Introduction, Difficulties and Perspectives Tutorial on Manifold Learning with Medical Images





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September 22, 2011

Manifold Learning Three seminal algorithms

Common Practical Problems

Breaking the implicit assumptions Determining the parameters Mapping new points Large data-sets

Conclusions



GOAL: dimensionality reduction

- For data lying on (or close to) a manifold ...
- find a new representation ...
- that is low dimensional ...
- allowing a more efficient processing of the data.

Isomap

- Locally Linear Embedding (LLE)
- Laplacian Eigenmaps (LapEigs)

[> Joshua Tenenbaum, Vin de Silva, John Langford. A Global Geometric Framework for Nonlinear Dimensionality Reduction, *Science*, 2000.]

[> Sam Roweis, Lawrence Saul, Nonlinear Dimensionality Reduction by Locally Linear Embedding, *Science*, 2000.]

[> M. Belkin, P. Niyogi. Laplacian Eigenmaps for Dimensionality Reduction and Data Representation. *Neural Computation*, June 2003; 15 (6):1373-1396.]



The data is assumed to lie on or close to a Manifold



Access is given only to a number of **samples** of the Manifold (data points)



Build a **neighborhood graph** using the samples.

The graph **approximates** the manifold



To complete the graph by determining **weights** on the edges (between every pair of neighbor nodes). The graph can then be expressed in a **matrix form**:

$\mathbf{W} =$	- 0	$\mathbf{w_{1,2}}$	$w_{1,3}$	0	0	0	0	0	0	0	0	0	0	0
	$w_{1,2}$	0	W2.3	$w_{2,4}$	$w_{2.5}$	0	0	0	0	0	0	0	0	0
	w1.3	$w_{2,3}$	0	0	W3.5	0	0	0	0	0	0	0	0	0
	0	W2.4	0	0	W4.5	0	W4.7	$w_{4.8}$	0	0	0	0	0	0
	0	W2.5	W3.5	w4.5	0	W5.6	W5.7	0	0	0	0	0	0	0
	0	0	0	0	W5.6	0	W6.7	0	0	0	0	0	0	0
	0	0	0	W4.7	W5.7	W6.7	0	W7.8	W7.9	0	0	0	0	0
	0	0	0	W4.8	0	0	W7.8	0	W8.9	W8.10	0	0	0	0
	0	0	0	0	0	0	W7.9	W8.9	0	W9,10	0	0	w _{9,13}	w9,14
	0	0	0	0	0	0	0	W8.10	W9.10	0	w10,11	$w_{10,12}$	0	0
	0	0	0	0	0	0	0	0	0	w10.11	0	W11.12	w11.13	0
	0	0	0	0	0	0	0	0	0	w10,12	$w_{11,12}$	0	W12.13	0
	0	0	0	0	0	0	0	0	W 9,13	0	w11,13	$w_{12,13}$	0	w13.14
	0	0	0	0	0	0	0	0	w9,14	0	0	0	w13.14	0



Find \mathcal{Y}^{\star} by optimizing some cost function \mathcal{J}

 $\mathcal{Y}^{\star} = \min_{\mathcal{Y}} \mathcal{J}(\mathcal{T}(\mathbf{W}), \mathcal{Y})$

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In spectral methods the optimization of $\mathcal J$ can be expressed in the form:

 $\min_{\mathbf{v}_l} \frac{\mathbf{v}_l^\top \mathcal{T}(\mathbf{W}) \mathbf{v}_l}{\mathbf{v}_l^\top \mathbf{v}_l} \quad \forall l \in \{1, \dots, d\} \quad (\text{Rayleigh Quotient})$





Isomap

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Algorithm: Locally Linear Embedding (LLE)

[> Sam Roweis & Lawrence Saul. Nonlinear Dimensionality Reduction by Locally Linear Embedding, Science, 2000.]



Algorithm: Locally Linear Embedding (LLE)



Find the new coordinates that preserve the reconstructing weights

$$\mathcal{J}(\mathbf{W}, \mathcal{Y}) = \sum_{\mathbf{y}_i} ||\mathbf{y}_i - \sum_{\mathbf{y}_j \in \mathcal{N}(\mathbf{y}_i)} w_{ij} \mathbf{y}_j||^2$$

Using the transformation:

$$\mathcal{T}(\mathbf{W}) = (\mathbf{I} - \mathbf{W})^{\top} (\mathbf{I} - \mathbf{W})$$

The solution is given by the d + 1 eigenvectors of $\mathcal{T}(\mathbf{W})$ corresponding to the smallest eigenvalues.

