

A Unifying Probabilistic Perspective on Spectral Approaches to Dimensionality Reduction

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Outline

Review

Maximum Entropy Unfolding

Relation to Laplacian Eigenmaps

Relation to Locally Linear Embedding

Relation to Isomap

Relation to GP-LVM

Experiments

Discussion and Conclusions

Notation

p	data dimensionality	
q	latent dimensionality	
n	number of data points	
$\mathbf{Y}$	<i>design matrix</i> containing our data	$n \times p$
$\mathbf{X}$	matrix of latent variables	$n \times q$
$\mathbf{D}$	matrix of interpoint squared distances	$n \times n$
$\mathbf{K}$	similarities/covariance/kernel	$n \times n$
$\mathbf{L}$	Laplacian matrix	$n \times n$

Row vector from matrix $\mathbf{A}$ given by $\mathbf{a}_{i,:}$; column vector $\mathbf{a}_{:,j}$ and element given by $a_{i,j}$.

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Distances and Similarities

- ▶ Typical scenario, a data set, $\mathbf{Y}$ stored in a matrix of dimension $n \times p$.
- ▶ Proximity data: a data set in form of distances, $\mathbf{D}$, or similarities $\mathbf{K}$. These matrices are dimension $n \times n$.
 - ▶ Similarity matrices have large entries when data points are close.
 - ▶ Distance matrices have large entries when points are far apart.

Multidimensional Scaling

- ▶ Multidimensional scaling (MDS) algorithms are dimensionality reduction for proximity matrices.
- ▶ We can move between similarity and squared distance as follows $d_{i,j} = k_{i,i} - 2k_{i,j} + k_{j,j}$.
 - ▶ In MDS this is known as the standard transformation (Mardia et al., 1979).
 - ▶ If $k_{i,j} = k(\mathbf{y}_{i,:}, \mathbf{y}_{j,:})$ is a “kernel” this is the “distance in feature space” (Schölkopf and Smola, 2001).
 - ▶ If $k_{i,j}$ is an element from a covariance matrix $\mathbf{K}$, it is the *expected squared distance* between two samples with that covariance.

Note: Centering and Squared Distances

- ▶ Consider matrix form of squared distance,

$$\mathbf{D} = \text{diag}(\mathbf{K}) \mathbf{1}^\top - 2\mathbf{K} + \mathbf{1} \text{diag}(\mathbf{K})^\top.$$

- ▶ A Centering matrix has the form

$$\mathbf{H} = \mathbf{I} - n^{-1} \mathbf{1} \mathbf{1}^\top : \quad \mathbf{H} \mathbf{1} = \mathbf{0}$$

- ▶ This implies:

$$-\frac{1}{2} \mathbf{H} \mathbf{D} \mathbf{H} = \mathbf{H} \mathbf{K} \mathbf{H}.$$

- ▶ i.e. centered distance matrix is closely related to centred similarity/kernel.

Spectral Dimensionality Reduction in Machine Learning

- ▶ Spectral approach to dimensionality reduction.
 1. Convert data to a matrix of dimension $n \times n$.
 2. Visualize data with eigenvectors of matrix.
- ▶ Examples:
 - ▶ Isomap (Tenenbaum et al., 2000),
 - ▶ locally linear embeddings (LLE, Roweis and Saul, 2000),
 - ▶ Laplacian eigenmaps (LE, Belkin and Niyogi, 2003) and
 - ▶ maximum variance unfolding (MVU, Weinberger et al., 2004).
 - ▶ Also kernel PCA (Schölkopf et al., 1998; Ham et al., 2004).

Classical Multidimensional Scaling Perspective

- ▶ Classical multidimensional scaling (CMDS)
 1. Compute an $n \times n$ squared distance matrix, $\mathbf{D}$.
 2. Form the centered “similarity matrix” $\mathbf{H}\mathbf{K}\mathbf{H} = -\frac{1}{2}\mathbf{H}\mathbf{D}\mathbf{H}$.
 3. Visualize through q principal eigenvectors (as latent matrix $\mathbf{X}$).
- ▶ This algorithm matches squared distances computed in $\mathbf{X}$ to those computed in $\mathbf{Y}$ through an L1 error.
- ▶ Our Argument:
 - ▶ Main innovation in ML work: how to compute the squared distance matrix $\mathbf{D}$.

