}_2) & \dots & k(\mathbf{x}_2, \mathbf{x}_n) \\ \vdots & \vdots & \ddots & \vdots \\ k(\mathbf{x}_n, \mathbf{x}_1) & k(\mathbf{x}_n, \mathbf{x}_2) & \dots & k(\mathbf{x}_n, \mathbf{x}_n) \end{bmatrix}$$

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Use top/bottom eigenvectors of Gram matrix as embedding

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Use top/bottom eigenvectors of Gram matrix as embedding

Works for fixed dataset $\mathbf{x}_1, \dots, \mathbf{x}_n$ -
but what is the embedding vector for a new data point $\mathbf{x}'$?

Inference on held-out data

Assume data drawn $\mathbf{x}_1, \ldots, \mathbf{x}_n \sim p(\mathbf{x})$. Gram matrix is approximation to linear operator:

$$\frac{1}{n}\mathbf{M}\begin{pmatrix} f(\mathbf{x}_1) \\ f(\mathbf{x}_2) \\ \vdots \\ f(\mathbf{x}_n) \end{pmatrix}_i = \frac{1}{n}\sum_j k(\mathbf{x}_i, \mathbf{x}_j) f(\mathbf{x}_j) \approx \mathbb{E}_{p(\mathbf{x})}[k(\mathbf{x}_i, \mathbf{x}) f(\mathbf{x})]$$

$$= \mathcal{K}_p[f](\mathbf{x}_i)$$

Bengio, Paiement, Vincent et al 2004

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Eigenvectors ϕ_k of $\mathbf{M}$ are approximation to eigenfunctions $\phi_k(\cdot)$ of linear operator $\mathcal{K}_p$

Bengio, Paiement, Vincent et al 2004

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$$= \quad \mathcal{K}_p[f](\mathbf{x}_i)$$

From eigenvalues $\lambda_1, \ldots, \lambda_k$ and eigenvectors $\phi_1, \ldots, \phi_k$ of $\mathbf{M}$, can approximate eigenfunction of $\mathcal{K}_p$ with Nyström method:

$$\phi_k(\mathbf{x}') \propto \sum_i \phi_{ki} k(\mathbf{x}_i, \mathbf{x}')$$

Bengio, Paiement, Vincent et al 2004

Trade-offs of manifold learning

☺ Exactly solvable by eigendecomposition

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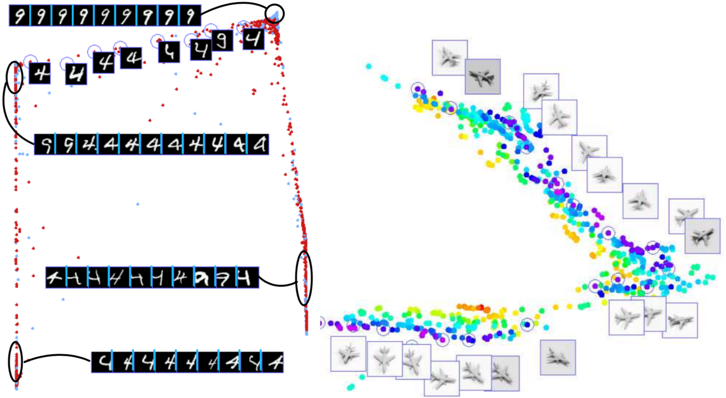
Other methods have become popular for low-dimensional visualization - especially t-SNE (Maaten and Hinton 2008)

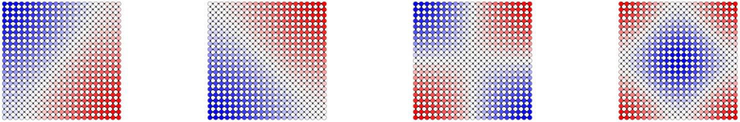
Collapsed embeddings



Hadsell, Chopra and LeCun 2006

Improving spectral embeddings

Bottom eigenfunctions of graph Laplacian of evenly-scaled grid are natural coordinates



Pfau and Burgess 2018

Improving spectral embeddings

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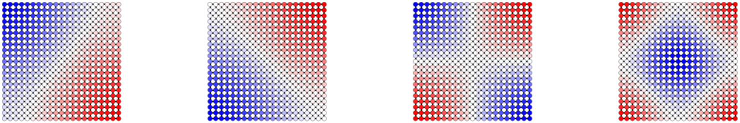

Bottom eigenfunctions of unevely-scaled grid are not

Pfau and Burgess 2018

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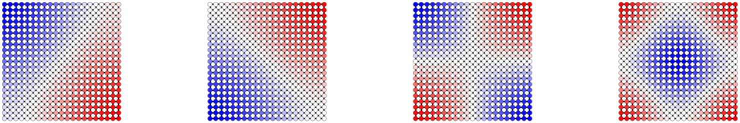

Bottom eigenfunctions of unevely-scaled grid are not

Eigenfunctions must be orthogonal, but can still be predictable, e.g. $\sin(2x)$ and $\sin(x)$ and $\cos(x)$.

Pfau and Burgess 2018

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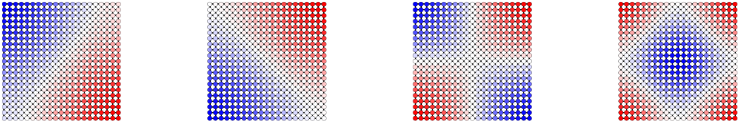


Bottom eigenfunctions of unevely-scaled grid are not

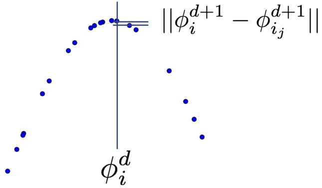
Eigenfunctions must be orthogonal, but can still be predictable, e.g. $\sin(2x)$ and $\sin(x)$ and $\cos(x)$.

Instead of using lowest eigenfunctions as embedding, use lowest eigenfunctions that are unpredictable from lower eigenfunctions

Pfau and Burgess 2018

Minimally redundant Laplacian eigenmaps

After adding eigenfunctions $\phi^1, \ldots, \phi^d$ to embedding, evaluate ϕ^{d+1} as candidate.



Pfau and Burgess 2018

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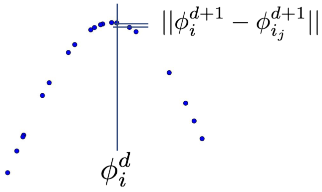
If value of ϕ^{d+1} at point i can be predicted from nearest neighbors of i in $\phi^1, \ldots, \phi^d$, eigenfunction is too predictable



Pfau and Burgess 2018

Minimally redundant Laplacian eigenmaps

NORB: Model dataset for studying invariance in object recognition

Pfau and Burgess 2018; LeCun, Huang and Bottou 2005

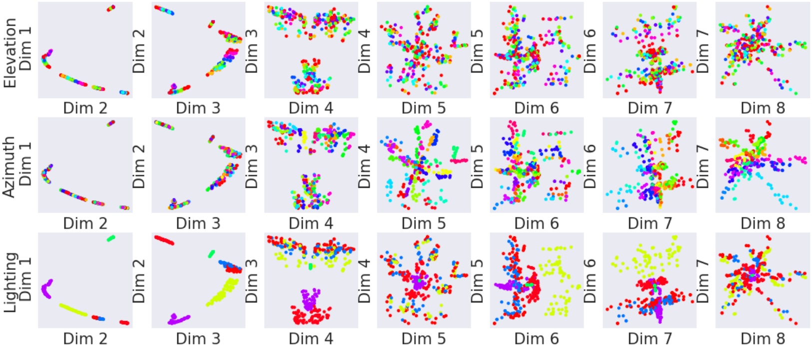
Minimally redundant Laplacian eigenmaps

NORB: Model dataset for studying invariance in object recognition

Consider a single object under different lighting and rotation

Pfau and Burgess 2018; LeCun, Huang and Bottou 2005

Minimally redundant Laplacian eigenmaps



Pfau and Burgess 2018

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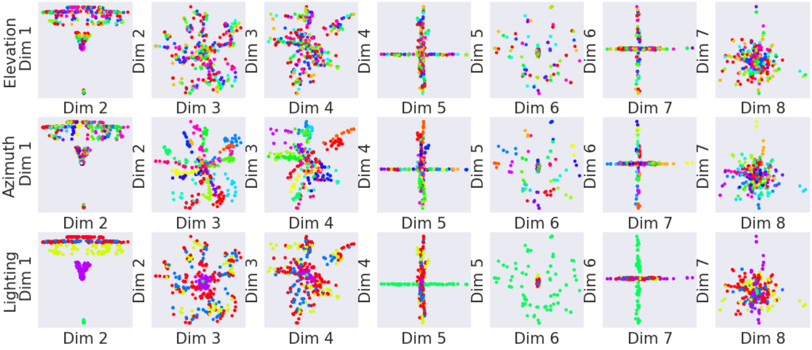

