Manifold Learning in the Age of Big Data

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Annual Plenary Meeting
Garching, 01/22/2019

Supervised, Unsupervised, Reinforcement Learning

- We are witnessing an AI/ML revolution
  - this is led by Supervised (speech recognition) and Reinforcement Learning (self-driving cars)
  - i.e. Prediction and Acting
- Unsupervised learning
  - cluster analysis, dimension reduction, explanatory models
  - is in a much more primitive state of development
  - it is harder conceptually: defining the objective is part of the problem
  - but everybody does it [in the sciences]
  - because exploration, explanation, understanding, uncovering the structure of the data are necessary
    in the language of the discipline
  - is the next big data challenge. . . ?

Unsupervised learning at scale and automatically validated

- Topics: Geometry and combinatorics
  - Non-linear dimension reduction
  - Topological data analysis
  - Graphs, rankings, clustering
- Algorithms and computation
- Mathematics/theory/theorems/models
  - validation/checking/guarantees
  - beyond discovering patterns

- Demands from practical problems stimulate good research
  - astronomy
  - chemistry and materials science

Basics of manifold learning algorithms

- Computational challenges

Metric Manifold Learning

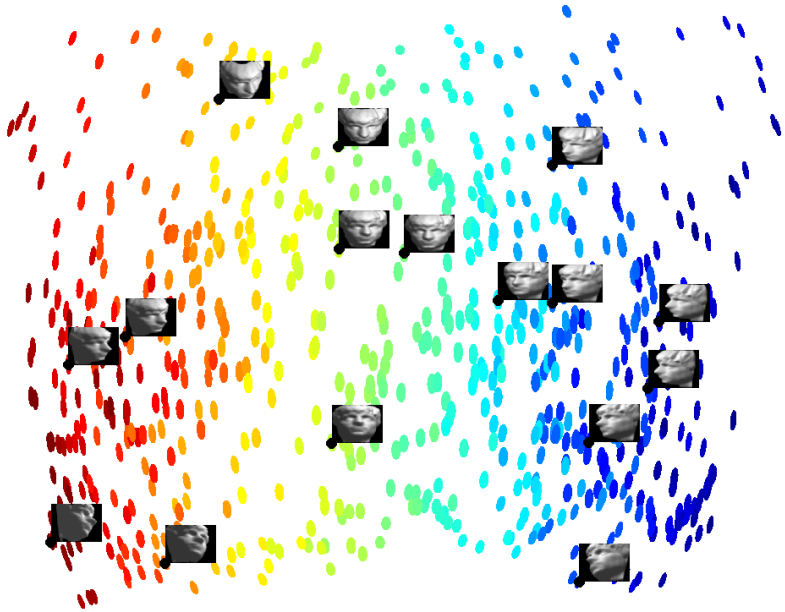
- Estimating the embedding distortion
- Estimating the kernel bandwidth

Scalable manifold learning

- Finding filaments in high dimensions
- More computational challenges ahead
- megaman

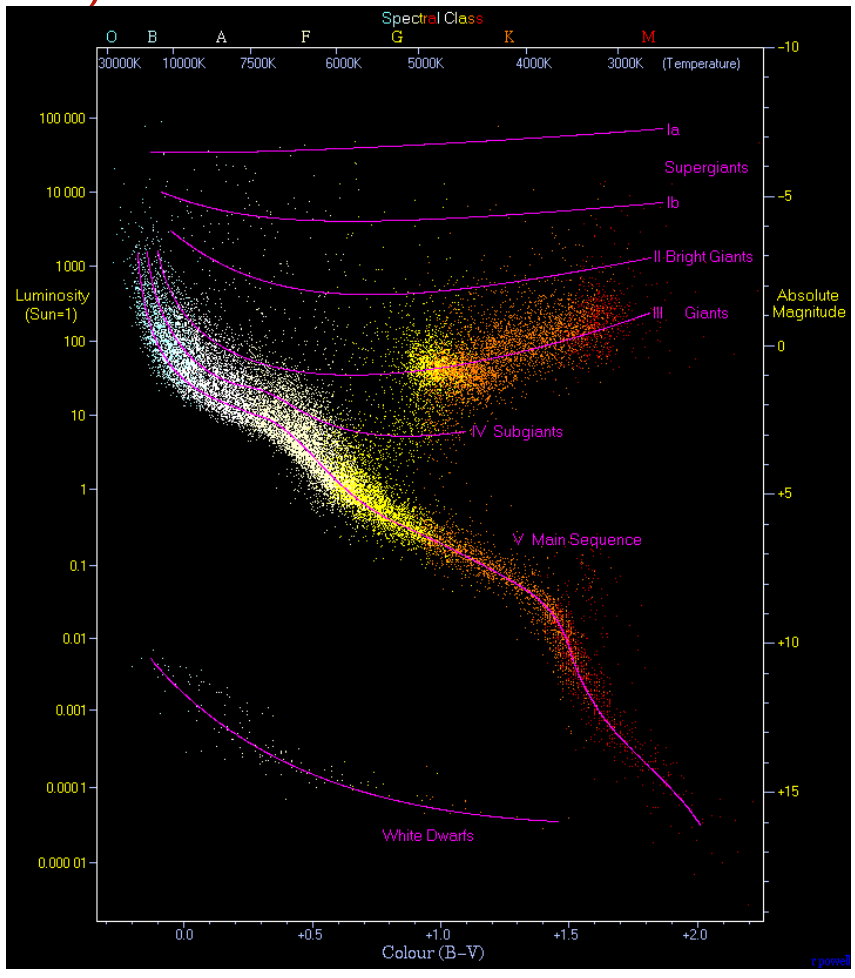
Outline

When to do (non-linear) dimension reduction



- high-dimensional data $p \in \mathbb{R}^D$, $D = 64 \times 64$
- can be described by a small number d of continuous parameters
- Usually, large sample size n

When to do (non-linear) dimension reduction

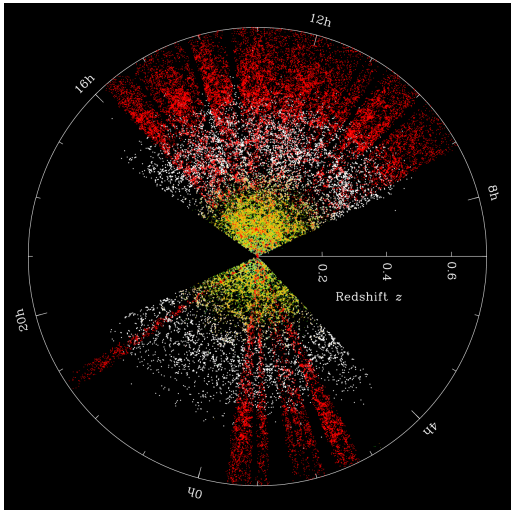


Why?

- To save space and computation
  - $n \times D$ data matrix $\rightarrow$ $n \times m$, $m \ll D$
- To use it afterwards in (prediction) tasks
- To understand the data better
  - preserve large scale features, suppress fine scale features

Spectra of galaxies measured by the Sloan Digital Sky Survey (SDSS)

www.sdss.org



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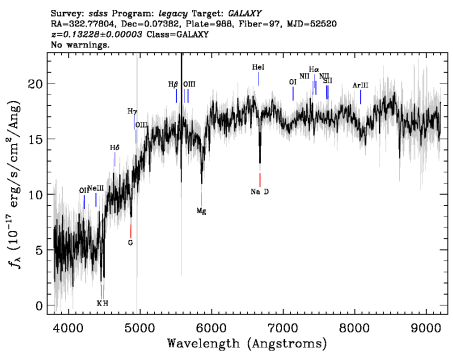
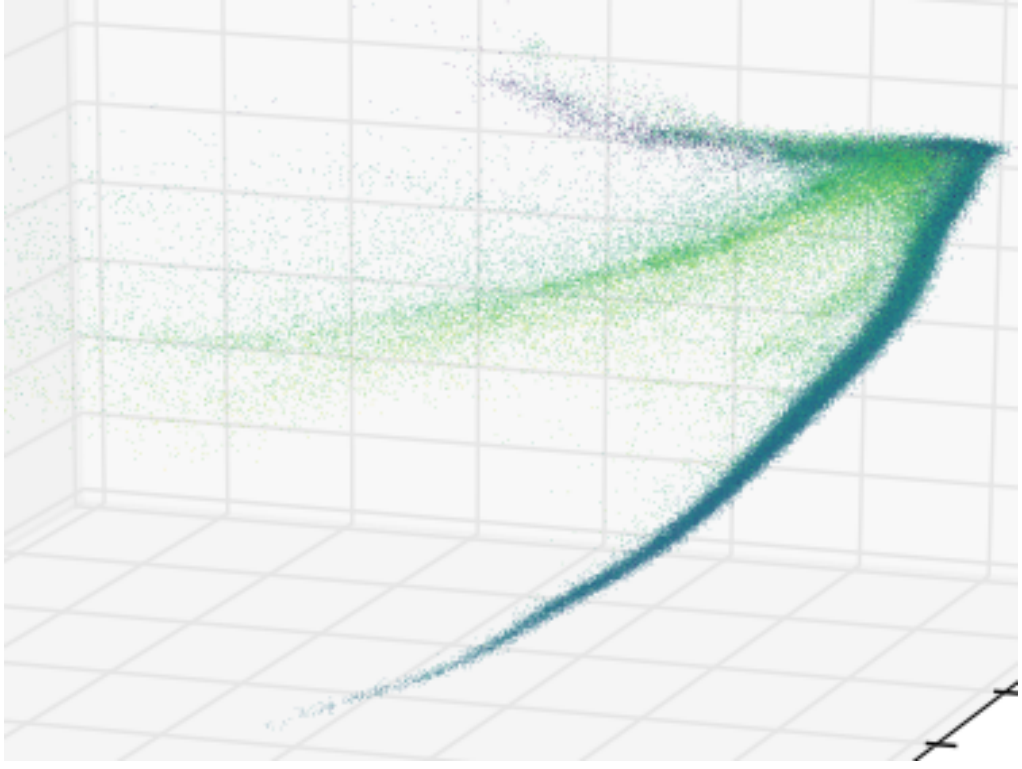
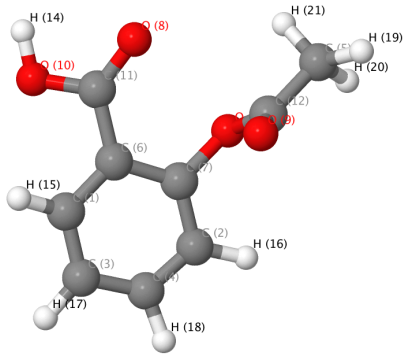


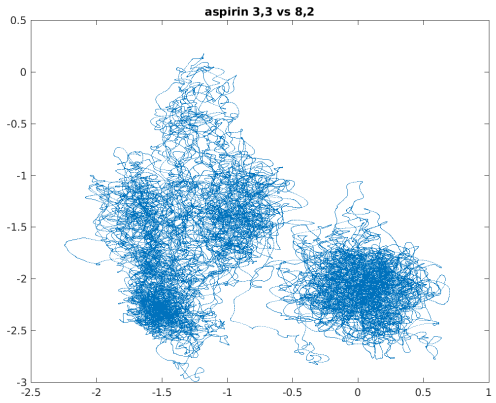
- Preprocessed by Jacob VanderPlas and Grace Telford
- $n = 675,000$ spectra $\times$ $D = 3750$ dimensions