This Talk

- ▶ Introduce probabilistic approach to constructing squared distance matrices.
- ▶ Relate isomap, LLE, LE and MVU to the approach.
- ▶ Wrap spectral methods in a unifying perspective of *Gaussian random fields* and CMDS.

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- ▶ Standard classical MDS gives a *linear* embedding in the Euclidean space implied by $\mathbf{D}$.
- ▶ This implies a linear transformation between $\mathbf{X}$ and $\mathbf{Y}$ (if squared distances are computed directly in $\mathbf{Y}$).
- ▶ Spectral approaches in machine learning give a *nonlinear* relationship between the data and the distances.
- ▶ This is done by not computing $\mathbf{D}$ directly in the space of $\mathbf{Y}$.
- ▶ This is very clear for kernel PCA, where $\mathbf{D}$ is computed in a feature space derived from $\mathbf{Y}$.

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- ▶ Kernel PCA squared distance is defined through a kernel:

$$d_{i,j} = k(\mathbf{y}_{i,:}, \mathbf{y}_{i,:}) - 2k(\mathbf{y}_{i,:}, \mathbf{y}_{j,:}) + k(\mathbf{y}_{j,:}, \mathbf{y}_{j,:}) \quad (1)$$

- ▶ $k(\cdot, \cdot)$ is a Mercer kernel (Ham et al., 2004).
- ▶ Kernel PCA (KPCA) recovers an $\mathbf{x}_{i,:}$ and a mapping from $\mathbf{Y}$ to $\mathbf{X}$ space.
- ▶ The mapping is induced through the choice of the *Mercer kernel*.

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Classical MDS and KPCA

- ▶ CMDS procedure performs eigenvalue problem on

$$\mathbf{B} = \mathbf{H}\mathbf{K}\mathbf{H}.$$

- ▶ This matches the KPCA algorithm (Schölkopf et al., 1998)¹.
- ▶ **However**, for the commonly used exponentiated quadratic kernel,

$$k(\mathbf{y}_{i,:}, \mathbf{y}_{j,:}) = \exp(-\gamma \|\mathbf{y}_{i,:} - \mathbf{y}_{j,:}\|_2^2),$$

KPCA actually *expands* the feature space (Weinberger et al., 2004).

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Learn a “Kernel” for Dimensionality Reduction

- ▶ In maximum variance unfolding (MVU) (Weinberger et al., 2004): learn a “kernel matrix” that will allow for dimensionality reduction.
- ▶ Preserve only *local* proximity relationships in the data.
 - ▶ Take a set of neighbors.
 - ▶ Construct a kernel matrix where only distances between neighbors match data distances.

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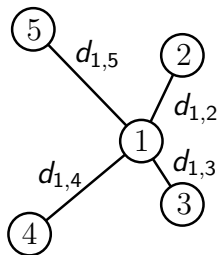
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Maximum Variance Unfolding

- ▶ Optimize elements of $\mathbf{K}$ by maximizing² $\text{tr}(\mathbf{K})$.



- ▶ Subject to squared distance constraints between neighbors

$$d_{i,j} = k_{i,i} - 2k_{i,j} + k_{j,j}$$

²The trace is the *total variance* of the data in feature space

Our Contribution

- ▶ Maximize *entropy* instead of variance (Jaynes, 1986): MEU (Lawrence, 2011, 2010).
- ▶ Entropy and variance are closely related.
- ▶ Maximum entropy leads to a *probabilistic model*.
- ▶ Each spectral approach approximates MEU in some way.

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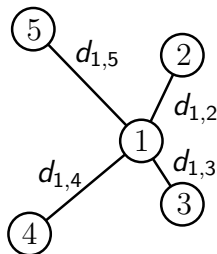
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Maximum Entropy Unfolding

- Find distribution with maximum entropy subject to constraints on *moments*.

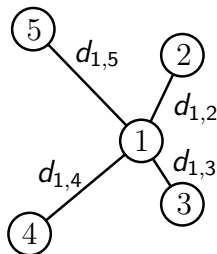


- MEU constraints are on expected distances between neighbors.

$$d_{i,j} = \langle \mathbf{y}_{i,:}^\top \mathbf{y}_{i,:} \rangle - 2 \langle \mathbf{y}_{i,:}^\top \mathbf{y}_{j,:} \rangle + \langle \mathbf{y}_{j,:}^\top \mathbf{y}_{j,:} \rangle$$

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$$d_{i,j} = k_{i,i} - 2k_{i,j} + k_{j,j}$$

which can be written in terms of the covariance.