With filtering by redundancy, all variation captured by 6 eigenfunctions

Pfau and Burgess 2018

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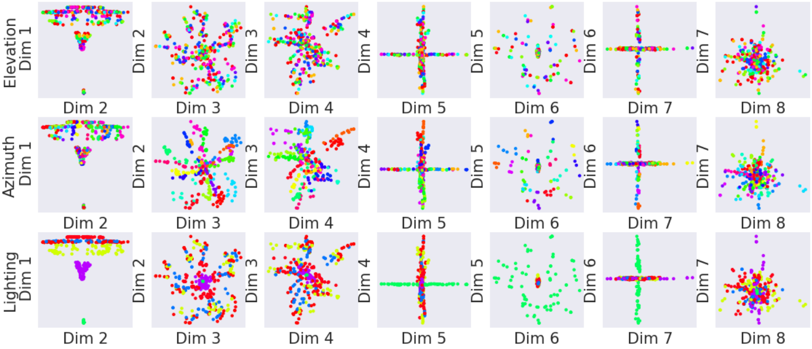
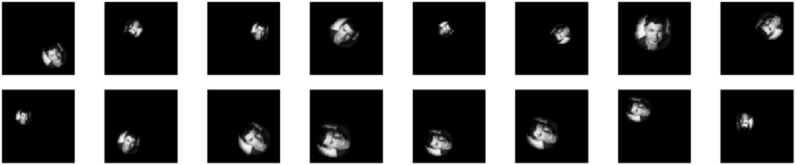


With filtering by redundancy, all variation captured by 6 eigenfunctions

Works with less than 1000 points!

Pfau and Burgess 2018

Minimally redundant Laplacian eigenmaps



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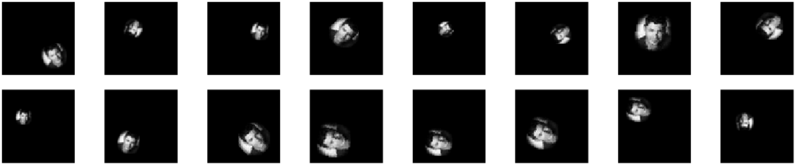
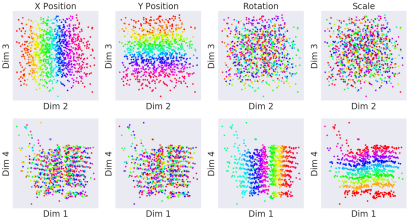


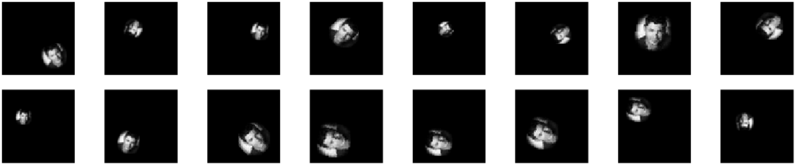


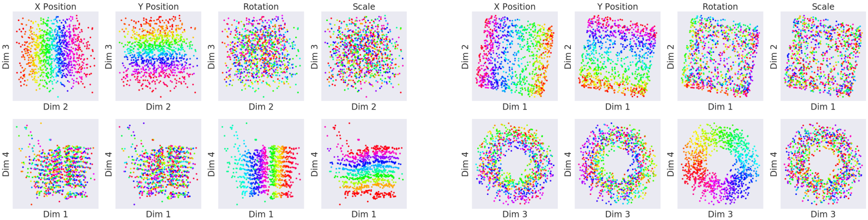
β-VAE

Disentangling VAEs learn the dimension but not the topology

Pfau and Burgess 2018

Minimally redundant Laplacian eigenmaps





β-VAE Laplacian eigenmaps

Disentangling VAEs learn the dimension but not the topology

Laplacian eigenmaps learns the topology but misses some dimensions

Pfau and Burgess 2018

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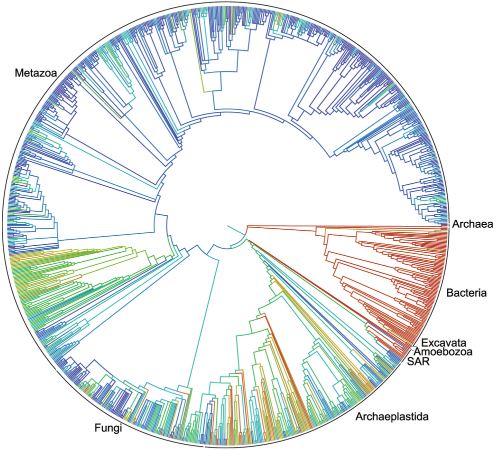
- ☺ Collapsed embeddings can be fixed by choice of eigenvector
- ☺ Can discover topology of data without prior assumptions

Embedding Hierarchies in Hyperbolic Spaces

Hierarchical data

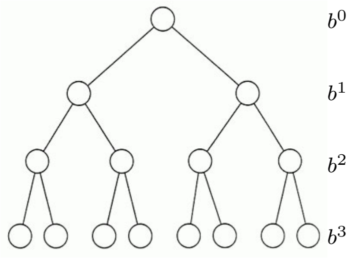
Some data can be embedded uniformly in flat space

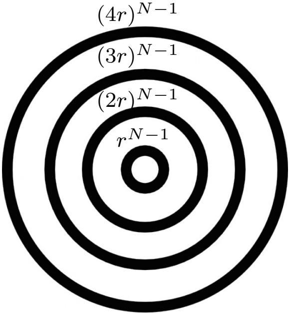
Hierarchical data



What about data with hierarchical structure?

Hierarchical data

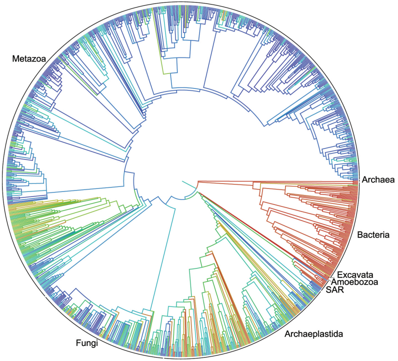


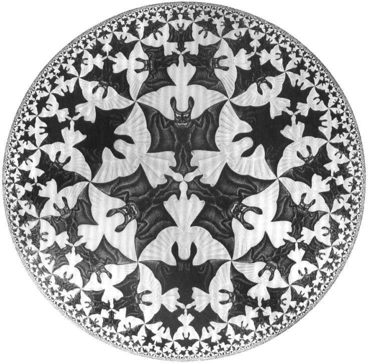


Tree with branching factor b has b^ℓ nodes at layer ℓ - exponential growth

Area of sphere in $\mathbb{R}^N$ with radius r grows as r^{N-1} - polynomial growth

Hierarchical data

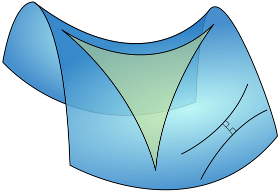




Idea: embed nodes in hierarchy in hyperbolic space instead of flat space

Hyperbolic geometry

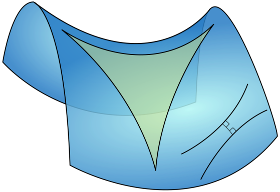
Hyperbolic space: manifold with constant negative curvature



Hyperbolic geometry

Hyperbolic space: manifold with constant negative curvature

Angles of triangle add to less than 180 degrees

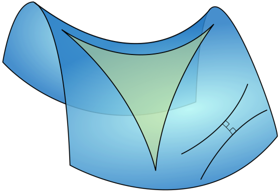


Hyperbolic geometry

Hyperbolic space: manifold with constant negative curvature

Angles of triangle add to less than 180 degrees

Surface area of spheres grows exponentially!