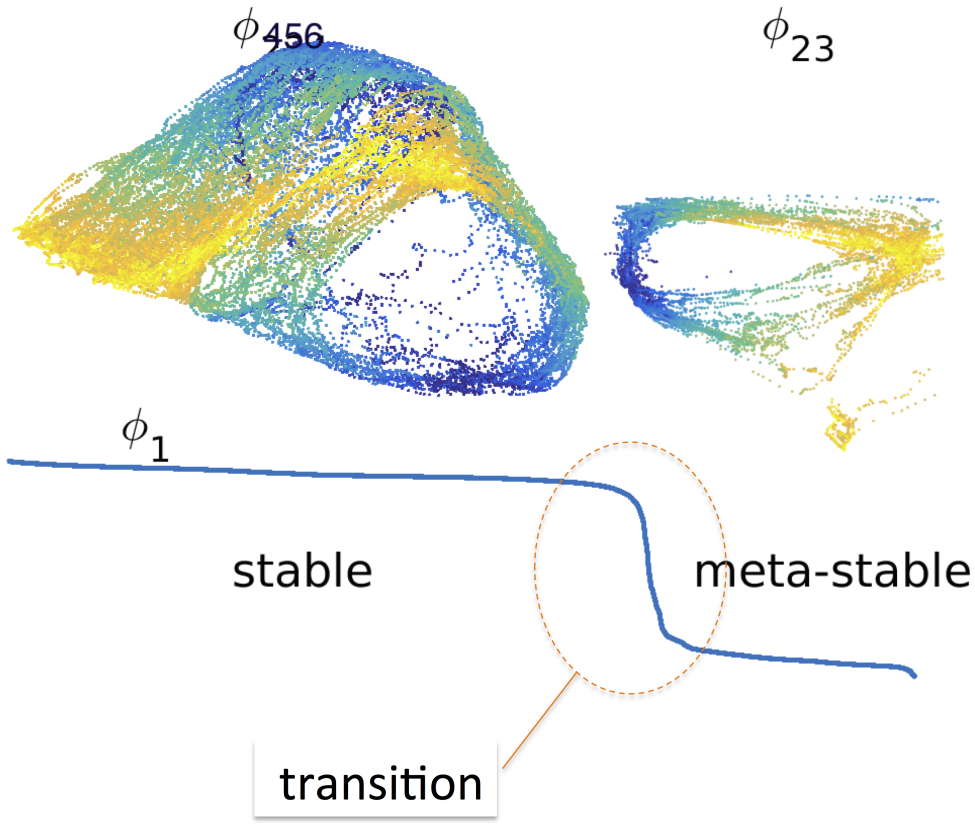
Molecular configurations

aspirin molecule



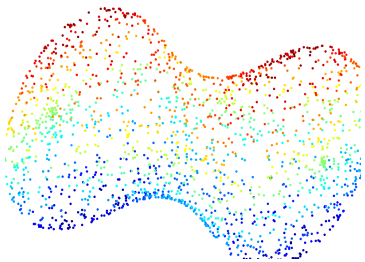


- Data from Molecular Dynamics (MD) simulations of small molecules by [Chmiela et al. 2016]
- $n \approx 200,000$ configurations $\times$ $D \sim 20 - 60$ dimensions



Brief intro to manifold learning algorithms

- **Input** Data $p_1, \ldots p_n$, embedding dimension m, neighborhood scale parameter ϵ



$p_1, \ldots p_n \subset \mathbb{R}^D$

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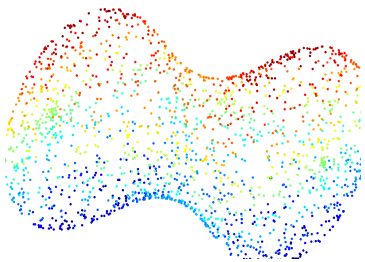

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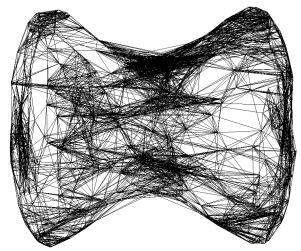

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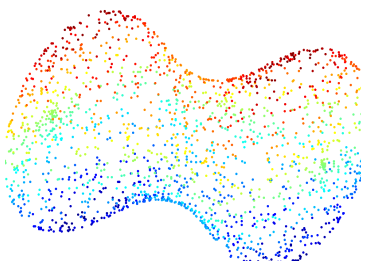

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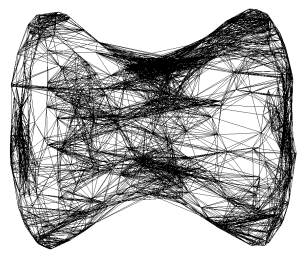

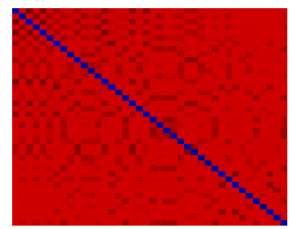

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Laplacian Eigenmaps/Diffusion Maps [Belkin,Niyogi 02,Nadler et al 05]

- Construct similarity matrix

$$S = [S_{pp'}]_{p,p' \in \mathcal{D}} \quad \text{with} \quad S_{pp'} = e^{-\frac{1}{\epsilon}||p-p'||^2} \quad \text{iff } p, p' \text{ neighbors}$$

- Construct Laplacian matrix $L = I - T^{-1}S$ with $T = \mathrm{diag}(S\mathbf{1})$
- Calculate $\phi^{1\ldots m}$ = eigenvectors of L (smallest eigenvalues)
- coordinates of $p \in \mathcal{D}$ are $(\phi^1(p), \ldots \phi^m(p))$

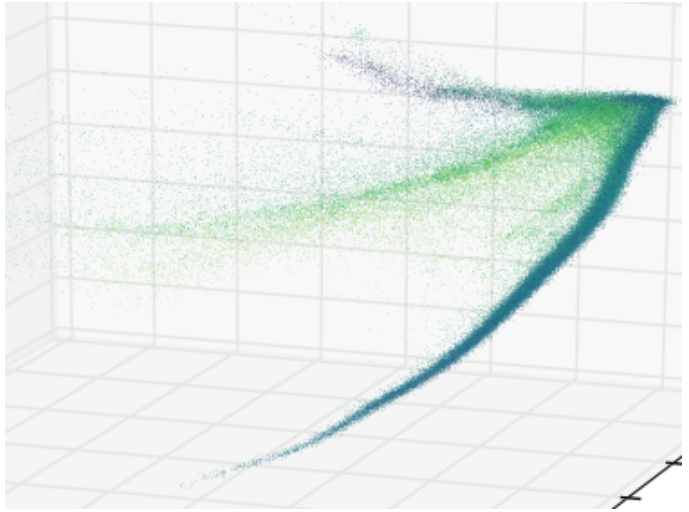
Manifold Learning is like choosing a basis

- Bases
  - Fourier
  - Finite Element
  - RHKS
  - SG
  - ...
- Trade dimension reduction vs. loss of information

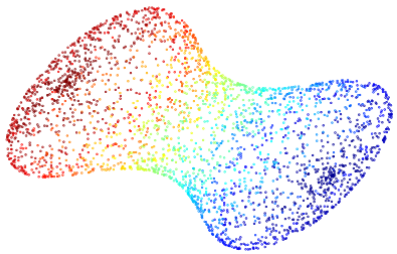
- Manifold Learning learns a basis from data
  - e.g. eigenfunctions of Δ operator in LaplacianEigenmaps/DiffusionMaps
  - Maps high D data to $m \ll D$ dimensions

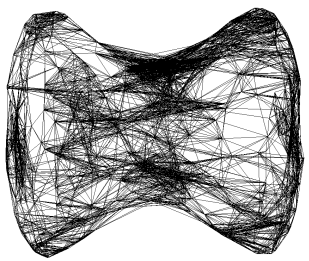
ML poses special computational challenges

SDDS spectra, $n = 0.7M$, $D = 3750$



- structure of computation not regular
  - and not known in advance
  - dictated by a random geometric graph
  - the graph represents the neighbohood relations between data points
  - affects storage, parallelization, run time (by unknown condition numbers)





ML poses special computational challenges

- intrinsic dimension d
  - data dimension D arbitrarily large as long as d small
  - d must be guessed/estimated
  - controls statistical and almost all numerical properties of ML algorithm
  - in particular, the density of the neighborhood graph is super-linear in d

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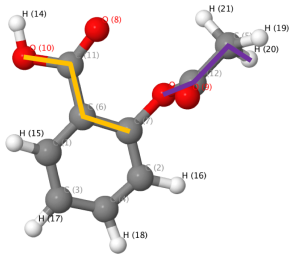
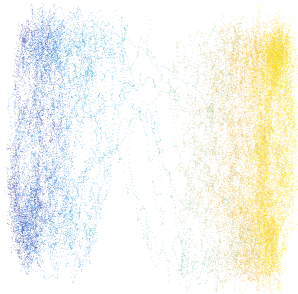
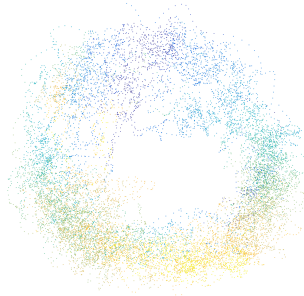
  - controls statistical and almost all numerical properties of ML algorithm
  - in particular, the density of the neighborhood graph is super-linear in d
- coordinate system is local

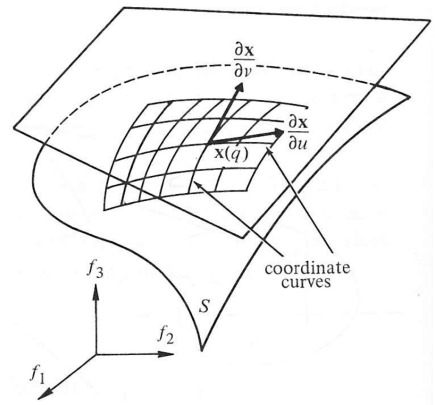




yellow



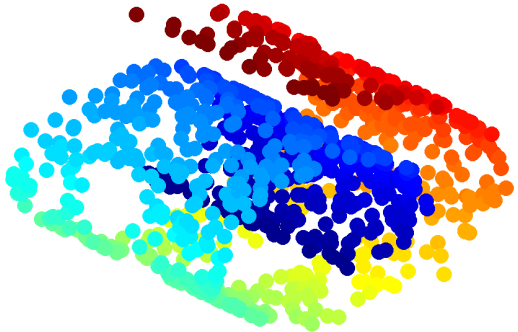
purple



- not easily parallelizable
- data partitioning is open problem
- problem of finding neighbors efficiently

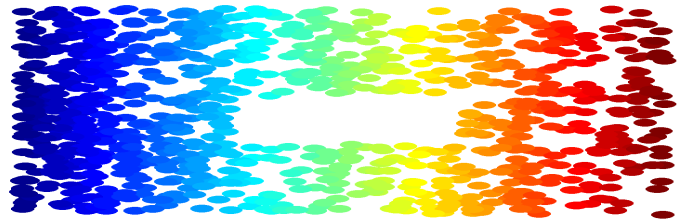
A toy example (the "Swiss Roll" with a hole)

points in $D \geq 3$ dimensions



Input

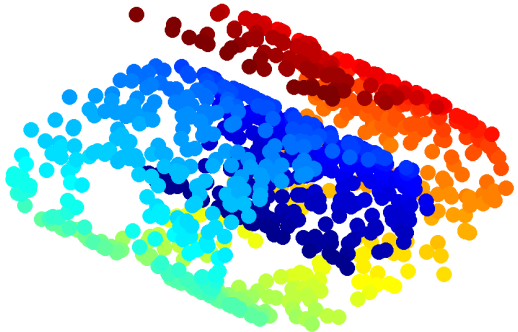
same points reparametrized in 2D



Desired output

A toy example (the "Swiss Roll" with a hole)