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Algorithm: Laplacian Eigenmaps (LapEig)



- 1. Neighborhood graph with similarity values w_{ij} (binary or Gaussian $w_{ij} = \exp(-\frac{||\mathbf{x}_i - \mathbf{x}_j||^2}{\sigma^2})$)
- 2. Define a cost that preserves neighborhood relations: if $\mathbf{x}_j \in \mathcal{N}(\mathbf{x}_i) \to \mathbf{y}_j \in \mathcal{N}(\mathbf{y}_i)$.

$$\mathcal{J}(\mathbf{W}, \mathcal{Y}) = \sum_{i} \sum_{j} w_{ij} (\mathbf{y}_i - \mathbf{y}_j)^2$$

3. Define $\mathbf{D} = \operatorname{diag}(d_1, \ldots, d_N)$, where $d_i = \sum_j w_{ij}$ and the Laplacian

 $\mathbf{L} = \mathcal{T}(\mathbf{W}) = \mathbf{D} - \mathbf{W}$

4. The min of $\mathcal{J}(\mathcal{Y})$ is given by the eigenvectors (corresp. to the smallest eigenvalues) of L.

- Isomap
- Locally Linear Embedding (LLE)
- Laplacian Eigenmaps (LapEigs)

Common Points and Differences

- Non-linear: build a non-linear mapping $\mathbb{R}^D \mapsto \mathbb{R}^d$
- Graph-based: Use a neighborhood graph to approx the manifold.
- Impose a preservation criteria:

Isomap: geodesic distances (the metric structure of the manifold). LLE: the local reconstruction weights. LapEig: the neighborhood relations.

- **Closed form** solution obtained through the spectral decomposition of a p.s.d. matrix (**spectral methods**).
- Global vs. Local:

Isomap : **global**, eigendecomposition of a **full** matrix. LLE, LapEig : **local**, eigendecomposition of a **sparse** matrix.

Other popular algorithms

• Kernel PCA

[> B. Schölkopf, A. Smola, and K.R. Müller. Nonlinear component analysis as a kernel eigenvalue problem. *Neural Computation*. 10, 5 (July 1998), 1299-1319.]

• LTSA (Local Tangent Space Alignment),

[> Z. Zhang and H. Zha. 2005. Principal Manifolds and Nonlinear Dimensionality Reduction via Tangent Space Alignment. SIAM J. Sci. Comput. 26, 1 (January 2005), 313-338.]

• MVU (Maximum Variance Unfolding or Semidefinite Embedding)



[D Weinberger, K. Q. Saul, L. K. An Introduction to Nonlinear Dimensionality Reduction by Maximum Variance Unfolding National Conf. on Artificial Intelligence (AAAI). 2006.]

Other popular probabilistic algorithms

• GTM (Generative Topographic Mapping),

[> C. M. Bishop, M. Svensén and C. K. I. Williams, GTM: The Generative Topographic Mapping, *Neural Computation*. 1998, 10:1, 215-234.]

GPLVM (Gaussian Process Latent Variable Models)

[> N. Lawrence, Probabilistic Non-linear Principal Component Analysis with Gaussian Process Latent Variable Models, Journal of Machine Learning Research 6(Nov):1783–1816, 2005.]

Diffusion maps

[> R.R. Coifman and S. Lafon. Diffusion maps. Applied and Computational Harmonic Analysis, 2006]

t-SNE (t-Distributed Stochastic Neighbor Embedding)

[> L.J.P. van der Maaten and G.E. Hinton. Visualizing High-Dimensional Data Using t-SNE. Journal of Machine Learning Research. 9(Nov):2579-2605, 2008.]

Laurens van der Maaten released a Matlab toolbox featuring 25 dimensionality reduction techniques

http://ticc.uvt.nl/~lvdrmaaten/Laurens_van_der_Maaten/ Home.html Manifold Learning Three seminal algorithms

Common Practical Problems

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Conclusions

- The manifold assumption
- The sampling assumption

The high-dimensional input data lies on or close to a lower-dimensional manifold.

Manifold definition

A manifold is a **topological space** that is **locally Euclidean**. [> Wolfram MathWorld]

- Does a low-dimensional manifold really exist?
- Does the data form clusters in low dimensional subspaces?
- How much noise can be tolerated?