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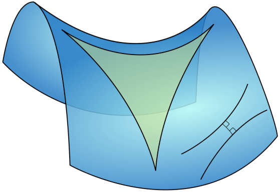
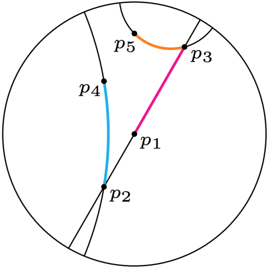
Surface area of spheres grows exponentially!

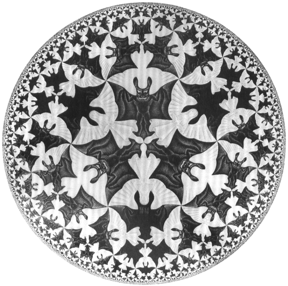
Many possible models of hyperbolic space



The Poincaré ball

Maps hyperbolic space to open ball $\mathbb{B}^N$





Nickel and Kiela 2017

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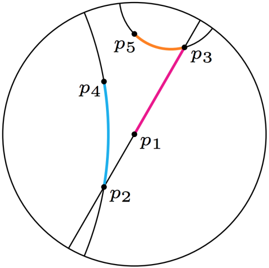
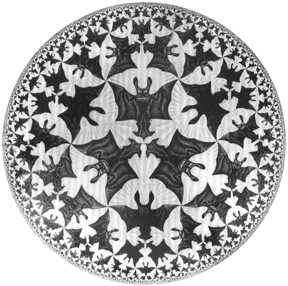
Metric: $\langle \mathbf{u}, \mathbf{v} \rangle_{T_{\mathbf{x}}\mathcal{P}} = \left(\frac{2}{1-\mathbf{x}^T\mathbf{x}} \right)^2 \mathbf{u}^T \mathbf{v}$





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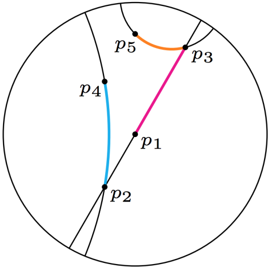
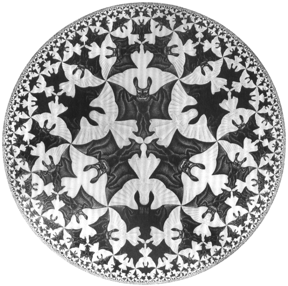
Geodesics: Circles that are orthogonal to boundary of ball





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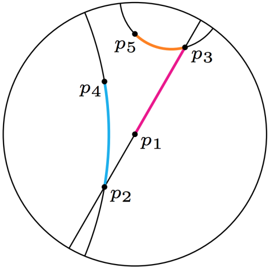
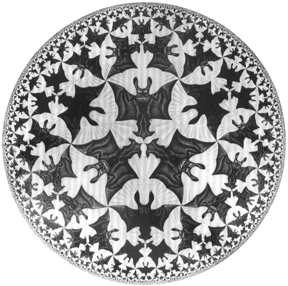
Geodesics: Circles that are orthogonal to boundary of ball

Distances:
$d(\mathbf{u}, \mathbf{v}) = \operatorname{arcosh}\left(1 + 2\frac{||\mathbf{u}-\mathbf{v}||^2}{(1-||\mathbf{u}||^2)(1-||\mathbf{v}||^2)}\right)$





Nickel and Kiela 2017

Poincaré embeddings for learning hierarchical representation

Given edges $\mathcal{E}$ from a graph, find an embedding $\mathbf{u}_i$ for vertex i that minimizes:

$$\sum_{i,j \in \mathcal{E}} \log \frac{e^{-d(\mathbf{u}_i, \mathbf{u}_j)}}{\sum_{j' \text{ st } ij' \notin \mathcal{E}} e^{-d(\mathbf{u}_i, \mathbf{u}_{j'})}}$$

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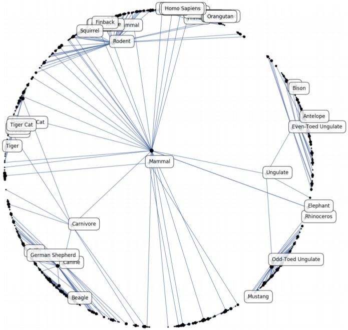

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			Dimensionality					
			5	10	20	50	100	200
WordNet Reconstruction	**Euclidean**	Rank	3542.3	2286.9	1685.9	1281.7	1187.3	1157.3
		MAP	0.024	0.059	0.087	0.140	0.162	0.168
	Translational	Rank	205.9	179.4	95.3	92.8	92.7	91.0
		MAP	0.517	0.503	0.563	0.566	0.562	0.565
	Poincaré	Rank	4.9	4.02	3.84	3.98	3.9	**3.83**
		MAP	0.823	0.851	0.855	0.86	0.857	**0.87**
WordNet Link Pred.	**Euclidean**	Rank	3311.1	2199.5	952.3	351.4	190.7	81.5
		MAP	0.024	0.059	0.176	0.286	0.428	0.490
	Translational	Rank	65.7	56.6	52.1	47.2	43.2	40.4
		MAP	0.545	0.554	0.554	0.56	0.562	0.559
	Poincaré	Rank	5.7	**4.3**	4.9	4.6	4.6	4.6
		MAP	0.825	0.852	0.861	**0.863**	0.856	0.855

State of the art results on link reconstruction and link prediction on WordNet noun dataset

Nickel and Kiela 2017

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Table 3: Spearman's ρ for Lexical Entailment on HYPERLEX.

	FR	**SLQS-Sim**	**WN-Basic**	**WN-WuP**	**WN-LCh**	**Vis-ID**	**Euclidean**	**Poincaré**
ρ	0.283	0.229	0.240	0.214	0.214	0.253	0.389	0.512

State of the art results on graded lexical entailment on HYPERLEX

Nickel and Kiela 2017

Trade-offs of Poincaré model

☺ Geodesics are simple

Trade-offs of Poincaré model

☺ Geodesics are simple

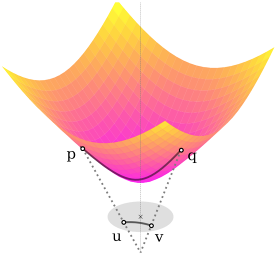
☺ Metric is diagonal

Trade-offs of Poincaré model

- ☺ Geodesics are simple
- ☺ Metric is diagonal
- ☹ Gradients of metric are unstable near boundary

The Lorentz model

Maps N-dim hyperbolic space to surface in $\mathbb{R}^{N+1}$



Nickel and Kiela 2018

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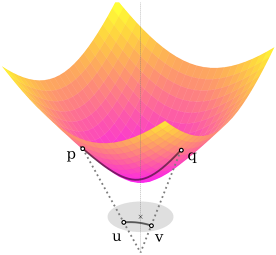
$\langle \mathbf{u}, \mathbf{v} \rangle_{\mathcal{L}} = -u_0 v_0 + \sum_{i=1}^{N+1} u_i v_i$



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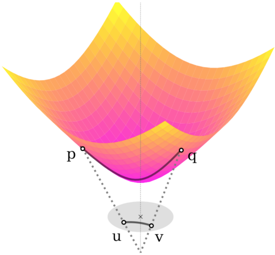

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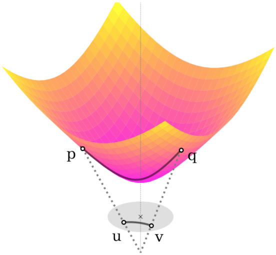

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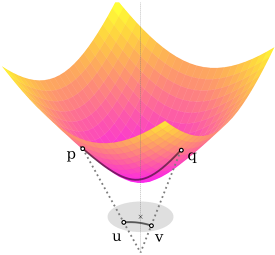
$$\exp_{\mathbf{x}}(t\mathbf{v}) = \cosh(t)\mathbf{x} + \sinh(t)\mathbf{v}$$



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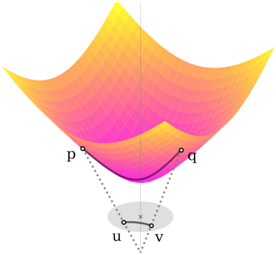
Projection: maps vectors onto tangent space:

$$\mathrm{proj}_{\mathbf{x}}(\mathbf{u}) = \mathbf{u} + \langle \mathbf{x}, \mathbf{u} \rangle_{\mathcal{L}}$$