points in $D \geq 3$ dimensions



Input

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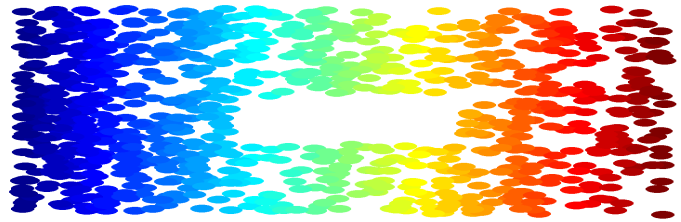
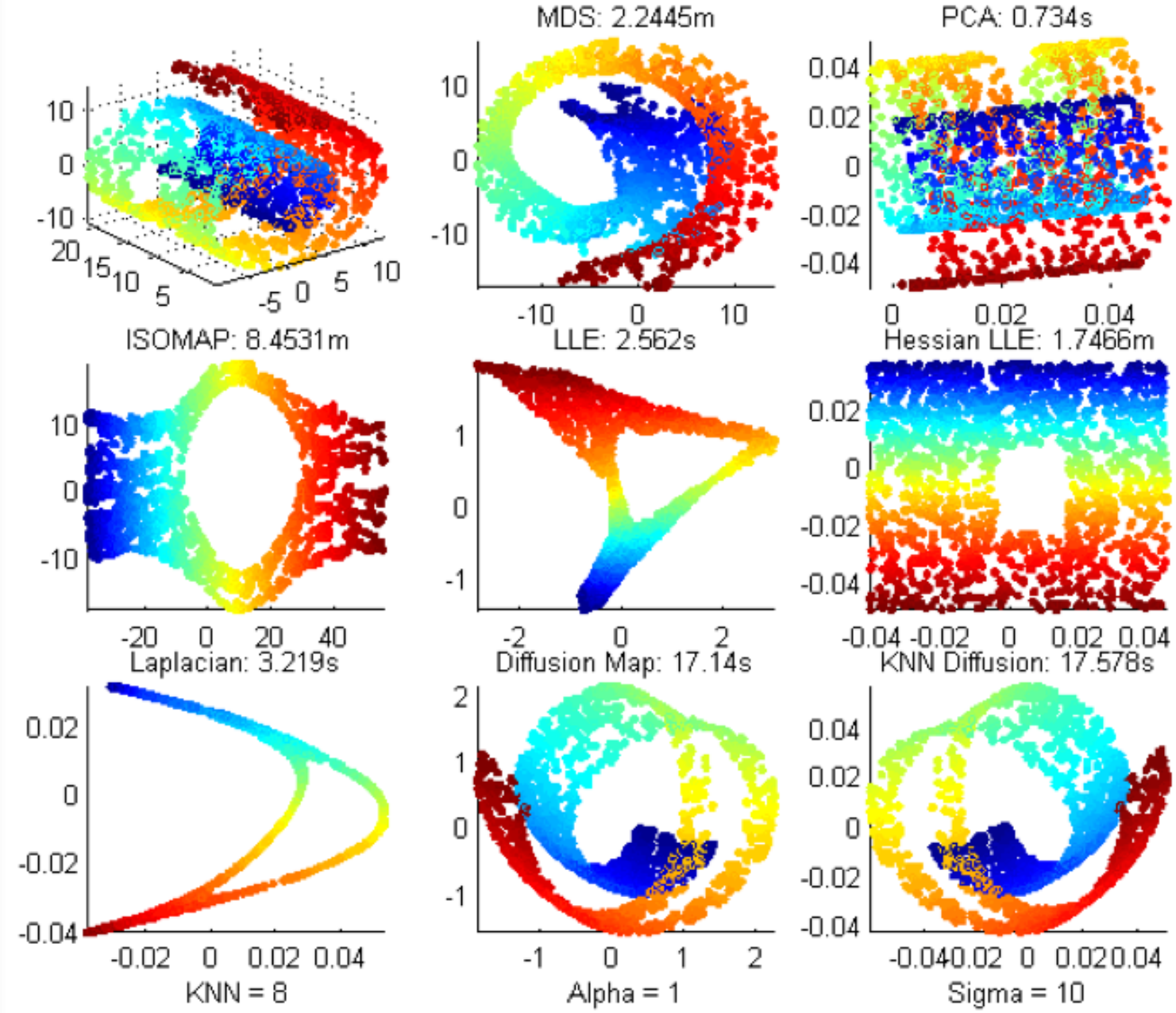


Desired output

...and a problem

Embedding in 2 dimensions by different manifold learning algorithms



Outline

Our approach: Metric Manifold Learning

[Perrault-Joncas,M 10]

Given

- mapping ϕ that preserves topology

true in many cases

Objective

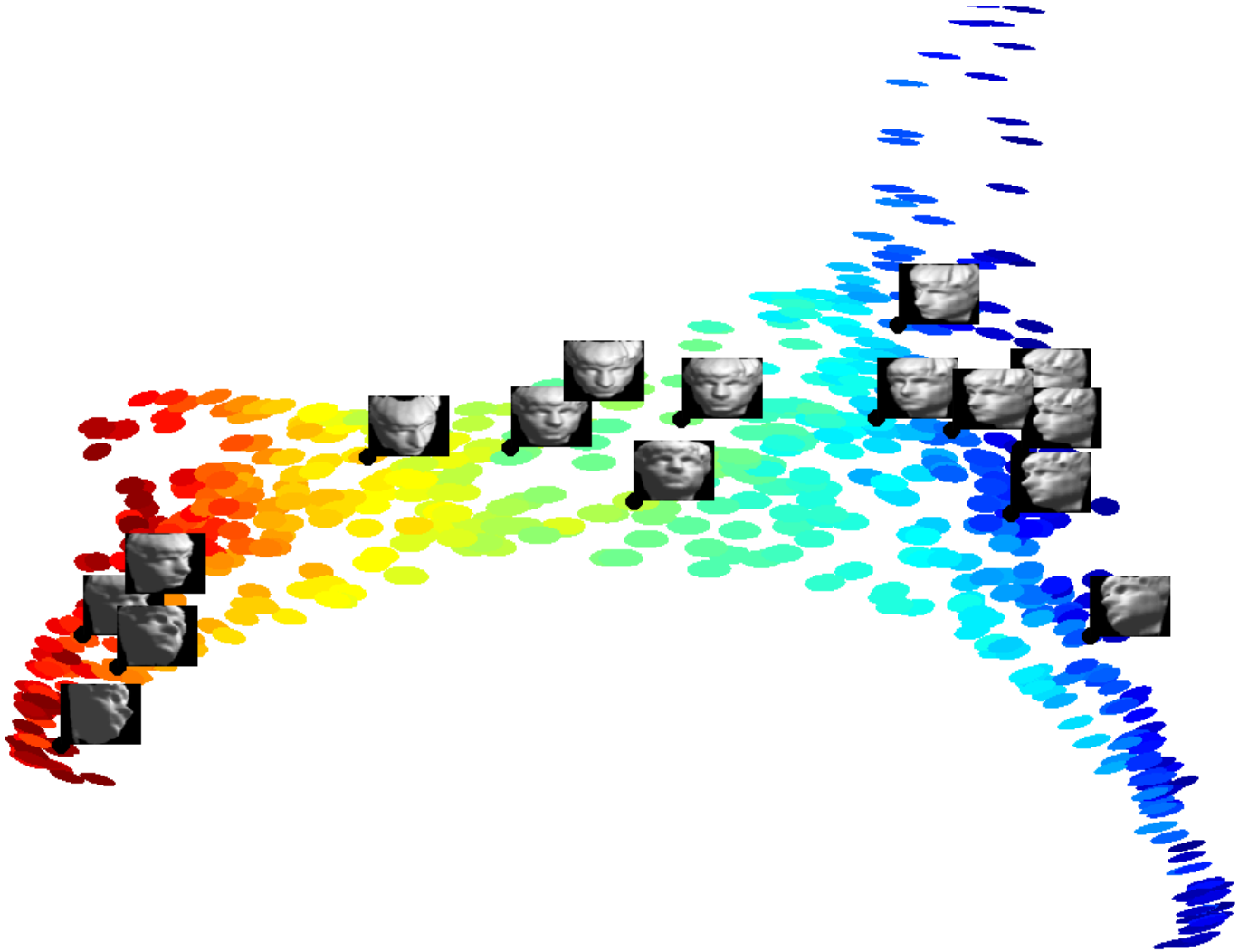
- augment ϕ with geometric information g so that (ϕ, g) preserves the geometry

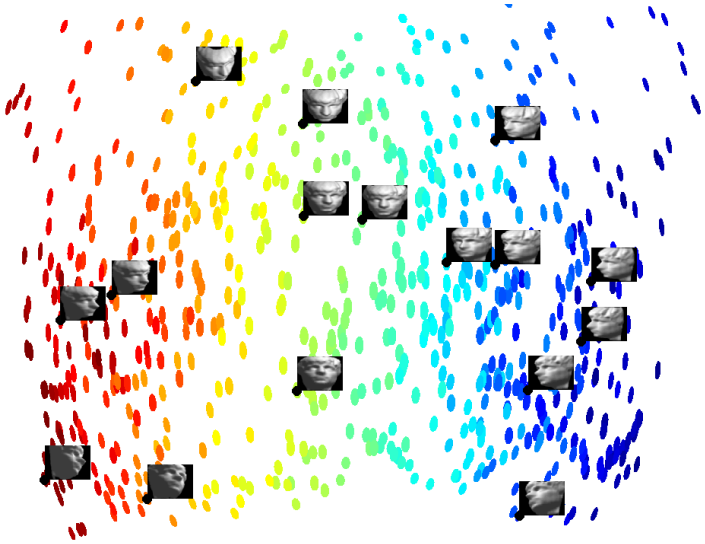
g is the Riemannian metric.

Dominique Perrault-Joncas

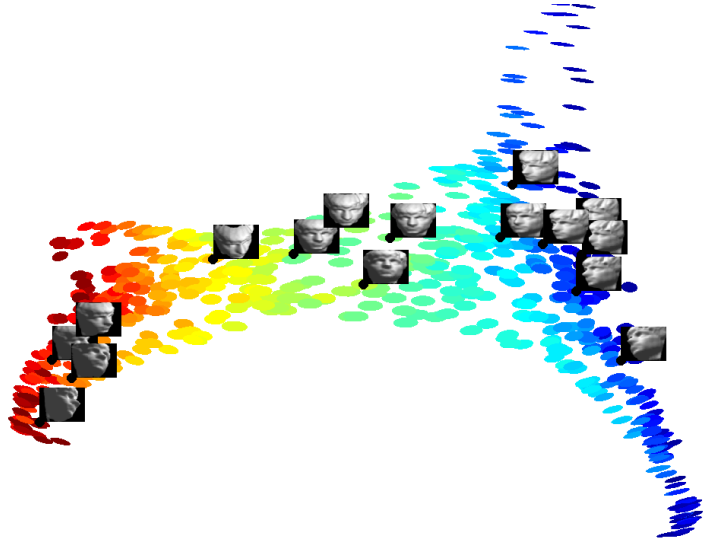
g for Sculpture Faces

- $n = 698$ with 64×64 gray images of faces
  - head moves up/down and right/left

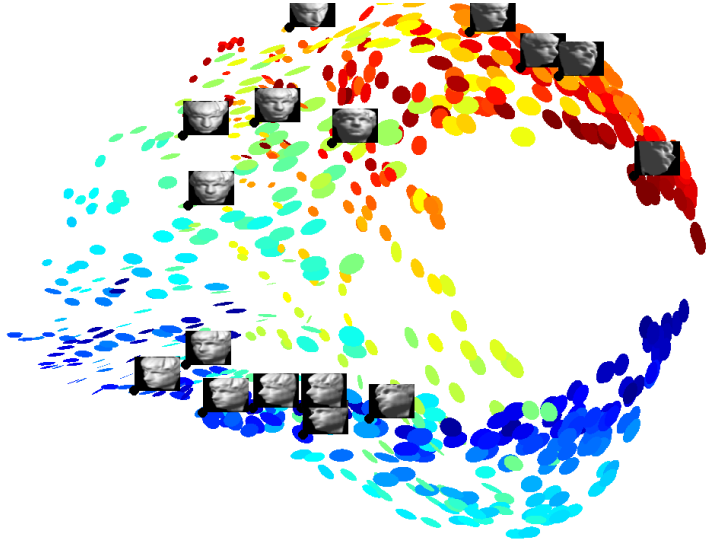




Isomap



LTSA



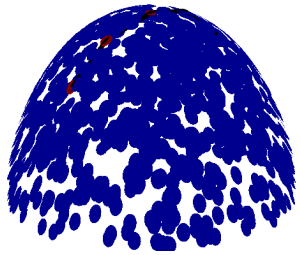
Laplacian Eigenmaps

Metric ML unifies embedding algorithms

- Distortions can now be corrected
  - implicitly: by integrating with the right length or volume element
  - locally: Locally Normalized Visualization
  - globally: Riemannian Relaxation
- Hence, all embedding algorithms preserve manifold geometry

Calculating distances in the manifold $\mathcal{M}$

Original



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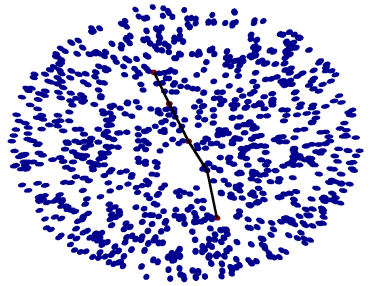