Problem In many cases we do not know in advance.

It is possible to acquire **enough** *data samples with* **uniform density** *from the manifold*



How many samples are really enough?

- Manifold assumption: Clusters!!!
- Sampling assumption: Low number of samples w.r.t. the complexity of the manifold
 - $\circ~$ Images of objects with deformations of high-order.
- $\rightarrow\,$ Disconnected components (good for clustering).
- $\rightarrow~$ Unexpected Results.
- $\rightarrow\,$ Not better than PCA or linear methods.

Good data examples

- Rythmic motions: motion capture walk, breathing/cardiac motions, musical pieces
- Images/motions with a reduced number of deformation "modes": MNIST dataset, population studies of a rigid organ.
- Images with **smooth changes** in viewpoint/lightning.





(walk.mp4)

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Conclusions

So far no standard principled way to automatically estimate the size of the neighborhood:

- Usually k-NN ϵ -ball neighborhoods are used.
- Attempts to make it adaptive to the local density of the points.
 - ▷ Jing Wang, Zhenyue Zhang. Adaptive Manifold Learning. NIPS. 2004
 - Zhang, Z.; Wang, J.; Zha, H.; PAMI. 2011

Determining the parameters: Dimensionality

What is the dimension of the manifold that best captures the structure of the data set?

Intuitively, the **intrinsic dimensionality** of the manifold is the **number of independent parameters** needed to pick out a unique point inside the manifold. Examples d = 2



(manifold-walk.mp4)

Determining the parameters: Dimensionality

- in PCA, and Isomap the dimensionality chosen by imposing a threshold over the residual variance (e.g. 95%).
- in general the error of minimized cost function \mathcal{J} does not decrease with increasing number of dimensions d.



Decrease in error as the dimensionality d of $\mathcal Y$ is increased in PCA and Isomap

[▷ Tenenbaum et.al., Science, 2000]

Determining the parameters: Dimensionality

Techniques for intrinsic dimensionality estimation.

- Eigenvalue-based estimation (like in PCA)
- Maximum Likelihood Estimator (MLE)

[▷ E. Levina and P. J. Bickel, Maximum Likelihood Estimation of Intrinsic Dimension, Advances in Neural Information Processing Systems (NIPS), 777-784, 2005.]

Correlation dimension (CorrDim)

[> P. Grassberger and I. Procaccia. Measuring the strangeness of strange attractors. *Physica D: Nonlinear Phenomena*, 9:189-208, 1983.]

Nearest neighbor evaluation (NearNb)

[> Costa, J.A.; Girotra, A.; Hero, A.O.; Estimating Local Intrinsic Dimension with k-Nearest Neighbor Graphs. *IEEE Workshop on Statistical Signal Processing*, 2005]

Packing numbers (PackingNumbers)

[> B. Kégl. Intrinsic dimension estimation using packing numbers. Advances in Neural Information Processing Systems (NIPS). 2002]

• Geodesic minimum spanning tree (GMST)

[> J. Costa, A. Hero, Manifold Learning with Geodesic Minimal Spanning Trees . Computing Research Repository - CORR. 2003]

- J. Theiler. Statistical precision of dimension estimators. Physical Review A, 41(6):3038-3051, 1990.
- ▷ F. Camastra. Data dimensionality estimation methods: a survey. Pattern Recognition, 36:2945- 2954, 2003.

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Mapping new points

I have a new point, how do I project it onto the low-dim representation? t_1 $\mathcal{Y} = \{\mathbf{y}_1, \dots, \mathbf{y}_N\}$ $\mathcal{X} = \{\mathbf{x}_1, \dots, \mathbf{x}_N\}$ \mathbb{R}^{D} \mathbb{R}^{d} y_{new} t_2 $\mathbf{o}_{\mathbf{x}_{new}}$

- There is no linear projection like in PCA, $\mathbf{y}_{new} = \mathbf{P} \mathbf{x}_{new}$.
- Most methods work with **batch data** and find directly (**without a projection step**) the coordinates of each data point in the low-dimensional space.





Find the neighborhood points of $\mathbf{x}_{\mathrm{new}}$

 $\mathbf{x}_j \in \mathcal{N}(\mathbf{x}_{new}) \quad \mathbf{x}_j \in \mathcal{X}$

Using a kernel function

 $k(\mathbf{x}_{new}, \mathbf{x}_j)$



 $\mathbf{x}_j \in \mathcal{N}(\mathbf{x}_{new}) \quad \mapsto \mathbf{y}_j$



Back-projection is only implemented for some techniques, e.g. GPLVM



Similarly, kernel regression can be used to find the map.