Nickel and Kiela 2018

Riemannian SGD

Scale Euclidean gradient by inverse metric:

$$\mathbf{h} = \mathbf{M}_{\mathbf{x}}^{-1} \nabla f(\mathbf{x})$$

Bonnabel 2013

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$$\mathrm{grad} f(\mathbf{x}) = \mathrm{proj}(\mathbf{h})$$

Bonnabel 2013

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Project gradient onto tangent space:

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Follow geodesic along Riemannian gradient:

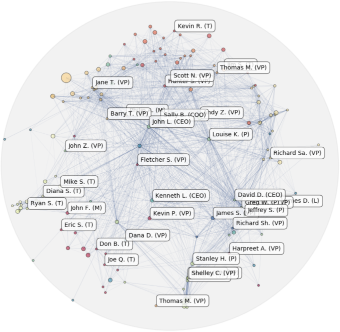
$$\mathbf{x} \leftarrow \exp_{\mathbf{x}}(-\eta \mathrm{grad} f(\mathbf{x}))$$

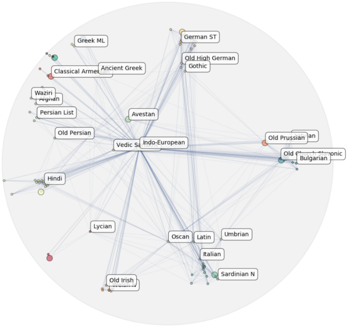
Bonnabel 2013

Learning continuous hierarchies in the Lorentz model

		WordNet Nouns			WordNet Verbs			EuroVoc			ACM			MeSH		
		2	5	10	2	5	10	2	5	10	2	5	10	2	5	10
MR	Poincaré	90.7	4.9	4.02	10.71	1.39	1.35	2.83	1.25	1.23	4.14	1.8	1.71	61.11	14.05	12.8
	Lorentz	22.8	3.18	2.95	3.64	1.26	1.23	1.63	1.24	1.17	3.05	1.67	1.63	38.99	14.13	12.42
	Δ%	74.8	35.1	36.2	66.0	9.6	8.9	42.4	6.1	3.4	26.3	7.2	4.8	36.2	-0.5	2.9
MAP	Poincaré	11.8	82.8	86.5	36.5	91.0	91.2	64.3	94.0	94.4	69.3	94.1	94.8	19.5	76.3	79.4
	Lorentz	30.5	92.3	92.8	57.9	93.5	93.3	87.1	95.8	96.5	82.9	96.6	97.0	34.8	77.7	79.9
	Δ%	61.3	10.3	6.8	58.6	2.7	2.3	35.6	1.6	2.0	19.6	2.7	2.3	43.9	1.8	0.6
ρ	Poincaré	13.8	57.2	58.5	11.0	54.1	55.1	37.5	57.5	61.4	59.8	63.5	62.9	42.2	69.9	74.9
	Lorentz	41.0	58.9	59.5	47.9	55.5	56.6	54.5	61.7	67.5	65.9	65.9	65.9	64.5	71.4	76.3

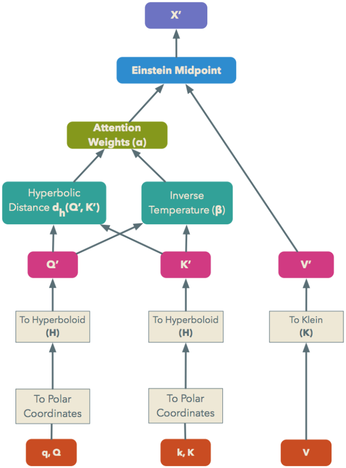
Significant improvement over Poincaré, especially in low dimensions





Nickel and Kiela 2018

Hyperbolic Attention Networks



Imposes hyperbolic geometry on activations of deep network with attention

Gulcehre, Denil, Malinowski et al 2018

Analyzing the Geometry of Deep Generative Models

What is the shape of latent space?

Higgins, Matthey, Pal et al 2017

What is the shape of latent space?

Are straight lines in latent space really straight?

Higgins, Matthey, Pal et al 2017

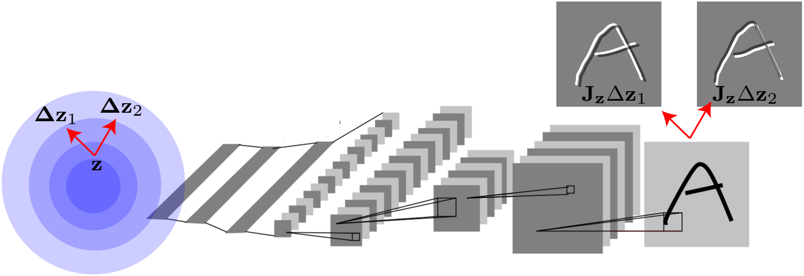
What is the shape of latent space?

Are straight lines in latent space really straight?

What is the right notion of distance in latent space?

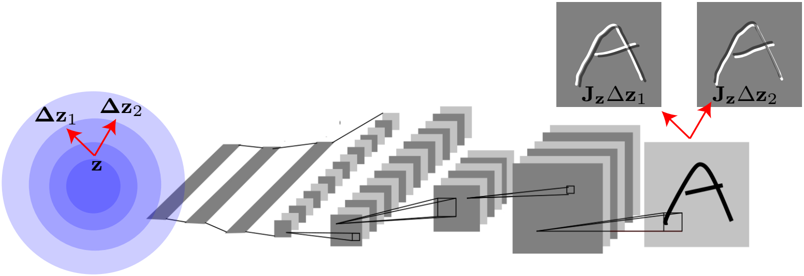
Higgins, Matthey, Pal et al 2017

Latent space metric



Deep generative model with decoder $f(\mathbf{z})$

Latent space metric



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Manifold $\mathcal{X}$ generated by f has tangent space $T_{\mathbf{z}}\mathcal{X} = \mathrm{span}(\mathbf{J_z})$ where $\mathbf{J_z}$ is Jacobian of f at $\mathbf{z}$

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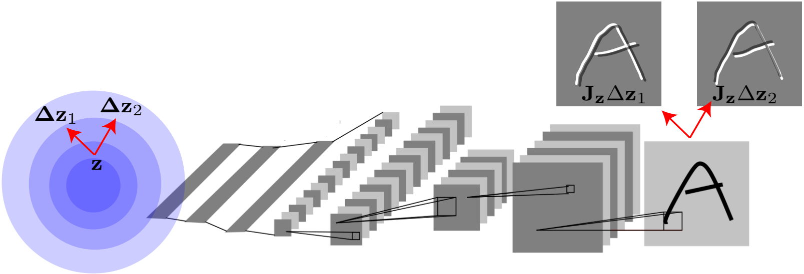

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Manifold $\mathcal{X}$ generated by f has tangent space $T_\mathbf{z}\mathcal{X} = \mathrm{span}(\mathbf{J_z})$ where $\mathbf{J_z}$ is Jacobian of f at $\mathbf{z}$

Use ℓ_2 metric in observation space as metric in latent space:

$$\langle \Delta\mathbf{z}_1, \Delta\mathbf{z}_2 \rangle_{T_\mathbf{z}\mathcal{X}} = \Delta\mathbf{z}_1^T \mathbf{J}_\mathbf{z}^T \mathbf{J_z} \Delta\mathbf{z}_2 = \Delta\mathbf{z}_1^T \mathbf{M_z} \Delta\mathbf{z}_2$$

Arvanitidis, Hansen and Hauberg 2018

Geodesic equation

How do we derive the geodesic equation from the introduction:

$$\ddot{\gamma} = -\mathbf{\Gamma}_{\gamma(t)} \left(\dot{\gamma}(t), \dot{\gamma}(t)\right)$$

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&= \min_{\gamma} \int_0^1 dt \left\langle \dot{\gamma(t)}, \dot{\gamma(t)} \right\rangle_{T_{\gamma(t)}\mathcal{X}}
\end{aligned}$$

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&= \min_{\gamma} \int_0^1 dt \sum_{ij} \mathbf{M}^{ij}_{\gamma(t)} \dot{\gamma}_i(t) \dot{\gamma}_j(t)
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Euler-Lagrange equation:

$$\frac{\partial L}{\partial \gamma^*} = \frac{d}{dt} \frac{\partial L}{\partial \dot{\gamma}^*}$$