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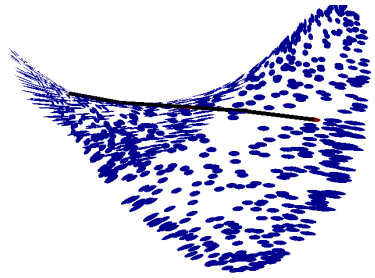
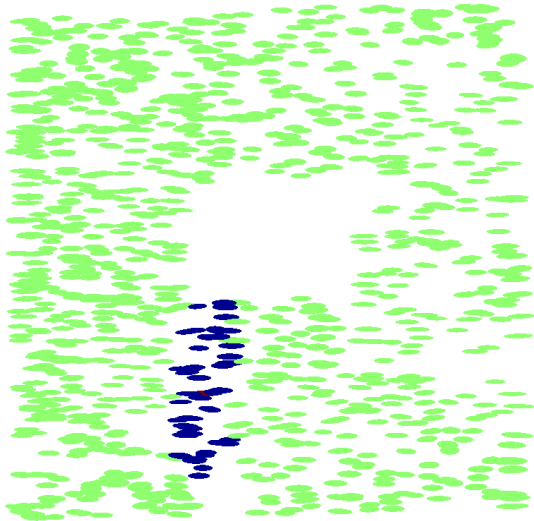


true distance $d = 1.57$

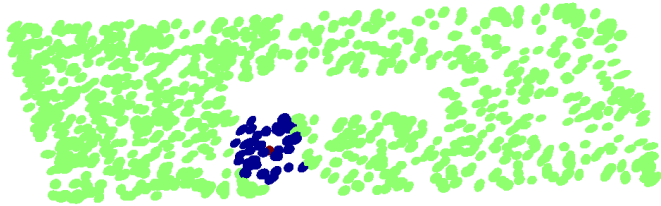
Embedding	$\|\|f(p) - f(p')\|\|$	Shortest Path $d_{\mathcal{G}}$	Metric $\hat{d}$	Rel. error
Original data	1.41	1.57	1.62	3.0%
Isomap $m = 2$	1.66	1.75	1.63	3.7%
LTSA $m = 2$	0.07	0.08	1.65	4.8%
LE $m = 2$	0.08	0.08	1.62	3.1%

$$l(c) = \int_a^b \sqrt{\sum_{ij} g_{ij} \frac{dx^i}{dt} \frac{dx^j}{dt}}\, dt,$$

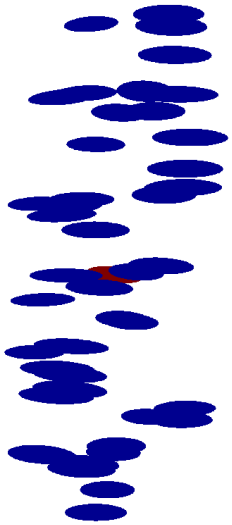
Locally Normalized Visualization

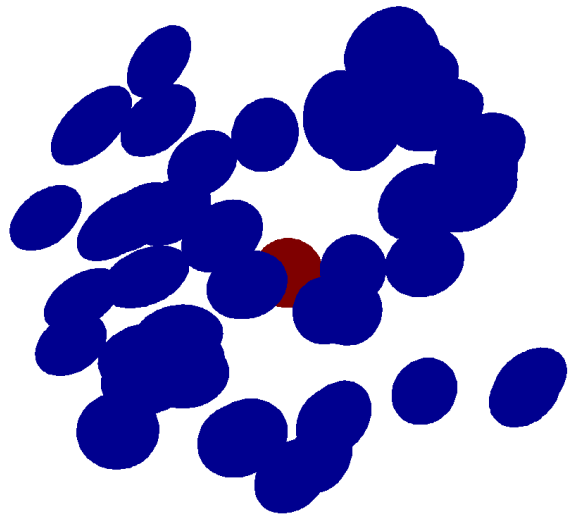


local neighborhood, unnormailzed

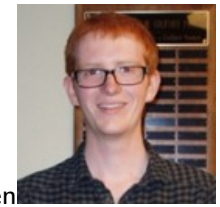


local neighborhood, Locally Normailzed





Riemannian Relaxation


James McQueen

Can we sometimes dispense with g?

Idea

- If embedding is isometric, then push-forward metric is identity

Idea, formalized

- Measure distortion from isometry by

$$\text{loss}(\phi) = \sum_{i=1}^{n} w_i ||G_i(\phi) - I_d||^2$$

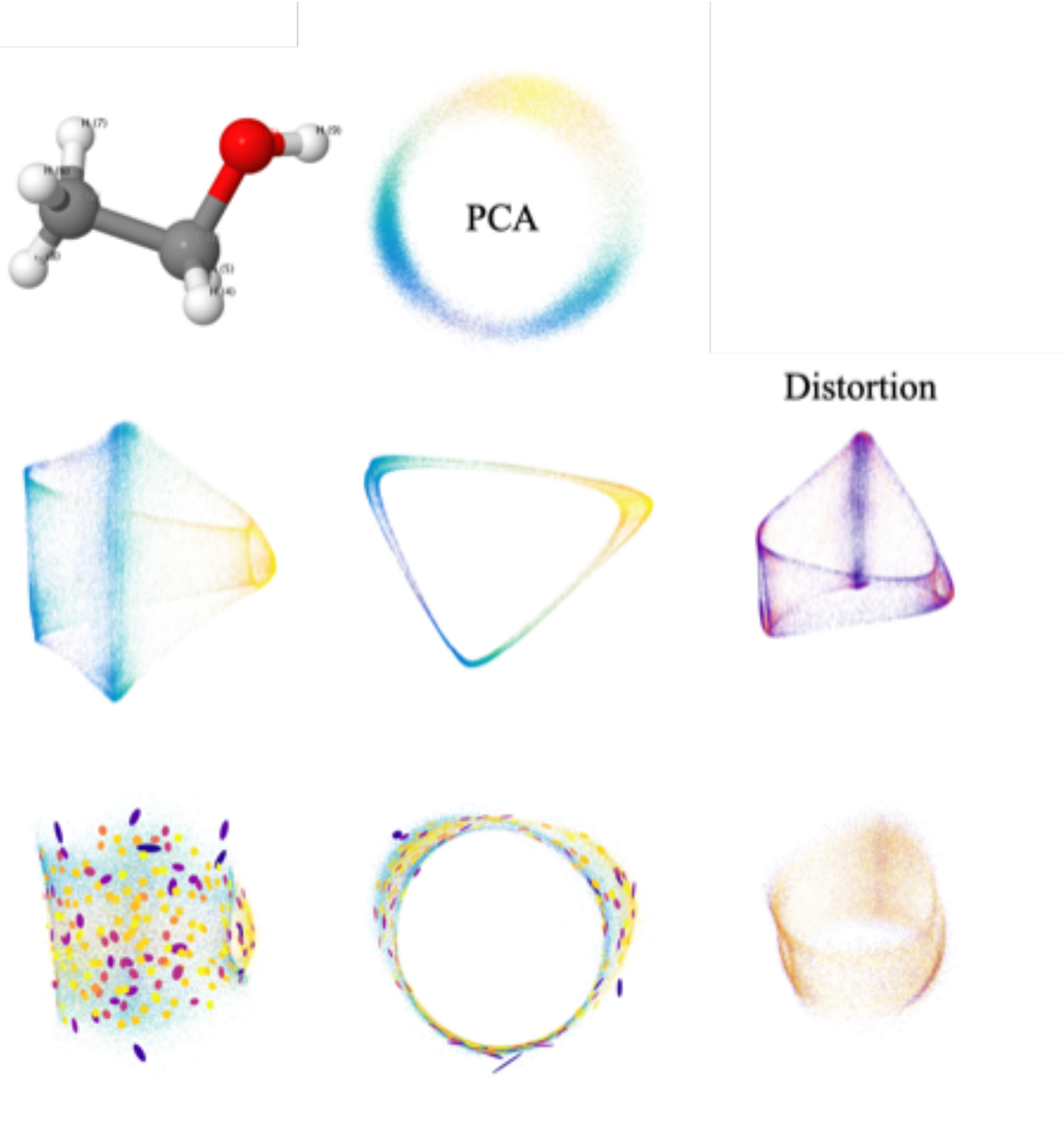
  - where G_i is Riemann metric estimate at point i
  - I_d is identity matrix
- Iteratively change embedding $\phi_{1:n}$ to minimize loss

Implementation

- Initialization with e.g Laplacian Eigenmaps
- Projected gradient descent to (local) optimum

Hourglass–Sphere

Riemannian Relaxation for Ethanol molecular configurations



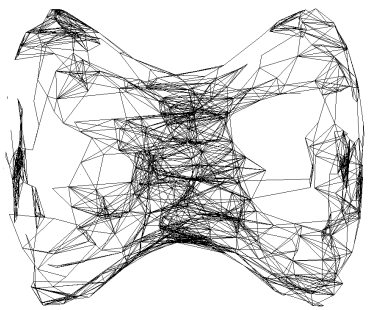
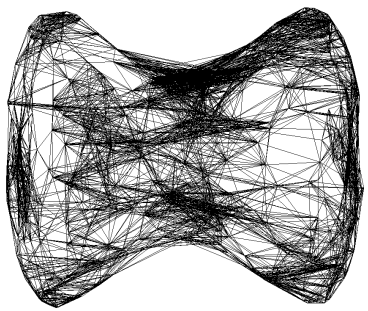
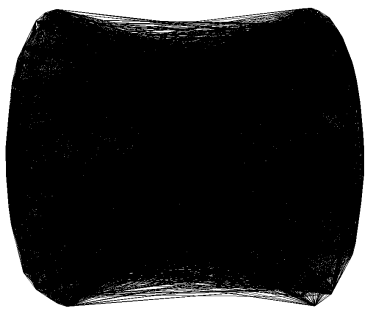
Self-consistent method of chosing ϵ

- Every manifold learning algorithm starts with a neighborhood graph
- Parameter $\sqrt{\epsilon}$
  - is neighborhood radius
  - and/or kernel banwidth

- For example, we use the kernel

  $K(p, p') = e^{-\frac{||p-p'||^2}{\epsilon}}$ if $||p - p'||^2 \leq \epsilon$ and 0 otherwise

- Problem: how to choose ϵ?

Our idea

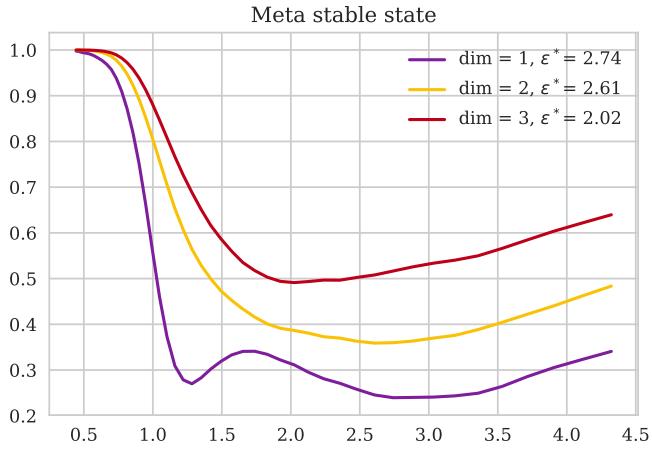
For given ϵ and data point p

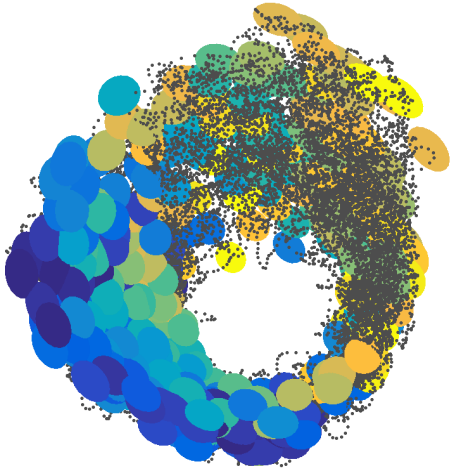
- Project neighbors of p onto tangent subspace
  - this "embedding" is approximately isometric to original data
- Calculate Laplacian $L(\epsilon)$) and estimate distortion $H_{\epsilon,p}$ at p
  - $H_{\epsilon,p}$ must be $\approx I_d$ identity matrix

- Idea: choose ϵ so that geometry encoded by L_ϵ is closest to data geometry
- Completely unsupervised