Gaussian Random Field

- ▶ The maximum entropy probability distribution is a *Gaussian random field*

$$p(\mathbf{Y}) = \prod_{j=1}^p \frac{1}{|\mathbf{K}|^{\frac{1}{2}} (2\pi)^{\frac{n}{2}}} \exp \left(-\frac{1}{2} \mathbf{y}_{:,j}^{\top} \mathbf{K}^{-1} \mathbf{y}_{:,j} \right),$$

- ▶ Covariance matrix is

$$\mathbf{K} = (\mathbf{L} + \gamma \mathbf{I})^{-1}$$

.

- ▶ Where $\mathbf{L}$ is the *Laplacian* matrix associated with the neighborhood graph.
- ▶ Off diagonal elements of the Laplacian are Lagrange multipliers from moment constraints.
- ▶ On diagonal elements given by negative sum of off-diagonal ($\mathbf{L}\mathbf{1} = \mathbf{0}$).

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Relationship to Laplacian Eigenmaps

- ▶ Laplacian eigenmaps (Belkin and Niyogi, 2003): graph Laplacian is specified across the data points.
- ▶ Laplacian has exactly the same form as our matrix $\mathbf{L}$.
- ▶ Parameters of the Laplacian are set either as constant or according to the distance between two points.
- ▶ Smallest eigenvectors of this Laplacian are then used for visualizing the data.

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Smallest Eigenvalues of Laplacian

- ▶ Eigendecomposition of the covariance is

$$\mathbf{K} = \mathbf{U}\mathbf{\Lambda}\mathbf{U}^T$$

- ▶ Eigendecomposition of the Laplacian is

$$\mathbf{L} = \mathbf{U}(\mathbf{\Lambda}^{-1} - \gamma\mathbf{I})\mathbf{U}^T$$

- ▶ Principal eigenvalues of $\mathbf{K}$ are smallest eigenvalues of $\mathbf{L}$.
 - ▶ (smallest eigenvalue of $\mathbf{L}$ is zero, but this is removed by the centering operation on $\mathbf{K}$, or discarded in LE)

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Laplacian Eigenmaps

- ▶ Set parameters of Laplacian.
- ▶ Perform CMDS on the implied matrix $\mathbf{K}$.
 1. No constraints are imposed in Laplacian eigenmaps so distances will not be preserved.
 2. LE gains significant computational advantage by not representing the covariance matrix explicitly.
 3. No matrix inverses required, eigenvalue problem sparse.

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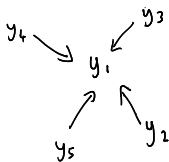
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LLE: Locally Linear Embeddings



Reconstruct a point
from its neighbours

$$y_1 \approx \sum_{j \in N(1)} w_j y_j$$

$$\sum_{j \in N(1)} w_j = 1$$

Constrain reconstruction
weights to sum to 1

Minimize

$$\|y_1 - \sum_{j \in N(1)} w_j y_j\|_2^2$$

Summing to 1
ensures translation
invariance

$$\|y_1 - \mu - \sum_{j \in N(1)} w_j (y_j - \mu)\|_2^2$$

$$= \|y_1 - \sum_{j \in N(1)} w_j y_j - (1 - \sum_{j \in N(1)} w_j) \mu\|_2^2$$

LLE 2

Objective

$$\sum_{i=1}^N \|y_{i,:} - \sum_{j \in \mathcal{N}(i)} w_j y_{j,:}\|_2^2$$

$$\sum_{j \in \mathcal{N}(i)} w_j = 1$$

$$\sum_{j=1}^d y_{i,j}^T (\mathbf{I} - \mathbf{W})(\mathbf{I} - \mathbf{W})^T y_{i,j}$$

in matrix form

$$= \text{Tr}(\mathbf{M} \mathbf{M}^T \mathbf{Y} \mathbf{Y}^T) \quad \mathbf{M} = \mathbf{I} - \mathbf{W}$$

Find a low dimensional dataset, $\mathbf{X}$, which respects the locally linear relationships between the data points.