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\end{aligned}$$

Euler-Lagrange equation:

$$\frac{\partial L}{\partial \gamma^*} = \frac{d}{dt} \frac{\partial L}{\partial \dot{\gamma}^*}$$

Exercise: Derive the left and right side of the Euler-Lagrange equation for $L(\gamma, \dot{\gamma}, t) = \sum_{ij} \mathbf{M}^{ij}_{\gamma(t)} \dot{\gamma}_i(t) \dot{\gamma}_j(t)$

Geodesic equation

$$\frac{\partial L}{\partial \gamma_i} = \sum_{jk} \frac{\partial \mathbf{M}^{jk}_{\gamma(t)}}{\partial \gamma_i} \dot{\gamma}_k(t) \dot{\gamma}_j(t)$$

Geodesic equation

$$\frac{\partial L}{\partial \gamma_i} = \sum_{jk} \frac{\partial \mathbf{M}^{jk}_{\gamma(t)}}{\partial \gamma_i} \dot{\gamma}_k(t) \dot{\gamma}_j(t)$$

$$\begin{aligned}
\frac{d}{dt}\frac{\partial L}{\partial \dot{\gamma}_i} = \frac{d}{dt}\left(2\sum_j \mathbf{M}^{ij}_{\gamma(t)} \dot{\gamma}_j(t)\right) \quad &= \quad 2\sum_j \left[\frac{\partial \mathbf{M}^{ij}_{\gamma(t)}}{\partial t} \dot{\gamma}_j(t) + \mathbf{M}^{ij}_{\gamma(t)} \ddot{\gamma}_j(t)\right] \\
&= \quad 2\sum_j \left[\sum_k \frac{\partial \mathbf{M}^{ij}_{\gamma(t)}}{\partial \gamma_k} \dot{\gamma}_k(t) \dot{\gamma}_j(t) + \mathbf{M}^{ij}_{\gamma(t)} \ddot{\gamma}_j(t)\right]
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\end{aligned}$$

$$\boxed{\ddot{\gamma}_j(t) = -\tfrac{1}{2} \sum_i \left(\mathbf{M}^{-1}_{\gamma(t)} \right)^{ij} \sum_k \left[\left(2 \tfrac{\partial \mathbf{M}^{ij}_{\gamma(t)}}{\partial \gamma_k} - \tfrac{\partial \mathbf{M}^{jk}_{\gamma(t)}}{\partial \gamma_i} \right) \dot{\gamma}_k(t) \dot{\gamma}_j(t) \right]}$$

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\frac{d}{dt}\frac{\partial L}{\partial \dot{\gamma}_i} = \frac{d}{dt}\left(2\sum_j \mathbf{M}^{ij}_{\gamma(t)} \dot{\gamma}_j(t)\right) \quad &= \quad 2\sum_j \left[\frac{\partial \mathbf{M}^{ij}_{\gamma(t)}}{\partial t} \dot{\gamma}_j(t) + \mathbf{M}^{ij}_{\gamma(t)} \ddot{\gamma}_j(t)\right] \\
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\end{aligned}$$

$$\boxed{\begin{gathered}
\ddot{\gamma}_j(t) = -\textstyle\sum_{ik} \mathbf{\Gamma}^{ik}_j(\gamma(t)) \dot{\gamma}_k(t) \dot{\gamma}_j(t) \\
\mathbf{\Gamma}^{ik}_j(x) = \frac{1}{2}\left(\mathbf{M}^{-1}_x\right)^{ij}\left(2\frac{\partial \mathbf{M}^{ij}_x}{\partial x_k} - \frac{\partial \mathbf{M}^{jk}_x}{\partial x_i}\right)
\end{gathered}}$$

Geodesic equation

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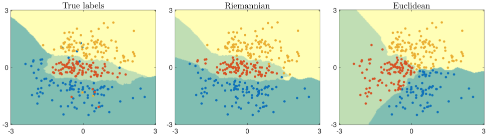
$\mathbf{\Gamma}^{ik}_j(x)$ are the parameters of the Levi-Civita connection: unique connection induced by the metric

The geodesics of deep generative models



Digits	Linear	Riemannian
$\{0, 1, 2\}$	$77.57(\pm 0.87)\%$	$\mathbf{94.28}(\pm\mathbf{1.14})\%$
$\{3, 4, 7\}$	$77.80(\pm 0.91)\%$	$\mathbf{89.54}(\pm\mathbf{1.61})\%$
$\{5, 6, 9\}$	$64.93(\pm 0.96)\%$	$\mathbf{81.13}(\pm\mathbf{2.52})\%$

Table 1: The F-measure results for k-means.

Classification from latent representations is better

Arvanitidis, Hansen and Hauberg 2018

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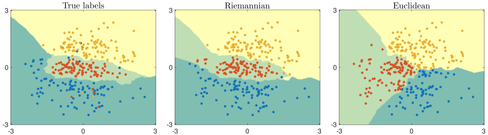

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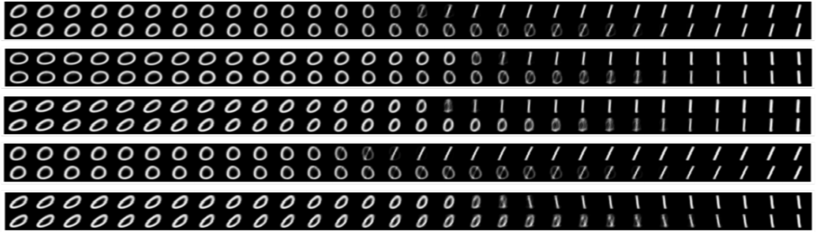

Transitions along geodesics are smoother

Arvanitidis, Hansen and Hauberg 2018

Summary

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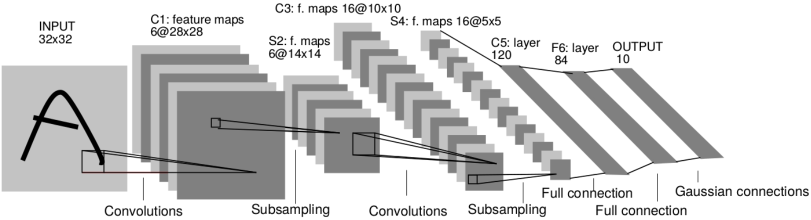
Part III

Spectral Deep Learning

Convolutions on Graphs and Manifolds

Key properties of CNNs



☺ Convolutional **(Translation invariance)**

LeCun et al. 1989

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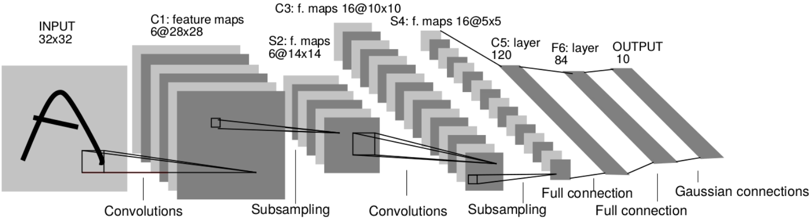

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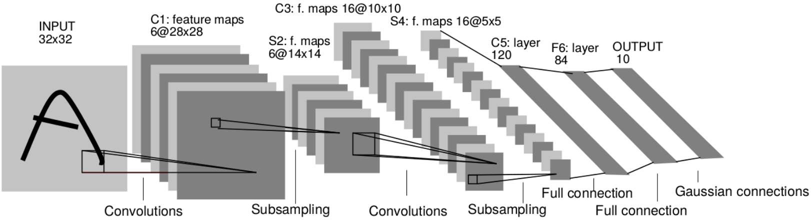

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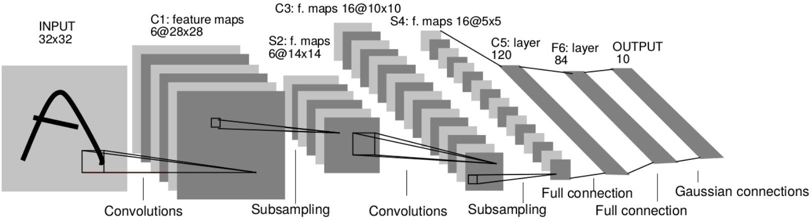