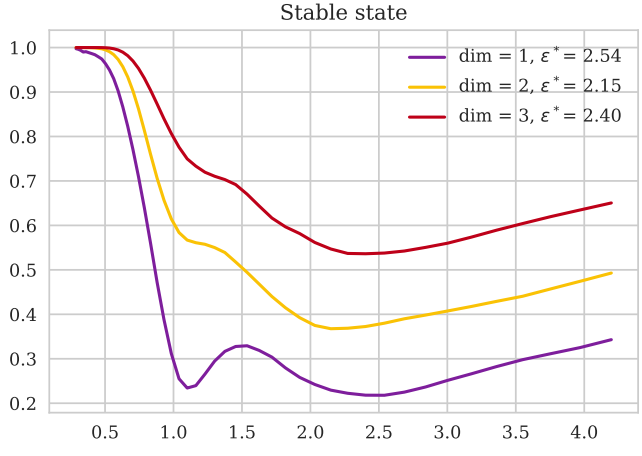
ϵ and distortion for aspirin

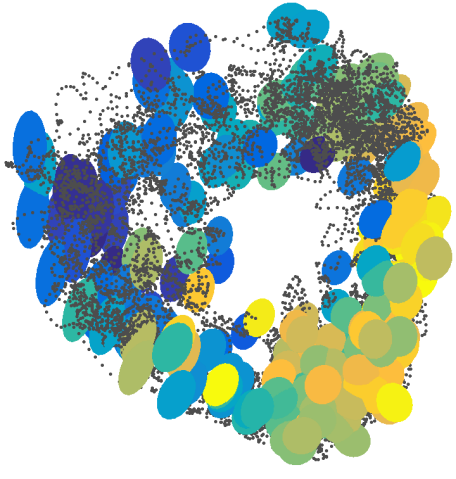
meta-stable cluster





stable cluster





Semisupervised learning benchmarks [Chapelle&al 08]

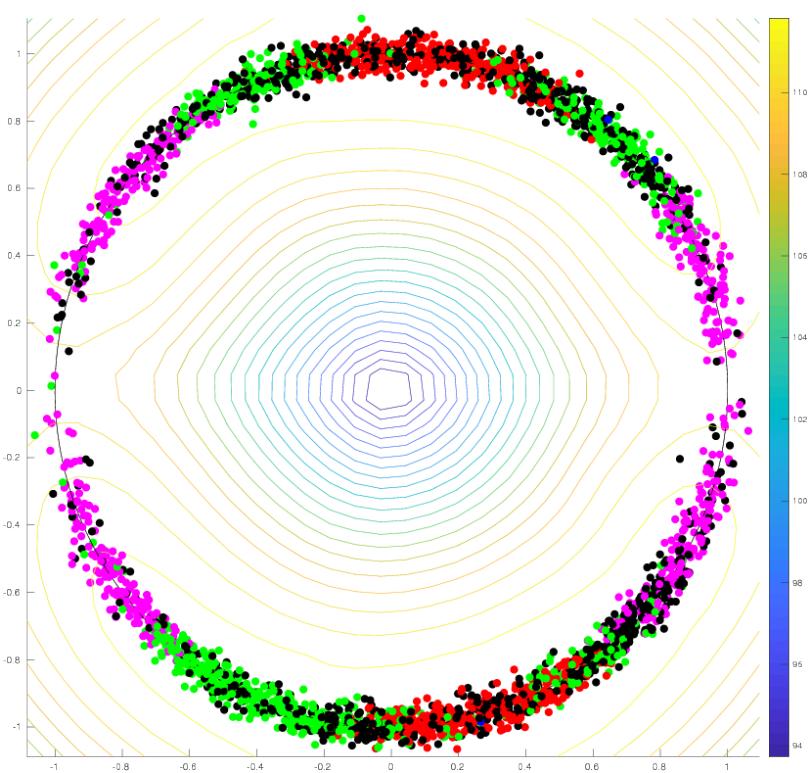
Multiclass classification problems

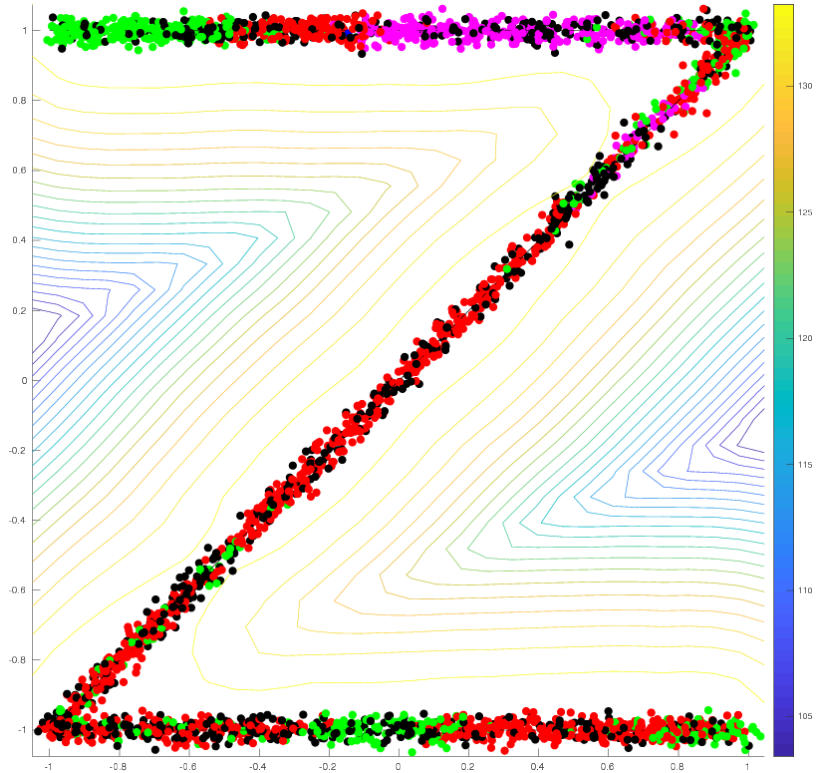
Classification error (%)

		Method	
Dataset	**CV**	[Chen&Buja]	**Ours**
Digit1	3.32	2.16	2.11
USPS	5.18	4.83	3.89
COIL	7.02	8.03	8.81
g241c	13.31	23.93	12.77
g241d	8.67	18.39	8.76
	superv.	fully unsupervised	

Outline

Finding filaments in high dimensions

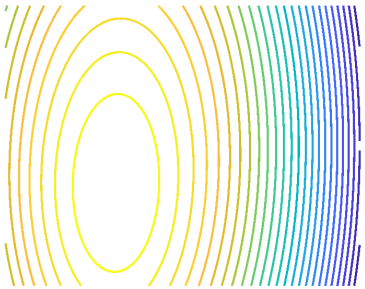




- data in $\mathbb{R}^D$ near a curve (or set of curves)
- wanted: track the ridge of the data density

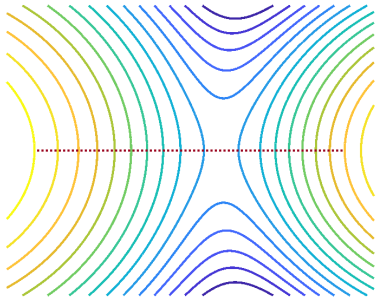
Mathematically,

Peak



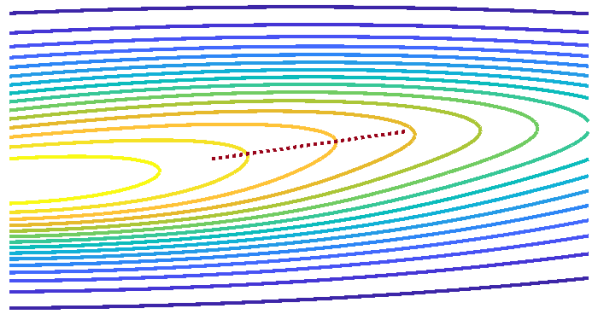
$\nabla p = 0$
$\nabla^2 p \prec 0$

Saddle



$\nabla p = 0$
$\nabla^2 p$ has $\lambda_1 > 0$,
$\lambda_{2:D} < 0$

Ridge



$\nabla p = 0$ in span$\{v_{2:D}\}$
v_j e-vector for λ_j, $j = 1 : D$
$\nabla^2 p$ has $\lambda_{2:D} < 0$

In other words, on a ridge

- $\nabla p \propto v_1$ direction of least negative curvature (LNC)
- $\nabla p, v_1$ are tangent to the ridge

SCMS Algorithm

SCMS = Subspace Constrained Mean Shift

Init any x^1 Density estimated by p =data $\star$ Gaussian kernel of width h

for $k = 1, 2, \ldots$

1. calculate $g^k \propto \nabla p(x^k)$ by Mean-Shift $\mathcal{O}(nD)$
2. $H^k = \nabla^2 p(x^k)$ $\mathcal{O}(nD^2)$
3. compute v_1 principal e-vector of H^k $\mathcal{O}(D^2)$
4. $x^{k+1} \leftarrow x^k + \text{Proj}_{v_1^\perp} g^k$ $\mathcal{O}(D)$

until convergence

- Algorithm SCMS finds 1 point on ridge; n restarts to cover all density
- Run time $\propto nD^2$/iteration
- Storage $\propto D^2$

Accelerating SCMS

- reduce dependency on n per iteration
  - index data (clustering, KD-trees, . . .)
  - we use FLANN [Muja,Lowe]
  - $n \leftarrow n'$ average number of neighbors
- reduce number iterations: track ridge instead of cold restarts
  - project ∇p on v_1 instead of $v_1^{\perp}$
  - tracking ends at critical point (peak or saddle)
- reduce dependence on D
  - $D^2 \leftarrow mD$ with $m \approx 5$

(Approximate) SCMS step without computing Hessian

Recall SCMS = Subspace Constrained Mean Shift

- Given $g \propto \nabla p(x)$
- Wanted $\text{Proj}_{v_1^\perp} g = (I - v_1 v_1^T) g$
- Need v_1

  principal e-vector of $H = -\nabla^2(\ln p)$ for $\lambda_1 =$ smallest e-value of H

  without computing/storing H

(Approximate) SCMS step without Hessian: First idea

- Wanted
  v_1 principal e-vector of $H = -\nabla^2(\ln p)$ for $\lambda_1 =$ smallest e-value of H

- First Idea
  1. use LBFGSS to approximate H^{-1} by $\hat{H^{-1}}$ of rank $2m$ [Nocedal & Wright]
  2. $\hat{v}_1$ obtained by $2m \times 2m$ SVD + Gram-Schmidt

- Run time $\propto Dm + m^2$ / iteration (instead of nD^2)
- Storage $\propto 2mD$ for $\{x^{k-l} - x^{k-l-1}\}_{l=1:m}$, $\{g^{k-l} - g^{k-l-1}\}_{l=1:m}$

- Problem v_1 too inaccurate to detect stopping

(Approximate) SCMS step without Hessian: Second idea

- Wanted
  v_1 principal e-vector of $H = -\nabla^2(\ln p)$ for $\lambda_1 =$ smallest e-value of H

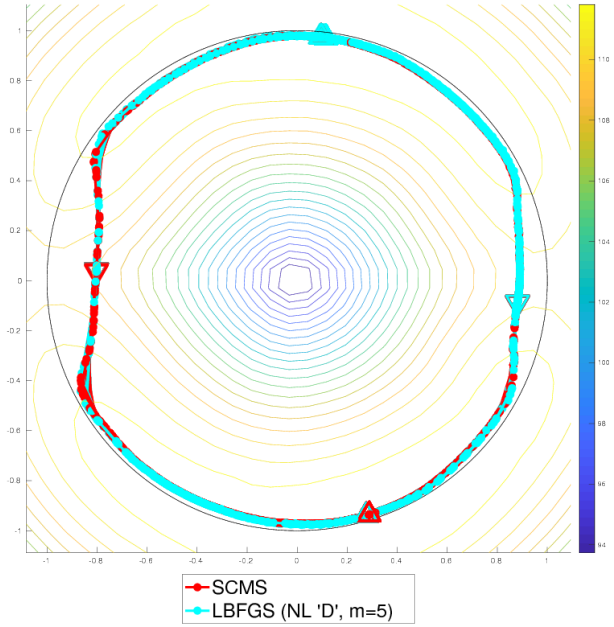
- Second Idea
  1. store $\{x^{k-l} - x^{k-l-1}\}_{l=1:m} \cup \{g^{k-l} - g^{k-l-1}\}_{l=1:m} = V$
  2. minimize $v^T H v$ s.t. $v \in \text{span } V$ where H is exact Hessian

- Possible because $H = \frac{1}{\sum c_i} \sum c_i u_i u_i^T - gg^T - \frac{1}{h^2} I$ with $c_{1:n}, u_{1:n}$ computed during Mean-Shift