Minimize

$$\text{Tr}(\mathbf{M} \mathbf{M}^T \mathbf{X} \mathbf{X}^T)$$

subject to

$$\mathbf{x}_{i,:}^T \mathbf{x}_{i,:} = 1$$

Eigenvalue Problem

Smallest eigenvectors of

$$\mathbf{M} \mathbf{M}^T$$

Locally Linear Embedding

- ▶ The Laplacian should be constrained positive definite.
- ▶ This constraint can be imposed by factorizing it as

$$\mathbf{L} = \mathbf{M}\mathbf{M}^\top$$

- ▶ To ensure it is a Laplacian, we need to constrain $\mathbf{M}^\top \mathbf{1} = \mathbf{0}$ giving $\mathbf{L}\mathbf{1} = \mathbf{0}$.
 - ▶ i.e. $m_{i,i} = -\sum_{j \in \mathcal{N}(i)} m_{j,i}$
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Locally Linear Embedding

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Point One

- ▶ For unit diagonals we have $\mathbf{M} = \mathbf{I} - \mathbf{W}$.
- ▶ Here the off diagonal sparsity pattern of $\mathbf{W}$ matches $\mathbf{M}$.
- ▶ Thus

$$(\mathbf{I} - \mathbf{W})^\top \mathbf{1} = \mathbf{0}.$$

- ▶ LLE proscribes that the smallest eigenvectors of

$$(\mathbf{I} - \mathbf{W})(\mathbf{I} - \mathbf{W})^\top = \mathbf{M}\mathbf{M}^\top = \mathbf{L}$$

(like Laplacian Eigenmaps).

- ▶ Equivalent to CMDS on the GRF described by $\mathbf{L}$.

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- Maximizing each conditional is equivalent to optimizing LLE objective.
- Constraint that LLE weights sum to one arises naturally because $w_{j,i}/m_{i,i}$ and $m_{i,i} = \sum_{j \in \mathcal{N}(i)} w_{j,i}$.
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LLE Approximates MEU

- ▶ LLE is an approximation to maximum likelihood.
- ▶ Laplacian has factorized form.
- ▶ Pseudolikelihood also allows for relatively quick parameter estimation.
 - ▶ ignoring the partition function removes the need to invert to recover the covariance matrix.
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Isomap

Shortest Path Algorithm



Squared Distance Matrix

$$D = \begin{bmatrix} 0 & d_{12} & d_{13} & d_{14} & d_{15} \\ d_{12}^2 & 0 & d_{23} & d_{24} & d_{25} \\ (d_{12} + d_{23})^2 & d_{23} & 0 & d_{34} & d_{35} \\ (d_{12} + d_{24})^2 & d_{24} & d_{34} & 0 & d_{45} \\ (d_{12} + d_{24} + d_{45})^2 & (d_{24} + d_{45})^2 & d_{34} & d_{45} & 0 \end{bmatrix}$$

Classical MDS on Resulting Squared Distances

① Center

$$B = -\frac{1}{2} H D H$$

$$(H = I - \frac{1}{N} \mathbf{1} \mathbf{1}^T)$$

② Eigenvalue problem on B

(if D is squared Euclidean distances
this is PCA)

Compare with MEU

- ▶ Both MVU and MEU can be thought of as starting with a sparse graph of (squared) distances.
- ▶ Fill in other distances by maximizing the total variance/entropy.
- ▶ Interneighbor distances in this graph are preserved just like in isomap.
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- ▶ GP-LVMs construct a Gaussian process by specifying a covariance function (Mercer kernel) in $\mathbf{X}$.
- ▶ A Gauss Markov random field can be specified by a Gaussian process through appropriate covariance functions

$$k(x, x') = \exp(-\|x - x'\|_1)$$

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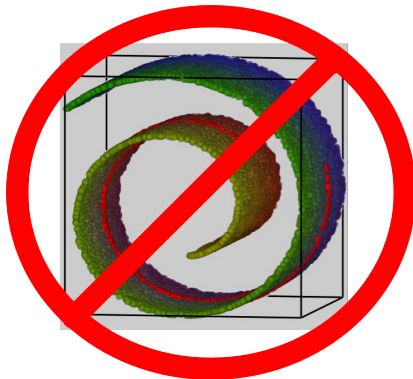
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Simple Experiments