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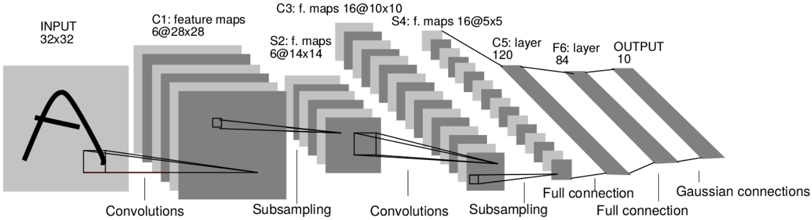

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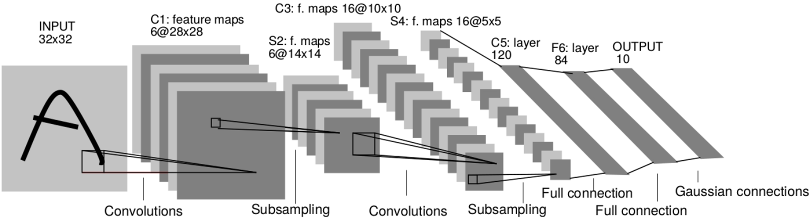

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- ☺ $\mathcal{O}(\log n)$ layers in classification tasks

LeCun et al. 1989

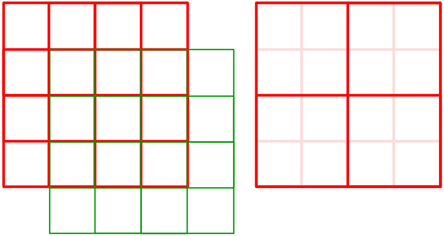
CNNs and Euclidean Geometry

CNNs are defined over Euclidean domains or Grids Ω. Two fundamental properties:

Translation Invariance (yielding convolutions).

Multiscale structure (yielding downsampling).

Inductive bias that exploits stationarity and deformation stability of many tasks.



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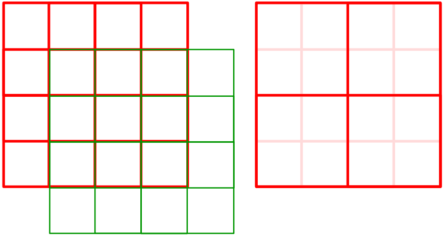

Roadmap: extend CNNs to non-Euclidean geometries by replacing filtering and pooling by appropriate operators

Convolution: Euclidean space

Given two functions $f, g : [-\pi, \pi] \to \mathbb{R}$ their convolution is a function

$$(f \star g)(x) = \int_{-\pi}^{\pi} f(x')g(x - x')dx'$$

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Efficient computation using FFT

Convolution Theorem

Convolution of two vectors $\mathbf{f} = (f_1, \ldots, f_n)^\top$ and $\mathbf{g} = (g_1, \ldots, g_n)^\top$

$$\mathbf{f} \star \mathbf{g} \quad = \quad \begin{bmatrix} g_1 & g_2 & \cdots & \cdots & g_n \\ g_n & g_1 & g_2 & \cdots & g_{n-1} \\ \vdots & \vdots & \ddots & \ddots & \vdots \\ g_3 & g_4 & \cdots & g_1 & g_2 \\ g_2 & g_3 & \cdots & \cdots & g_1 \end{bmatrix} \begin{bmatrix} f_1 \\ \vdots \\ f_n \end{bmatrix}$$

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Spectral convolution

Spectral convolution of $\mathbf{f}, \mathbf{g} \in L^2(\mathcal{V})$ can be defined by analogy

$$\mathbf{f} \star \mathbf{g} \quad = \quad \sum_{k \geq 1} \langle \mathbf{f}, \boldsymbol{\phi}_k \rangle_{L^2(\mathcal{V})} \langle \mathbf{g}, \boldsymbol{\phi}_k \rangle_{L^2(\mathcal{V})} \, \boldsymbol{\phi}_k$$

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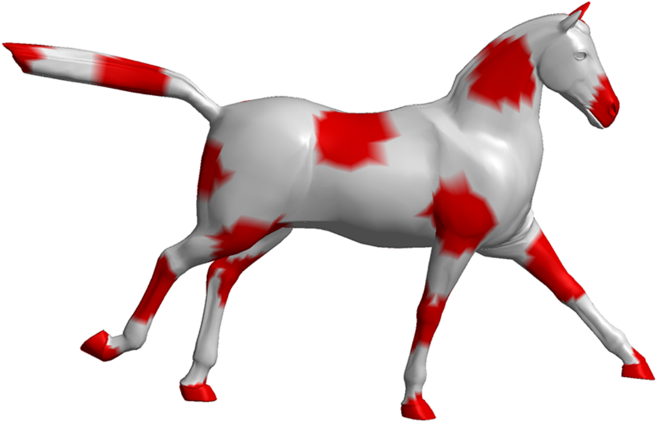
Filter coefficients depend on basis $\boldsymbol{\phi}_1, \ldots, \boldsymbol{\phi}_n$

Effect of spectral convolution



Function $\mathbf{f}$

Effect of spectral convolution

'Edge detecting' spectral filter $\mathbf{\Phi G \Phi^\top f}$

Effect of spectral convolution

Same spectral filter, different basis $\mathbf{\Psi} \mathbf{G} \mathbf{\Psi}^\top \mathbf{f}$

Effect of spectral convolution

High-frequency Laplacian eigenvector ϕ_{50}

Spectral Graph Convolutional Neural Networks

Spectral graph CNN

Convolution expressed in the spectral domain

$$\mathbf{g} = \mathbf{\Phi} \mathbf{W} \mathbf{\Phi}^\top \mathbf{f}$$

where $\mathbf{W}$ is $n \times n$ diagonal matrix of learnable spectral filter coefficients

Bruna, Zaremba, Szlam, LeCun 2014

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- ☹ No guarantee of spatial localization of filters

Bruna, Zaremba, Szlam, LeCun 2014

Localization and Smoothness

Vanishing moments: In the Euclidean setting

$$\int_{-\infty}^{+\infty} |x|^{2k} |f(x)|^2 dx = \int_{-\infty}^{+\infty} \left| \frac{\partial^k \hat{f}(\omega)}{\partial \omega^k} \right|^2 d\omega$$

Bruna, Zaremba, Szlam, LeCun 2014; Henaff, Bruna, LeCun 2015

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Application of the filter

$$\tau(\mathbf{\Delta})\mathbf{f} = \mathbf{\Phi}\tau(\mathbf{\Lambda})\mathbf{\Phi}^\top \mathbf{f}$$

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Parametrize the filter using a smooth spectral transfer function $\tau(\lambda)$

Application of the filter

$$\tau(\mathbf{\Delta})\mathbf{f} = \mathbf{\Phi} \begin{pmatrix} \tau(\lambda_1) & & \\ & \ddots & \\ & & \tau(\lambda_n) \end{pmatrix} \mathbf{\Phi}^\top \mathbf{f}$$

Bruna, Zaremba, Szlam, LeCun 2014; Henaff, Bruna, LeCun 2015

Localization and Smoothness

Vanishing moments: In the Euclidean setting

$$\int_{-\infty}^{+\infty} |x|^{2k}|f(x)|^2 dx = \int_{-\infty}^{+\infty} \left| \frac{\partial^k \hat{f}(\omega)}{\partial \omega^k} \right|^2 d\omega$$

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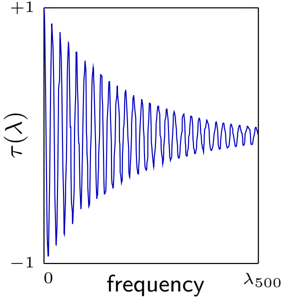
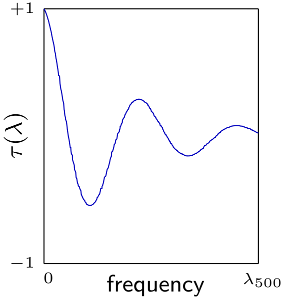


Non-smooth spectral filter (delocalized in space)

Localization and smoothness



Smooth spectral filter (localized in space)

Spectral graph CNN with polynomial filters (ChebNet)