Learn mappings along

- GPLVM: iterative, slow convergence.
- DRLIM [> Dimensionality Reduction by Learning an Invariant Mapping, CVPR 2006]
 - Uses contrastive learning
 - $\circ\;$ Defines a parametric function to map from $\mathbb{R}^D\mapsto\mathbb{R}^d$
 - Convolutional neural networks.
- P-DRUR [▷ Parametric Dimensionality Reduction by Unsupervised Regression, CVPR, 2010]
 - Learns both mappings $\mathbb{R}^D \mapsto \mathbb{R}^d$ and $\mathbb{R}^d \mapsto \mathbb{R}^D$
 - Mappings are radial basis function expansions
 - Variational problem
- Kernel Map [> Gerber, S.; Tasdizen, T.; Whitaker, R.; Dimensionality reduction and principal surfaces via Kernel Map Manifolds, ICCV, 2011.]



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Conclusions

For N samples:

- Find nearest neighbors: $O(N^2)$
- Spectral decomposition of *T*(*W*) (symmetric positive semi-definite matrix) : *O*(*N*³).

 $\mathcal{T}(\mathbf{W})\lambda=\mathbf{v}\lambda$

Iterative methods (Jacobi, Arnoldi, Hebbian), but

- $\circ~$ Need matrix-vector products and several passes over data
- Not suitable for large dense matrices (Isomap), better for sparse matrices (LapEig).

1. Hashing-based nearest neighbors

[▷ W. Liu, J. Wang, S. Kumar and S.F. Chang, Hashing with Graphs, ICML, 2011]

2. Use landmarks

• Randomly chosen and linear reconstruction for the remanning points.



[> V.D. Silva, J.B. Tenenbaum, Global versus local methods in nonlinear dimensionality reduction, Advances in neural information processing systems (NIPS), 2003.]

 Setting a sparse regression problem based on preserving the principal angles.

> [> J Silva, J.S. Marques, J. Miranda Lemos. Selecting Landmark Points for Sparse Manifold Learning. Neural Information Processing Systems (NIPS). 2005.]

Large data-sets: some solutions

3. Sampling-based approximation methods for the spectral decomposition.

- ▷ S. Kumar, M. Mohri, and A.Talwalkar. On sampling-based approximate spectral decomposition. ICML. 2009.
- ▷ K. Zhang, I. Tsang, J. Kwok. Improved Nyström Low Rank Approximation and Error Analysis. ICML. 2008.



- Nyström: $\tilde{\mathbf{A}}_{Nys} = \mathbf{C}\mathbf{B}^{-1}\mathbf{C}^{\top} \rightarrow O(l^3 + nld)$
- Column-sampling: $\tilde{\mathbf{A}}_{col} = \mathbf{C} \left(\left[\frac{l}{n} \mathbf{C}^{\top} \mathbf{C} \right]^{1/2} \right)^{-1} \mathbf{C}^{\top} \rightarrow O(nl^2)$

Different methods to sample: uniform, adaptive, ensemble, ...

Large data-sets: some solutions



[> Talwalkar, Kumar & Rowley, Large-Scale Face Manifold Learning, CVPR. 2008.]

4. Random Projections

Variant of the k-d tree which automatically adapts to intrinsic low dimensional structure in data.



- Y. Freund, S. Dasgupta, M. Kabra, N. Verma. Learning the structure of manifolds using random projections. Neural Information Processing Systems (NIPS), 2007.
- C. Hegde, R. Baraniuk. Random Projections for Manifold Learning. Neural Information Processing Systems (NIPS), 2007.
- Goldberg. Online semi-supervised learning. (ECML). 2008

Checklist to verify before using a manifold learning method

- Do I need a non-linear mapping?
- How likely is the data actually leaves close to a manifold?
- Can I acquire a **reasonable amount of samples** in accordance to the manifold complexity?
- Do I have any a-priori information on the **intrinsic dimensionality** of the manifold?
- Is all the data available at once or do new points need to be mapped?
- Is the optimization of the map (\mathcal{J}) coherent with my task?

Recall that some solutions exist in case of

- Need to map new points.
- Large data-sets.

Thanks for your attention!