- ▶ Consider two real data sets.
- ▶ We apply each of the spectral methods we have reviewed.
- ▶ Apply the MEU framework.
- ▶ Follow the suggestion of Harmeling (Harmeling, 2007) and use the GPLVM likelihood (Lawrence, 2005) for embedding quality.
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Motion Capture Data

- ▶ Data consists of a 3-dimensional point cloud of the location of 34 points from a subject performing a run.
- ▶ 102 dimensional data set containing 55 frames of motion capture.
- ▶ Subject begins the motion from stationary and takes approximately three strides of run.
- ▶ Should see this structure in the visualization: a starting position followed by a series of loops.
- ▶ Data was made available by Ohio State University.
- ▶ The two dominant eigenvectors are visualized in following figures.

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- ▶ Visualize data.

PCA on Stick Man

- First two principal components of stick man data.

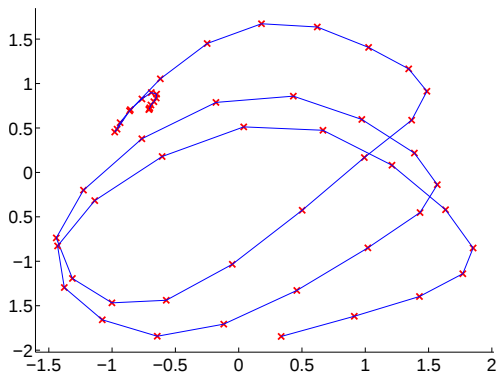


Figure: Stick man data projected onto their first two principal components. `demStickPpca1`.

Laplacian Eigenmaps and LLE

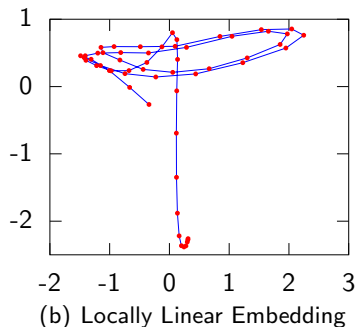
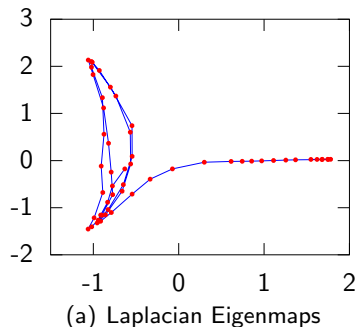


Figure: Models capture either the cyclic structure or the structure associated with the start of the run or both parts.

Isomap and MVU

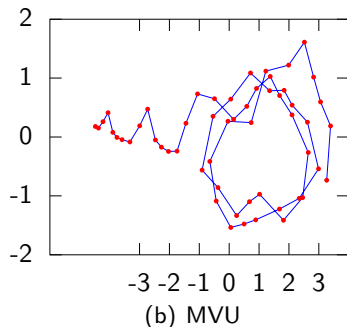
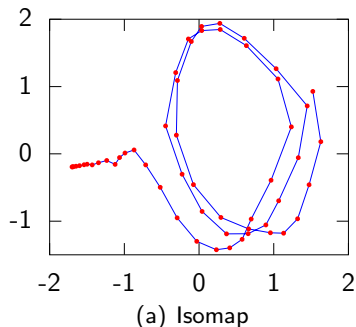


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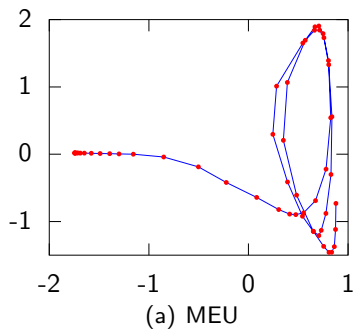


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Motion Capture: Model Scores

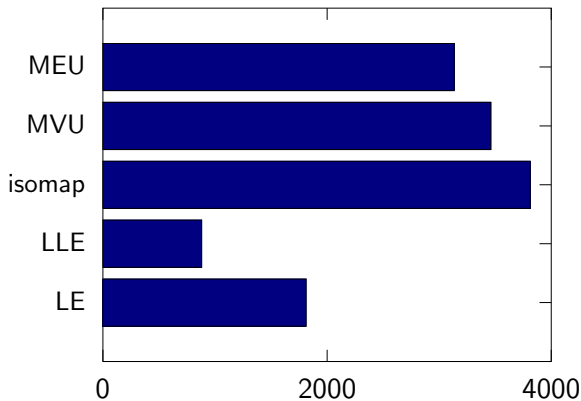


Figure: Model score for the different spectral approaches.