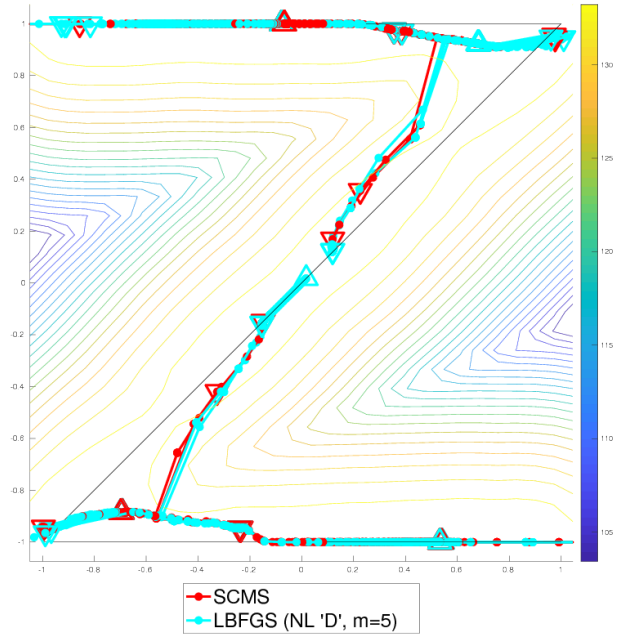
- Run time $\propto n' Dm + m^2$ / iteration (instead of nD^2)
- Storage $\propto 2mD$

- Much more accurate

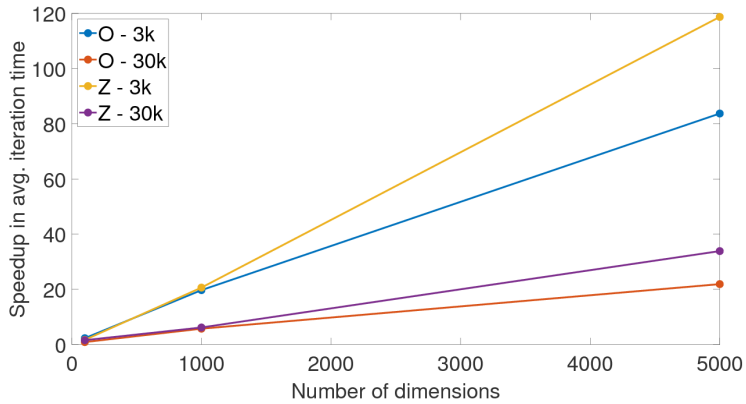
Principal curves SCMS vs. L-SCMS

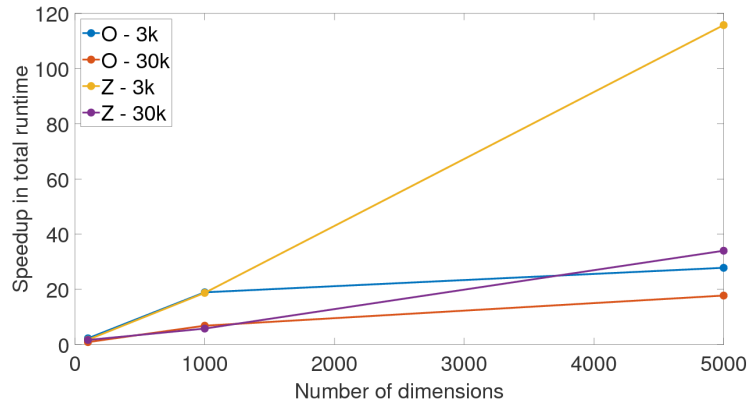


Speedup per iteration



Total speedup w.r.t. SCMS





For large n neighbor search dominates

Scaling: Statistical viewpoint

- Manifold estimation is non-parametric
  - model becomes more complex when more data available
  - provided ϵ kernel bandwidth decreases slowly with n
- Rates of convergence for manifold estimation as $n \longrightarrow \infty$
  - rate of Laplacian $n^{-\frac{1}{d+6}}$ [Singer 06], and of its eigenvectors $n^{-\frac{2}{(5d+6)(d+6)}}$ [Wang 15]
  - minimax rate of manifold learning $n^{-\frac{2}{d+2}}$ [Genovese et al. 12]
- Compare with rate of convergence for parametric estimation $n^{-\frac{1}{2}}$

- Hence,
  - for non-parametric models, accuracy improves very slowly with n
  - manifold learning **REQUIRES** big data

Scaling: Computational viewpoint

Laplacian Eigenmaps revisited

1. Construct similarity matrix

   $S = [S_{pp'}]_{p,p' \in \mathcal{D}}$ with $S_{pp'} = e^{-\frac{1}{\epsilon}||p-p'||^2}$

   iff p, p' neighbors

2. Construct Laplacian matrix
   $L = I - T^{-1}S$ with $T = \mathrm{diag}(S\mathbf{1})$
3. Calculate $\psi^{1\ldots m}$ = eigenvectors of L
   (smallest eigenvalues)
4. coordinates of $p \in \mathcal{D}$ are
   $(\psi^1(p), \ldots \psi^m(p))$

Nearest neighbor search in high dimensions

Sparse Matrix Vector multiplication

Principal eigenvectors

- of sparse, symmetric, (well conditioned) matrix

- With bandwidth ϵ estimation
  - overhead not larger than single embedding

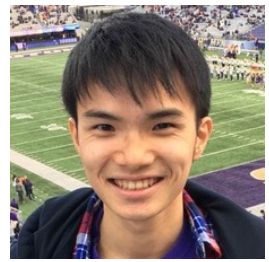
Manifold Learning and Clustering with millions of points

https://www.github.com/megaman

James McQueen | Jake VanderPlas | Jerry Zhang | Grace Telford | Yu-chia Chen





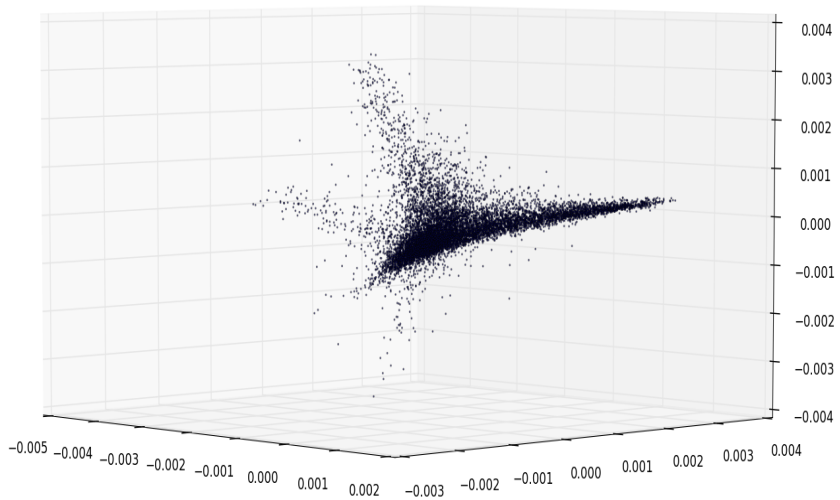


- Implemented in python, compatible with scikit-learn
- Statistical/methodological novelty
  - implements recent advances in the statistical understanding of manifold learning, e.g radius based neighborhoods [Hein 2007], consistent graph Laplacians [Coifman 2006], Metric learning
- Designed for performance
  - sparse representation as default
  - incorporates state of the art FLANN package[1]
  - uses amp, lobpcg fast sparse eigensolver for SDP matrices
  - exposes/caches intermediate states (e.g. data set index, distances, Laplacian, eigenvectors)
- Designed for extensions

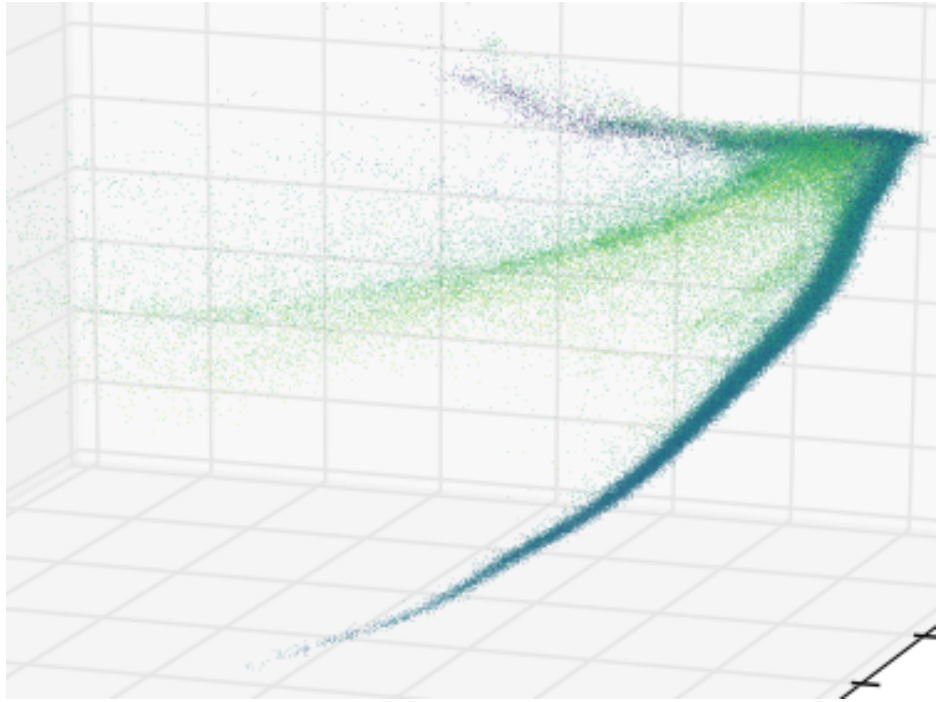
[1] Fast Approximate Nearest Neighbor search

Scalable Manifold Learning in python with megaman

https://www.github.com/mmp2/megaman



English words and phrases taken from Google news (3,000,000 phrases originally represented in 300 dimensions by the Deep Neural Network word2vec [Mikolov et al])



Main sample of galaxy spectra from the Sloan Digital Sky Survey (675,000 spectra originally in 3750 dimensions).

preprocessed by Jake VanderPlas and Grace Telford

megaman on Theta

- Parallelism support (OpenMP)
  - Nearest neighbors (brute force)
  - Eigenproblem: SLEPc added
- Commonly used kernels for MD included and tested
  - SOAP, SLATM
- (in progress) Highly parallelizable random projection based graph Laplacian construction

Computational challenges ahead

- Computing the neighborhood graphs
  - K-nearest neighbors vs. radius neighbors
- Partitioning the data
- Estimation of d and embedding dimension m in preprocessing

K-nearest neighbors vs. radius neighbors

- k-nearest neighbors graph: each node has degree k
- radius neighbors graph: p, p' neighbors iff $||p - p'|| \leq r$

- Does it matter?

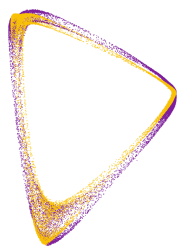
K-nearest neighbors vs. radius neighbors

- k-nearest neighbors graph: each node has degree k
- radius neighbors graph: p, p' neighbors iff $||p - p'|| \leq r$

- Does it matter?

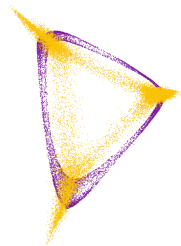
- Yes, for estimating the Laplacian and distortion
  - Why? [Hein 07, Coifman 06, Ting 10, . . .] k-nearest neighbor Laplacians do not converge to Laplace-Beltrami operator Δ
  - but to $\Delta + 2\nabla(\log p) \cdot \nabla$ (bias due to non-uniform sampling)
- Renormalization of Laplacian also necessary

configurations of ethanol $d = 2$



Radius k-NN

K-nearest neighbor



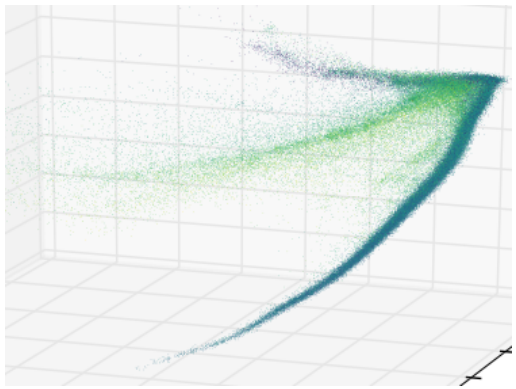
Renormalized Normalized

without renormalization

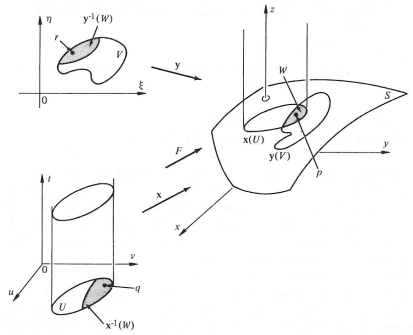
Challenge: radius neighborhood graph

- Scalable radius neighborhood graph construction needed
  - existing scalable software (FLANN) finds k-nearest neighbors
  - in progress: scalable approximate radius neighbors search by Locality Sensitive Hashing [Charikar, Siminelakis 18]