Represent spectral transfer function as a polynomial or order r

$$\tau_{\boldsymbol{\alpha}}(\lambda) = \sum_{j=0}^{r} \alpha_j \lambda^j$$

where $\boldsymbol{\alpha} = (\alpha_0, \ldots, \alpha_r)^\top$ is the vector of filter parameters

Defferrard, Bresson, Vandergheynst 2016; Kipf, Welling 2016

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- ☺ No explicit computation of $\mathbf{\Phi}^\top, \mathbf{\Phi} \Rightarrow \mathcal{O}(nr)$ computational complexity

Defferrard, Bresson, Vandergheynst 2016; Kipf, Welling 2016

Example: citation networks

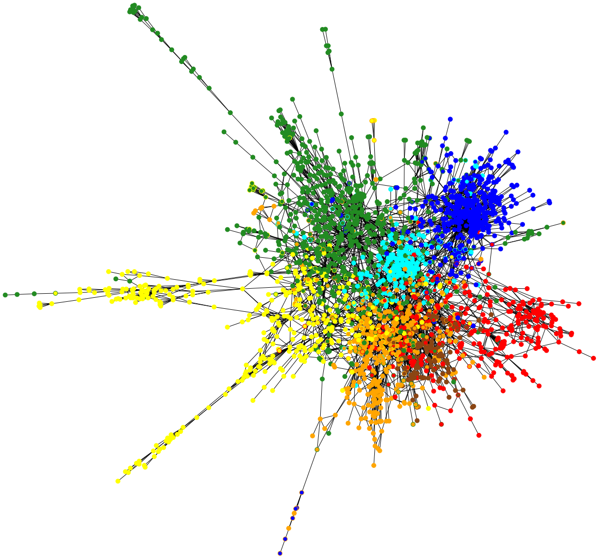


Figure: Monti, Boscaini, Masci, Rodolà, Svoboda, Bronstein 2017

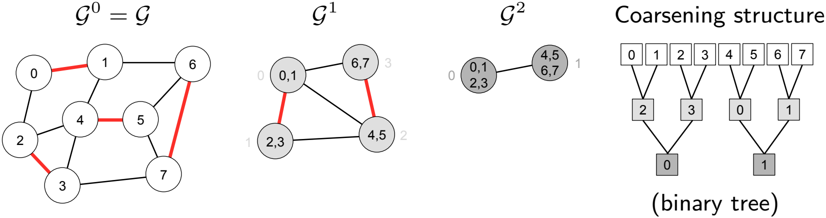
Example: citation networks

Method	**Cora**[1]	**PubMed**[2]
Manifold Regularization[3]	59.5%	70.7%
Semidefinite Embedding[4]	59.0%	71.1%
Label Propagation[5]	68.0%	63.0%
DeepWalk[6]	67.2%	65.3%
Planetoid[7]	75.7%	77.2%
Spectral graph CNN[8]	**81.6%**	**78.7%**

Classification accuracy of different methods on citation network datasets

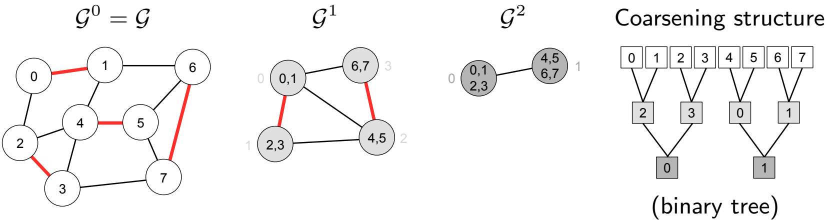
Data: [1,2]Sen et al. 2008; methods: [3]Belkin et al. 2006; [4]Weston et al. 2012; [5]Zhu et al. 2003; [6]Perozzi et al. 2014; [7]Yang et al. 2016; [8]Kipf, Welling 2016 (simplification of ChebNet)

Graph pooling



Produce a sequence of coarsened graphs

Graph pooling



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Max or average pooling of collapsed vertices

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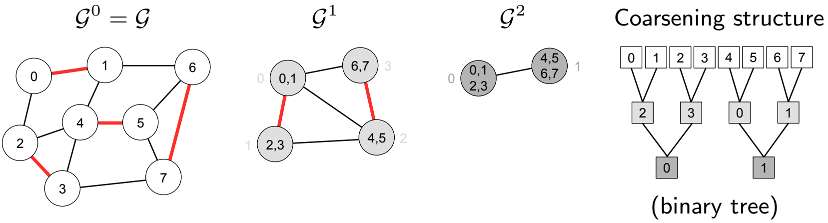

Produce a sequence of coarsened graphs

Max or average pooling of collapsed vertices

Binary tree arrangement of node indices

Limitations of spectral graph CNNs

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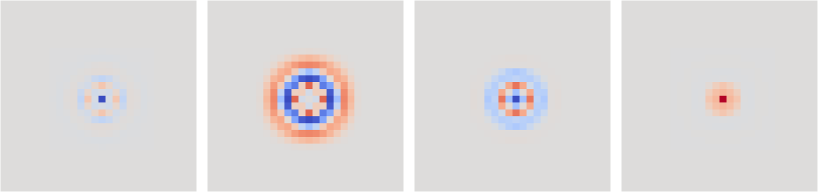
Only rotationally-symmetric kernels!



Example of Chebyshev filters (order $r = 7$) on Euclidean grid

Anisotropic kernels on manifolds

Scale t Orientation θ Elongation α

Examples of anisotropic heat kernels on a manifold

Boscaini, Masci, Rodolà, Bronstein, Cremers 2016

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- ☹ Only undirected graphs, as symmetry of the Laplacian matrix is assumed

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Different formulations of non-Euclidean CNNs

Spectral domain

Spatial domain

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Spatial domain

Geometric Deep Learning Tutorial: NIPS 2017

https://vimeo.com/248497329

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Pooling operation can be replaced with graph pooling

Inference in Spectral Learning with Deep Networks

Manifold learning (again)

Basic pattern:

Construct Gram matrix from kernel $k(\mathbf{x}, \mathbf{x}')$

$$\mathbf{M} = \begin{bmatrix} k(\mathbf{x}_1, \mathbf{x}_1) & k(\mathbf{x}_1, \mathbf{x}_2) & \dots & k(\mathbf{x}_1, \mathbf{x}_n) \\ k(\mathbf{x}_2, \mathbf{x}_1) & k(\mathbf{x}_2, \mathbf{x}_2) & \dots & k(\mathbf{x}_2, \mathbf{x}_n) \\ \vdots & \vdots & \ddots & \vdots \\ k(\mathbf{x}_n, \mathbf{x}_1) & k(\mathbf{x}_n, \mathbf{x}_2) & \dots & k(\mathbf{x}_n, \mathbf{x}_n) \end{bmatrix}$$

Use top/bottom eigenvectors of Gram matrix as embedding

Use Nyström approximation for inference on held-out data:
$\phi_k(\mathbf{x}') \propto \sum_i \phi_{ki} k(\mathbf{x}_i, \mathbf{x}')$

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Why not just learn parameterized $\phi_k(\mathbf{x})$ directly?

Deep learn all the things

A successful strategy: take a branch of machine learning and fit the model using a deep network

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Spectral Learning: ????