Robot Navigation Example

- ▶ Second data set: series of recordings from a robot as it traces a square path in a building.
- ▶ It records the strength of WiFi signals (see Ferris et al., 2007, for an application).
- ▶ Robot only in two dimensions, the inherent dimensionality of the data should be two.
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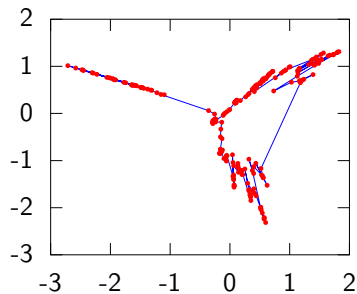
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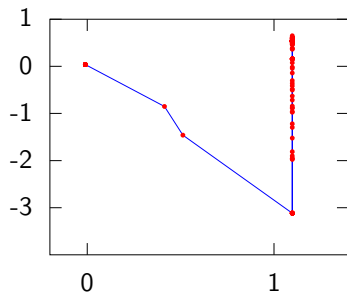
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Laplacian Eigenmaps and LLE



(a) Laplacian Eigenmaps



(b) Locally Linear Embedding

Figure: Models show loop closure but smooth the trace to different degrees.

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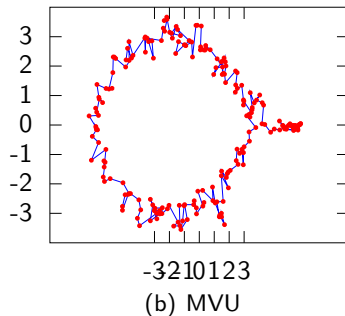
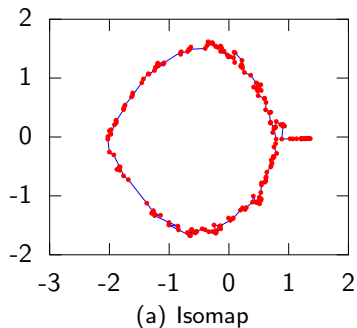


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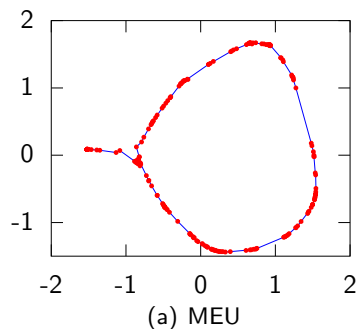


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Robot Navigation: Model Scores

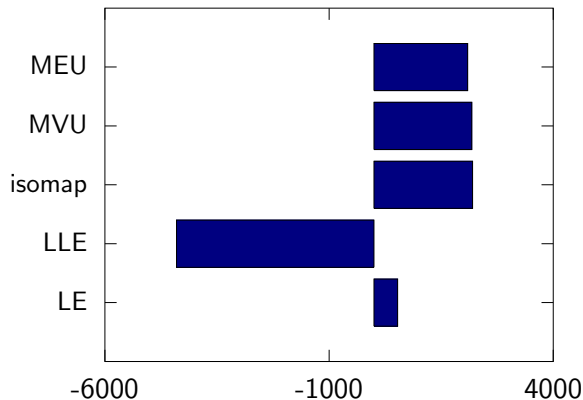


Figure: Model score for the different spectral approaches.

Outline

Review

Maximum Entropy Unfolding

Relation to Laplacian Eigenmaps

Relation to Locally Linear Embedding

Relation to Isomap

Relation to GP-LVM

Experiments

Discussion and Conclusions

- ▶ New perspective on dimensionality reduction algorithms based around maximum entropy.
- ▶ Start with MVU and end with GRFs.
- ▶ Hope that this perspective on dimensionality reduction will encourage new strands of research at the interface of these areas.