- Laplacian less tractable numerically
  - number of non-zeros in each row depends on data density



Challenge: data partitioning

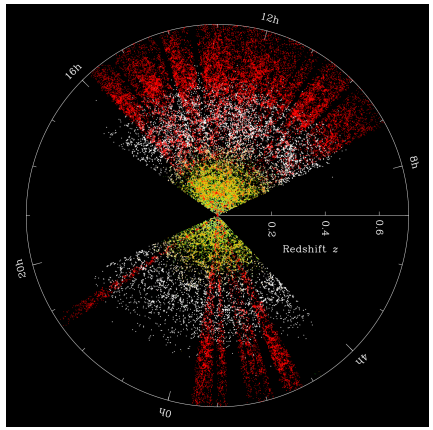


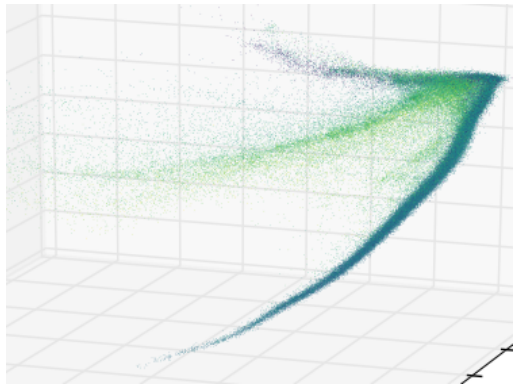
- When data does not fit in memory
- Manifold framework naturally suited

- Problem: data must be (re)organized by locality
  - a point and its neighbors are in the same partition
  - by e.g. clustering

- No systematic work in this area yet

www.sdss.org



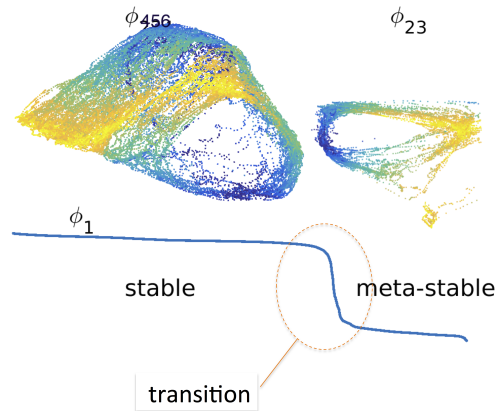


Estimating d and m before embedding

- d is intrinsic dimension
  - estimating d not completely solved
- m is embedding dimension
  - $m = \#$ coordinates needed to embed data $= \#$ eigenvectors of L
- Theoretically
  - $m \leq 2d$ to embed $\mathcal{M}$ continuously
  - $m \sim d^3$ to embed $\mathcal{M}$ isometrically
- Practically
  - (some eigenfunctions are "harmonics" of previous eigenfunctions)
  - data contains K clusters

    $\leq K - 1$ additional dimensions needed
  - data is union of several manifolds

    $m \leq m_1 + m_2 + \ldots$
- Chicken and egg problem `[ lambda, V ] = eigs( L, m )`
  - need to analyze data to find `m`!
- Heuristics: start with clustering subset of data, locally estimate d, ...
- Open?
- estimate principal eigenvalues and eigengaps before `eigs()`



Manifold learning for sciences and engineering

Manifold learning should be like PCA

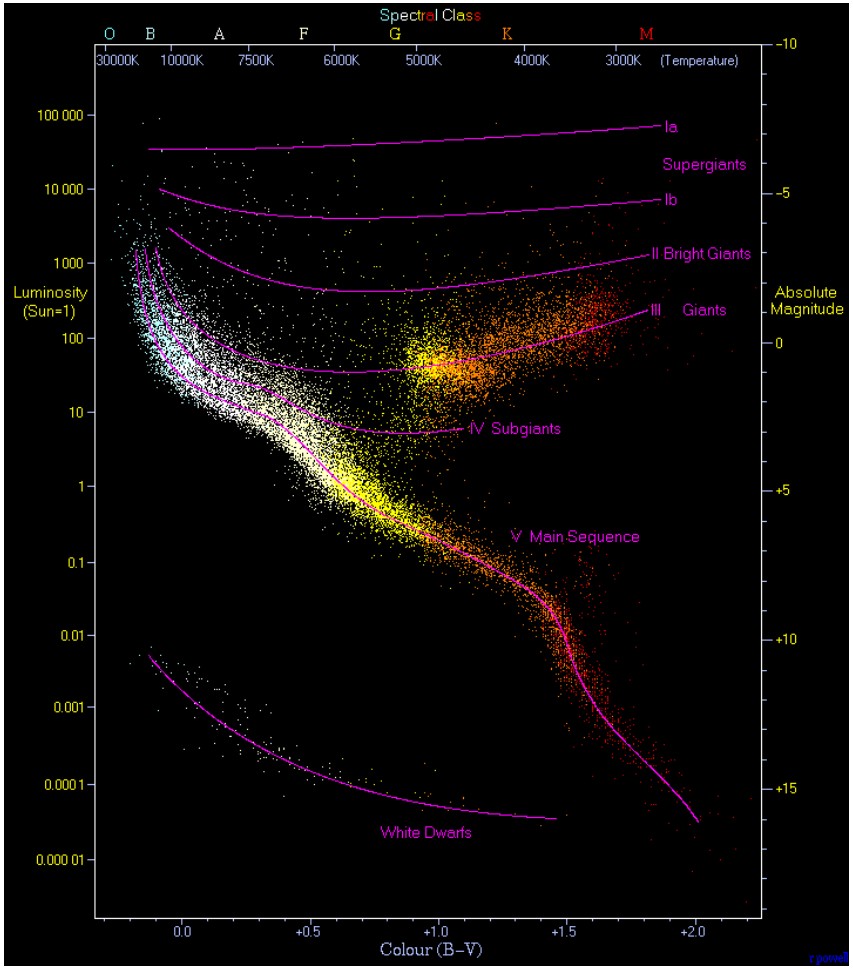
- tractable/scalable
- "automatic" – minimal burden on human
- first step in data processing pipe-line

  should not introduce artefacts

More than PCA

- estimate richer geometric/topological information
- dimension
- borders, stratification
- clusters
- Morse complex
- meaning of coordinates/continuous parametrization

Manifold Learning for engineering and the sciences



- manifold learning as preprocessing for other tasks (learning the basis)
- "physical laws through machine learning"
- scientific discovery by quantitative/statistical data analysis

Samson Koelle, Yu-Chia Chen, Hanyu Zhang, Alon Milchgrub
Dominique-Perrault Joncas (Google), James McQueen (Amazon)

Jacob VanderPlas, Grace Telford (UW Astronomy)
Jim Pfaendtner (UW), Chris Fu (UW)
A. Tkatchenko (Luxembourg), S. Chmiela (TU Berlin), A. Vasquez-Mayagoitia (ALCF)

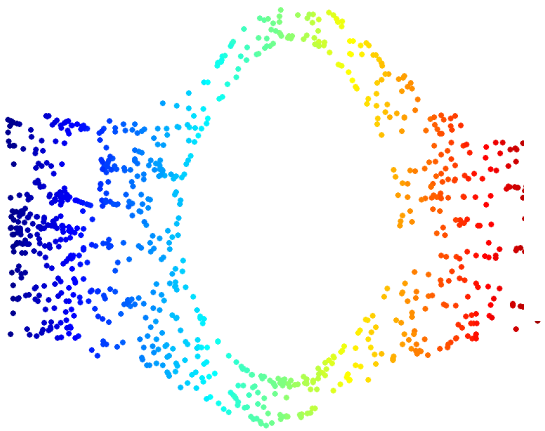
Thank you

Preserving topology vs. preserving (intrinsic) geometry

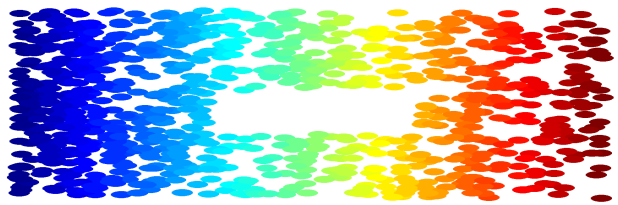
- Algorithm maps data $p \in \mathbb{R}^D \longrightarrow \phi(p) = x \in \mathbb{R}^m$

- Mapping $\mathcal{M} \longrightarrow \phi(\mathcal{M})$ is diffeomorphism
  preserves topology
  often satisfied by embedding algorithms
- Mapping ϕ preserves
  - distances along curves in $\mathcal{M}$
  - angles between curves in $\mathcal{M}$
  - areas, volumes
    . . . i.e. ϕ is isometry
    For most algorithms, in most cases, ϕ is not isometry

Preserves topology



Preserves topology + intrinsic geometry



Previous known results in geometric recovery

Positive results

- Nash's Theorem: Isometric embedding is possible.
- Diffusion Maps embedding is isometric in the limit [Besson 1994]
- algorithm based on Nash's theorem (isometric embedding for very low d) [Verma 11]
- Isomap [Tennenbaum,]recovers flat manifolds isometrically
- Consistency results for Laplacian and eigenvectors
  - [Hein & al 07,Coifman & Lafon 06, Singer 06, Ting & al 10, Gine & Koltchinskii 06]
  - imply isometric recovery for LE, DM in special situations

Negative results

- obvious negative examples
- No affine recovery for normalized Laplacian algorithms [Goldberg&al 08]
- Sampling density distorts the geometry for LE [Coifman& Lafon 06]

Our approach: Metric Manifold Learning

[Perrault-Joncas,M 10]

Given

- mapping ϕ that preserves topology

true in many cases

Objective

- augment ϕ with geometric information g so that (ϕ, g) preserves the geometry

g is the Riemannian metric.

Dominique Perrault-Joncas

The Riemannian metric g

Mathematically

- $\mathcal{M}$ = (smooth) manifold
- p point on $\mathcal{M}$
- $T_p\mathcal{M}$ = **tangent subspace** at p
- g = Riemannian metric on $\mathcal{M}$

  g defines inner product on $T_p\mathcal{M}$

$$< v, w >= v^T g_p w \quad \text{for } v, w \in T_p\mathcal{M} \text{ and for } p \in \mathcal{M}$$

  - g is symmetric and positive definite tensor field
  - g also called first fundamental form
  - $(\mathcal{M}, g)$ is a Riemannian manifold

Computationally at each point $p \in \mathcal{M}$, g_p is a positive definite matrix of rank d

All (intrinsic) geometric quantities on $\mathcal{M}$ involve g

- Volume element on manifold

$$Vol(W) = \int_W \sqrt{\det(g)} dx^1 \dots dx^d .$$

- Length of curve c

$$l(c) = \int_a^b \sqrt{\sum_{ij} g_{ij} \frac{dx^i}{dt} \frac{dx^j}{dt}} dt,$$

- Under a change of parametrization, g changes in a way that leaves geometric quantities invariant

- Current algorithms estimate $\mathcal{M}$
- This talk: estimate g along with $\mathcal{M}$

  (and in the same coordinates)