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Spectral Learning: **Spectral Inference Networks**

Pfau, Petersen, Agarwal, Barrett and Stachenfeld 2018

Trade-offs of manifold learning

- ☺ Exactly solvable by eigendecomposition
- ☺ Data efficient (works with $\mathcal{O}(1000)$ data points)
- 😐 Unsupervised learning without a generative model
- ☹ Learning scales as $\mathcal{O}(n \log n)$ with size of training data
- ☹ Inference scales as $\mathcal{O}(n)$ with size of training data
- ☹ Performance degrades for noisy or clustered data
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Spectral inference networks trade the first two for the second two

Eigendecomposition as optimization

Rayleigh quotient has top eigenvector as argmax:

$$\max_{\boldsymbol{\phi}} \frac{\boldsymbol{\phi}^T \mathbf{A} \boldsymbol{\phi}}{\boldsymbol{\phi}^T \boldsymbol{\phi}}$$

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Generalize to multiple eigenvectors (up to rotation):

$$\max_{\boldsymbol{\Phi}} \mathrm{Tr}\left((\boldsymbol{\Phi}^T \boldsymbol{\Phi})^{-1} \boldsymbol{\Phi}^T \mathbf{A} \boldsymbol{\Phi} \right)$$

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$$\max_{\boldsymbol{\phi}} \operatorname{Tr}\left(\mathbb{E}_{\mathbf{x}} \left[\boldsymbol{\phi}(\mathbf{x}) \boldsymbol{\phi}(\mathbf{x})^T \right]^{-1} \mathbb{E}_{\mathbf{x},\mathbf{x}'} \left[k(\mathbf{x}, \mathbf{x}') \boldsymbol{\phi}(\mathbf{x}) \boldsymbol{\phi}(\mathbf{x}')^T \right] \right)$$

Replace A_{ij} with $k(\mathbf{x}, \mathbf{x}')$ and sums with expectations

Pfau, Petersen, Agarwal, Barrett and Stachenfeld 2018

Eigendecomposition as optimization

Most machine learning:

$$\max_{\theta} \mathbb{E}_{\mathbf{x}}[f_{\theta}(\mathbf{x})]$$

Empirical gradient in unbiased

Pfau, Petersen, Agarwal, Barrett and Stachenfeld 2018

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Pfau, Petersen, Agarwal, Barrett and Stachenfeld 2018

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Empirical gradient is biased

Solution: use moving average of gradient of $\phi_\theta \phi_\theta^T$ term

Pfau, Petersen, Agarwal, Barrett and Stachenfeld 2018

Spectral inference network gradients

Objective is of the form $\mathrm{Tr}(\mathbf{\Sigma}^{-1}\mathbf{\Pi})$

Pfau, Petersen, Agarwal, Barrett and Stachenfeld 2018

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Gradient is of the form $\mathrm{Tr}\left(\mathbf{\Sigma}^{-1}\nabla_\theta\mathbf{\Pi}\right) - \mathrm{Tr}\left(\mathbf{\Sigma}^{-1}\mathbf{\Pi}\mathbf{\Sigma}^{-1}\nabla_\theta\mathbf{\Sigma}\right)$

Pfau, Petersen, Agarwal, Barrett and Stachenfeld 2018

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Pfau, Petersen, Agarwal, Barrett and Stachenfeld 2018

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To reduce bias in the gradient, use moving average for $\mathbf{\Sigma}$ and $\nabla_\theta\mathbf{\Sigma}$

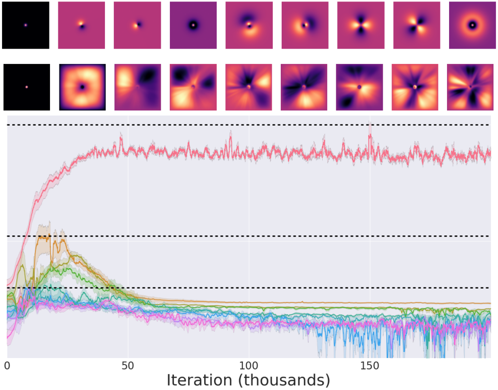
Pfau, Petersen, Agarwal, Barrett and Stachenfeld 2018

Spectral inference networks

Sanity check: the Schrödinger equation

$$E\psi(\mathbf{x}) = -\frac{\hbar}{2m}\nabla^2\psi(\mathbf{x}) - \frac{\psi(\mathbf{x})}{|\mathbf{x}|}$$

Without bias correction:



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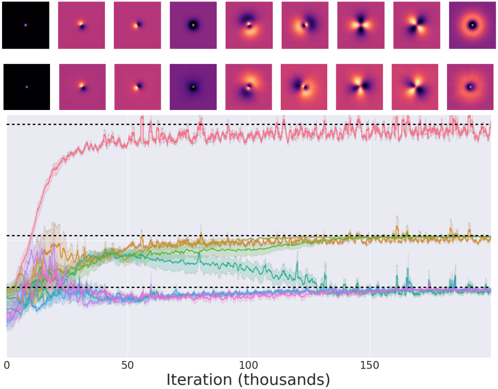

Pfau, Petersen, Agarwal, Barrett and Stachenfeld 2018

Approximating Laplacian eigenmaps

Objective:

$$k(\mathbf{x}, \mathbf{x}')\boldsymbol{\phi}(\mathbf{x})\boldsymbol{\phi}(\mathbf{x})^T = (\boldsymbol{\phi}(\mathbf{x}) - \boldsymbol{\phi}(\mathbf{x}'))(\boldsymbol{\phi}(\mathbf{x}) - \boldsymbol{\phi}(\mathbf{x}'))^T$$

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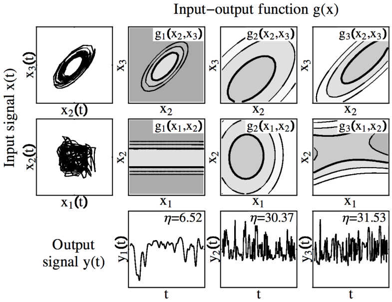
If $\mathbf{x}$, $\mathbf{x}'$ are sequential video frames, equivalent to Slow Feature Analysis



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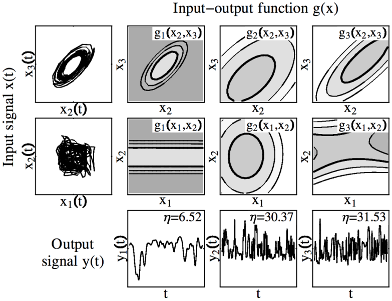

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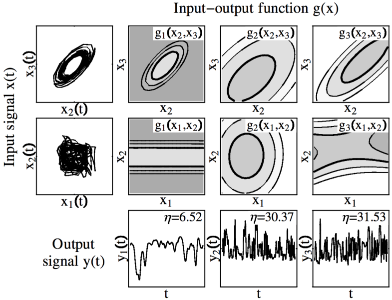


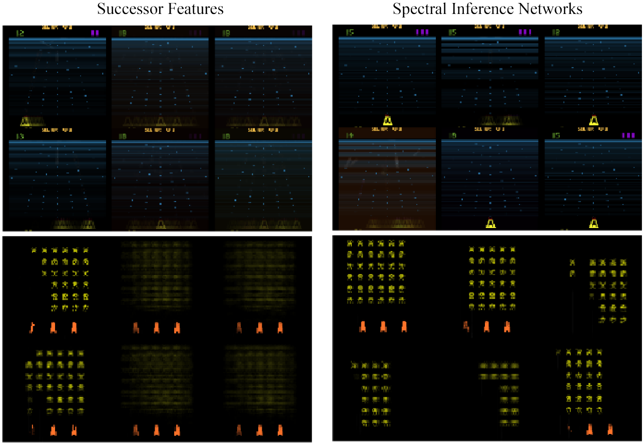
SFA learned layer-by-layer rather than end-to-end

SFA learned feature-by-feature rather than fully online

Wiskott and Sejnowski 2002; Sprekeler 2011

Spectral inference networks on Atari

More interpretable features compared to other approaches when trained on random policies on Atari games



Pfau, Petersen, Agarwal, Barrett and Stachenfeld 2018

Summary

Eigenfunctions can be learned by stochastic gradient descent with function approximation

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Slow feature analysis is a special case of Spectral Inference Networks

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Eigenfunctions can be learned by stochastic gradient descent with function approximation

Slow feature analysis is a special case of Spectral Inference Networks

While less efficient than standard spectral algorithms, it is far more scalable

Future challenges in manifold and spectral learning

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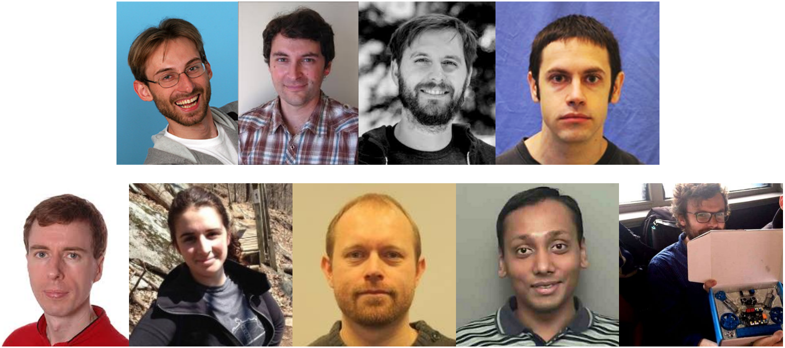
Can we better connect spectral learning with probabilistic models?

Acknowledgements



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