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Stages of Spectral Dimensionality Reduction

- ▶ Our perspective shows there are three separate stages used in existing spectral dimensionality algorithms.
 1. A neighborhood between data points is selected. Normally k -nearest neighbors or similar algorithms are used.
 2. Interpoint distances between neighbors are fed to the algorithms which provide a similarity matrix. The way the entries in the similarity matrix are computed is the main difference between the different algorithms.
 3. The relationship between points in the similarity matrix is visualized using the eigenvectors of the similarity matrix.

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Our Perspective

- ▶ Each step is somewhat orthogonal.
- ▶ Neighborhood relations need not come from nearest neighbors: can use structure learning.
- ▶ Main difference between approaches is how similarity matrix entries are determined.
- ▶ Final step attempts to visualize the similarity using eigenvectors. This is just one possible approach.
- ▶ There is an entire field of graph visualization proposing different approaches to visualizing such graphs.

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Advantages of Existing Approaches

- ▶ Conflating the three steps allows faster complete algorithms.
- ▶ E.g. mixing 2nd & 3rd allows speed ups by never computing the similarity matrix.
- ▶ We still can understand the algorithm from the unifying perspective while exploiting the computational advantages offered by this neat shortcut.

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Acknowledgements

Conversations with John Kent, Chris Williams, Brenden Lake, Joshua Tenenbaum and John Lafferty have influenced the thinking in this work.

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Outline

Learning the Neighborhood

Final Experiment: Structure Learning

- ▶ Test the ability of L1 regularization of the random field to learn the neighborhood.
- ▶ Considered the motion capture data and used the DRILL with a neighborhood size of 20 and full connectivity.
- ▶ L1 regularization on the parameters: vary regularization size and seek a maximum under the GPLVM.

Structure Learning from Neighborhood of 20

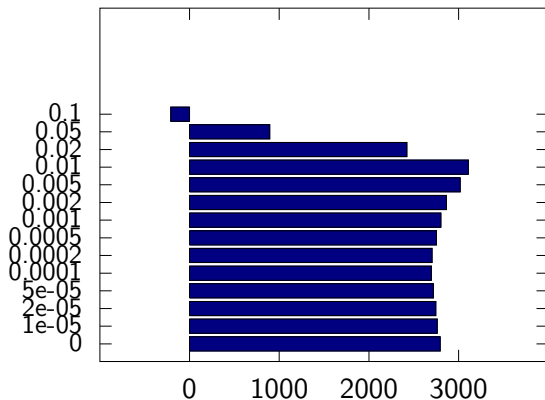


Figure: Model scores for different regularization coefficients.

Structure Learning from Neighborhood of 20

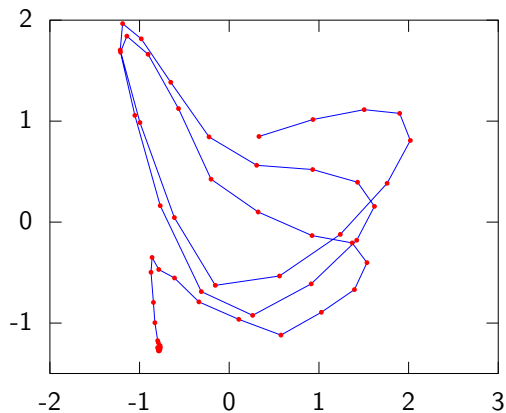


Figure: Visualization associated with highest model score.