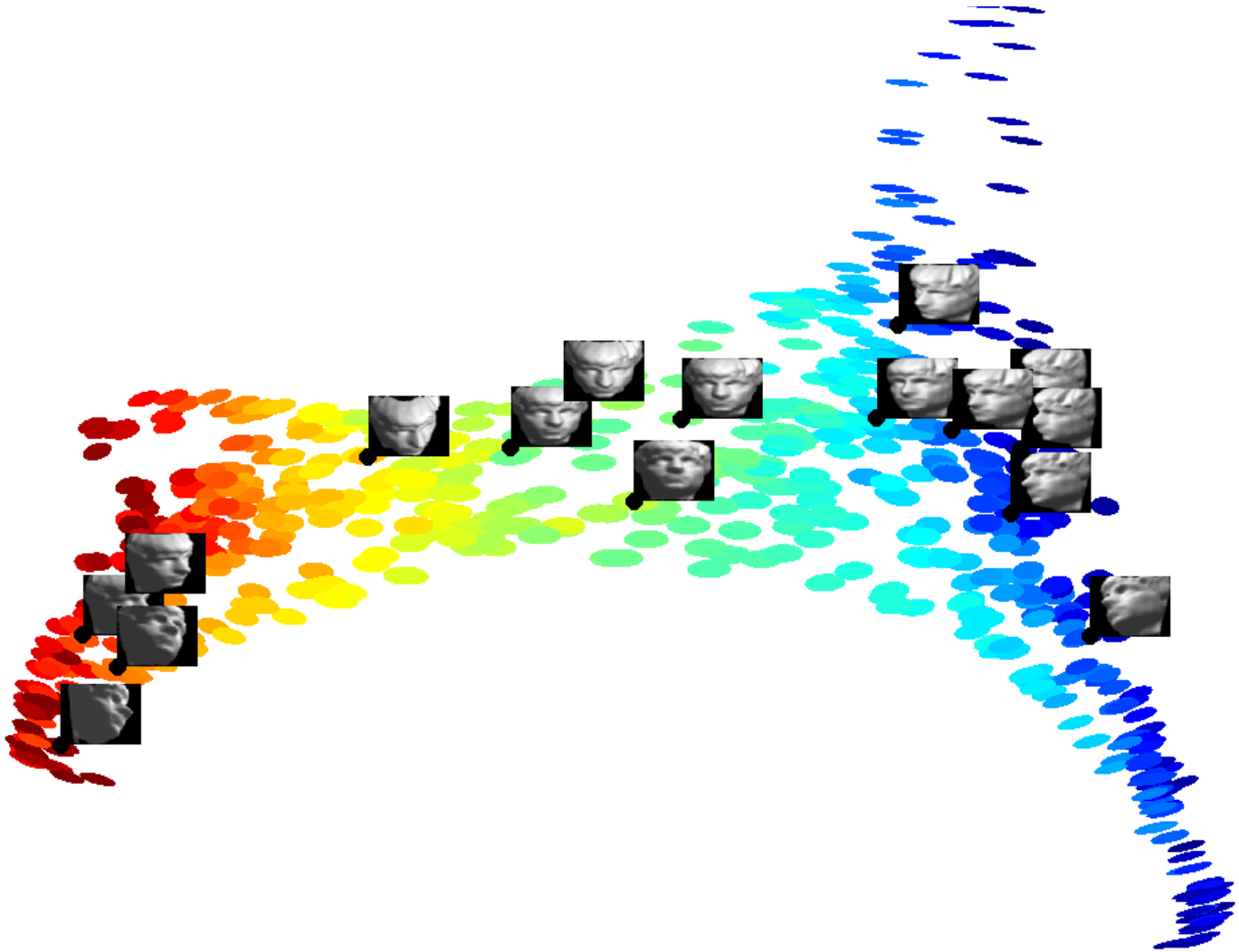
Problem formulation

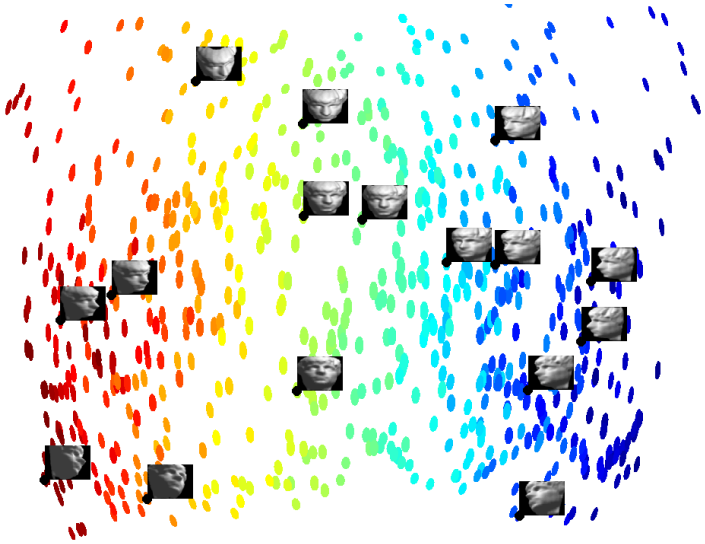
- Given:
  - data set $\mathcal{D} = \{p_1, \dots p_n\}$ sampled from manifold $\mathcal{M} \subset \mathbb{R}^D$
  - embedding $\{ x_i = \phi(p_i),\ p_i \in \mathcal{D} \}$
    by e.g LLE, Isomap, LE, ...
- Estimate $G_i \in \mathbb{R}^{m \times m}$ the (pushforward) Riemannian metric for $p_i \in \mathcal{D}$
  in the embedding coordinates ϕ

- The embedding $\{x_{1:n}, G_{1:n}\}$ will preserve the geometry of the original data

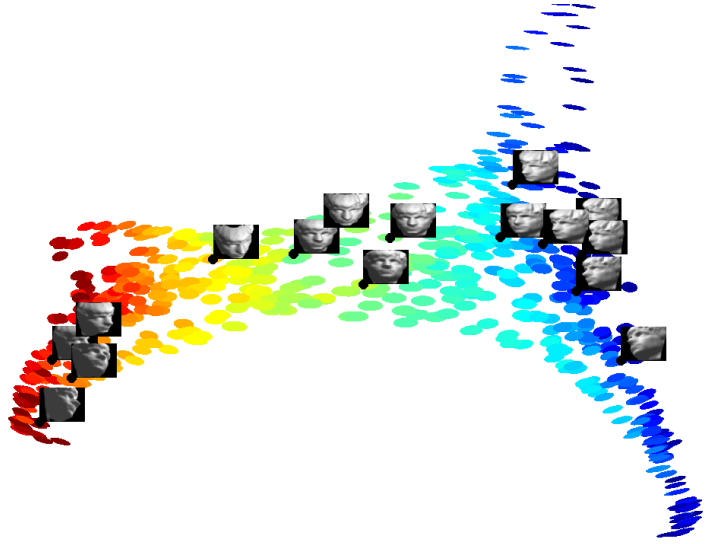
g for Sculpture Faces

- $n = 698$ gray images of faces in $D = 64 \times 64$ dimensions
  - head moves up/down and right/left

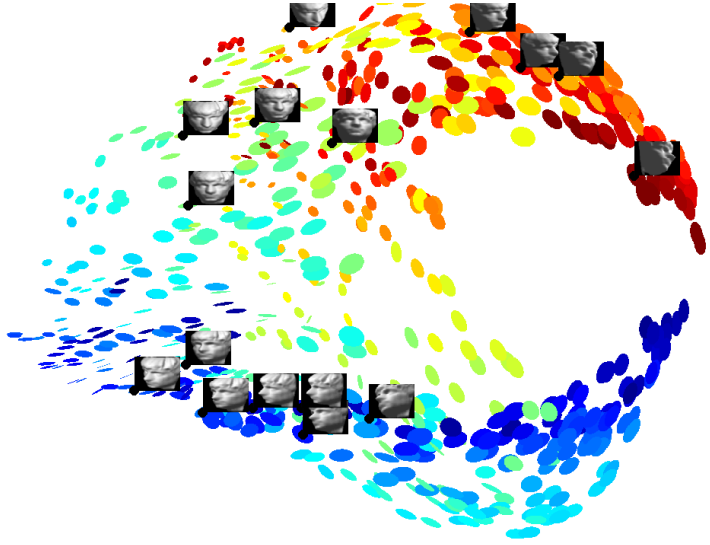




Isomap



LTSA



Laplacian Eigenmaps

Relation between g and Δ

- $\Delta =$ Laplace-Beltrami operator on $\mathcal{M}$
  - $\Delta = \mathrm{div} \cdot \mathrm{grad}$
  - on C^2, $\Delta f = \sum_j \frac{\partial^2 f}{\partial x_j^2}$
  - on weighted graph with similarity matrix S, and $t_p = \sum_{pp'} S_{pp'}$, $\Delta = \mathrm{diag}\{t_p\} - S$

Proposition 1 (Differential geometric fact)

$$\Delta f = \sqrt{\det(h)} \sum_l \frac{\partial}{\partial x^l} \left(\frac{1}{\sqrt{\det(h)}} \sum_k h_{lk} \frac{\partial}{\partial x^k} f \right) ,$$

Estimation of g

Proposition 2 (Main Result 1)

Let Δ be the Laplace-Beltrami operator on $\mathcal{M}$. Then

$$h_{ij}(p) = \frac{1}{2}\Delta(\phi_i - \phi_i(p))(\phi_j - \phi_j(p))|_{\phi_i(p),\phi_j(p)}$$

where $h = g^{-1}$ (matrix inverse) and $i, j = 1, 2, \ldots m$ are embedding dimensions

Intuition:

- at each point $p \in \mathcal{M}$, $g(p)$ is a $d \times d$ matrix
- apply Δ to embedding coordinate functions $\phi_1, \ldots \phi_m$
- this produces $g^{-1}(p)$ in the given coordinates
- our algorithm implements matrix version of this operator result
- consistent estimation of Δ is solved [Coifman&Lafon 06,Hein&al 07]

Algorithm to Estimate Riemann metric g (Main Result 2)

Given dataset $\mathcal{D}$

1. Preprocess (construct neighborhood graph, ...)
2. Find an embedding ϕ of $\mathcal{D}$ into $\mathbb{R}^m$
3. Estimate discretized Laplace-Beltrami operator $L \in \mathbb{R}^{n \times n}$
4. Estimate $H_p = G_p^{-1}$ and $G_p = H_p^{\dagger}$ for all $p \in \mathcal{D}$

Output (ϕ_p, G_p) for all p

Algorithm to Estimate Riemann metric g (Main Result 2)

Given dataset $\mathcal{D}$

1. Preprocessing (construct neighborhood graph, ...)
2. Find an embedding ϕ of $\mathcal{D}$ into $\mathbb{R}^m$
3. Estimate discretized Laplace-Beltrami operator L
4. Estimate $H_p = G_p^{-1}$ and $G_p = H_p^\dagger$ for all p
   - 4.1 For $i, j = 1 : m$,
     $$H^{ij} = \frac{1}{2}\left[L(\phi_i * \phi_j) - \phi_i * (L\phi_j) - \phi_j * (L\phi_i)\right]$$
     where $X * Y$ denotes elementwise product of two vectors $X, Y \in \mathbb{R}^N$
   - 4.2 For $p \in \mathcal{D}$, $H_p = [H_p^{ij}]_{ij}$ and $G_p = H_p^\dagger$

Output (ϕ_p, G_p) for all p

Algorithm MetricEmbedding

Input data $\mathcal{D}$, m embedding dimension, ϵ resolution

1. Construct neighborhood graph p, p' neighbors iff $||p - p'||^2 \leq \epsilon$
2. Construct similary matrix
   $S_{pp'} = e^{-\frac{1}{\epsilon}||p-p'||^2}$ iff p, p' neighbors, $S = [S_{pp'}]_{p,p' \in \mathcal{D}}$
3. Construct (renormalized) Laplacian matrix [Coifman & Lafon 06]
   3.1 $t_p = \sum_{p' \in \mathcal{D}} S_{pp'}$, $T = \operatorname{diag} t_p$, $p \in \mathcal{D}$
   3.2 $\tilde{S} = I - T^{-1} S T^{-1}$
   3.3 $\tilde{t}_p = \sum_{p' \in \mathcal{D}} \tilde{S}_{pp'}$, $\tilde{T} = \operatorname{diag} \tilde{t}_p, p \in \mathcal{D}$
   3.4 $P = \tilde{T}^{-1} \tilde{S}$.
4. Embedding $[\phi_p]_{p \in \mathcal{D}} = \text{GenericEmbedding}(\mathcal{D}, m)$
5. Estimate embedding metric H_p at each point
   denote $Z = X * Y$, $X, Y \in \mathbb{R}^N$ iff $Z_i = X_i Y_i$ for all i
   5.1 For $i, j = 1 : m$, $H^{ij} = \frac{1}{2}\left[P(\phi_i * \phi_j) - \phi_i * (P\phi_j) - \phi_j * (P\phi_i)\right]$ (column vector)
   5.2 For $p \in \mathcal{D}$, $\tilde{H}_p = [H_p^{ij}]_{ij}$ and $H_p = \tilde{H}_p^{\dagger}$

Ouput $(\phi_p, H_p)_{p \in \mathcal{D}}$

Metric Manifold Learning summary

Metric Manifold Learning = estimating (pushforward) Riemannian metric G_i along with embedding coordinates x_i

Why useful

- Measures local distortion induced by any embedding algorithm
  $G_i = I_d$ when no distortion at p_i
- Algorithm independent geometry preserving method
- Outputs of different algorithms on the same data are comparable
- Models built from compressed data are more interpretable

Applications

- Correcting distortion
  - Integrating with the local volume/length units based on G_i
  - Riemannian Relaxation (coming next)
- Estimation of neighborhood radius [Perrault-Joncas,M,McQueen NIPS17]
- and of intrinsic dimension d (variant of [Chen,Little,Maggioni,Rosasco])
- Accelerating Topological Data Analysis (in progress)