Full Structure Learning

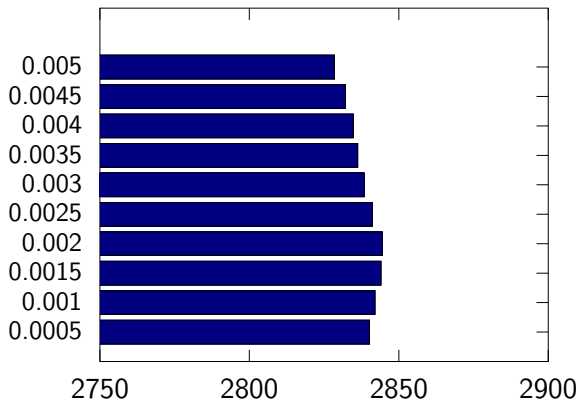


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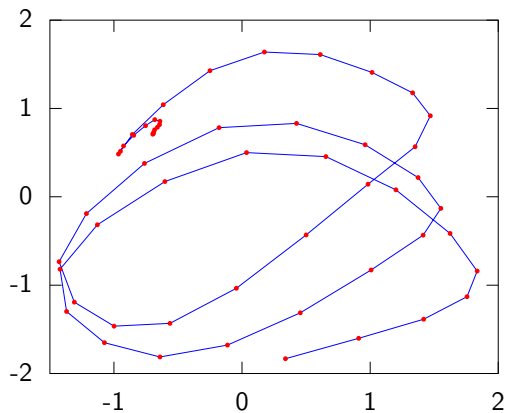


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Different Neighborhood Scores

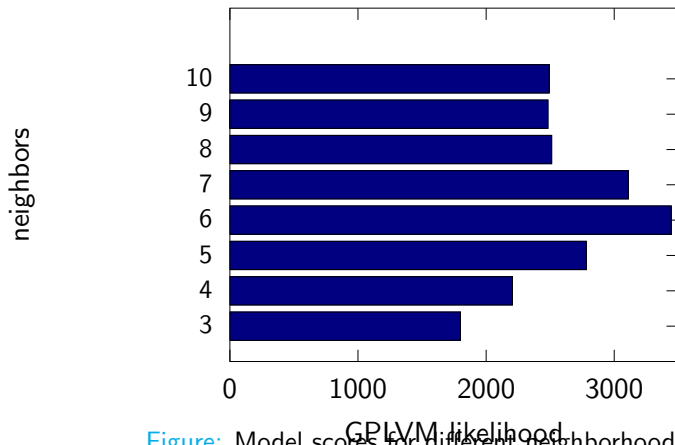


Figure: Model scores for different neighborhood sizes.

Different Neighborhood Scores

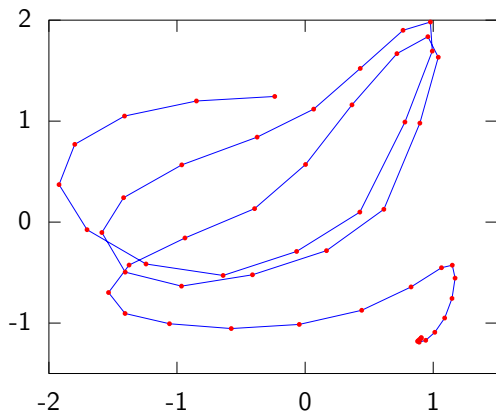


Figure: Visualization associated with highest model score.

Structure Learning from Neighborhood of 6

regularization coefficient

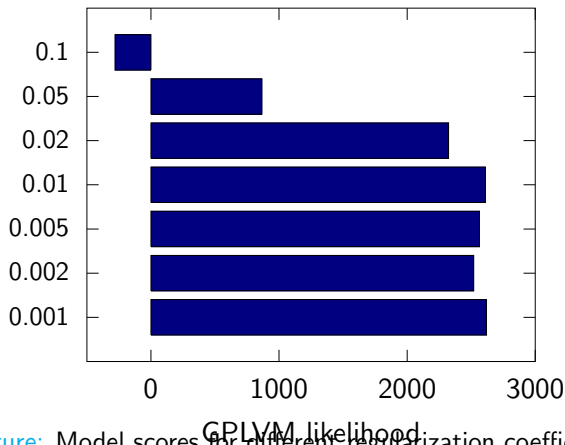


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Structure Learning from Neighborhood of 6

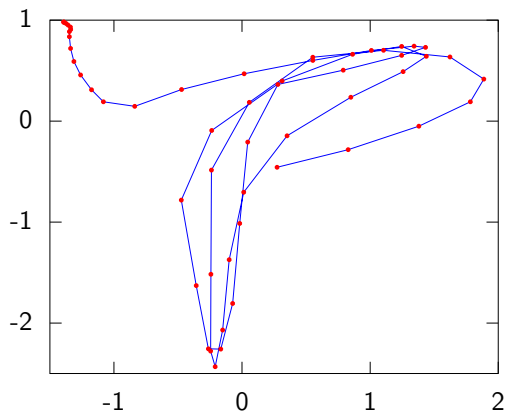


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