A Unifying Probabilistic Perspective on Spectral Approaches to Dimensionality Reduction

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Talk at Workshop on Manifold Learning
Hausdorff Research Institute for Mathematics, Bonn

31st May 2011

Outline

Notation

p	data dimensionality	
q	latent dimensionality	
n	number of data points	
$\mathbf{Y}$	*design matrix* 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 $a_{i,j}$.

Outline

Distances and Similarities

- Typical scenario, a data set, **Y** stored in a matrix of dimension $n \times p$.
- Proximity data: a data set in form of distances, **D**, orsimilarities **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,

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

- 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" $\mathbf{HKH} = -\frac{1}{2}\mathbf{HDH}$.
  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.

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

Spectral Approaches

- 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

- Kernel PCA squared distance is defined through a kernel:

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

- $k(\cdot, \cdot)$ 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
$$\mathbf{B} = \mathbf{HKH}.$$
- This matches the KPCA algorithm (Schölkopf et al., 1998)[1].
- **However**, for the commonly used exponentiated quadratic kernel,
$$k(y_{i,:}, y_{j,:}) = \exp(-\gamma \left\|\mathbf{y}_{i,:} - \mathbf{y}_{j,:}\right\|_2^2),$$
KPCA actually *expands* the feature space (Weinberger et al., 2004).

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Maximum Variance Unfolding

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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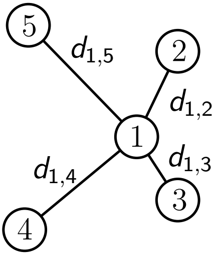
Maximum Variance Unfolding

- Optimize elements of $\mathbf{K}$ by maximizing[2] $\text{tr}(\mathbf{K})$.



- Subject to squared distance constraints between neighbors

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

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

Maximum Entropy Unfolding

Our Contribution

- Maximize *entropy* instead of variance (Jaynes, 1986): MEU.
- 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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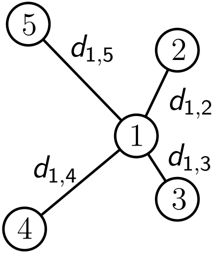
- Find distribution with maximum entropy subject to constraints on *moments*.



- MEU constraints are on expected distances between neighbors.

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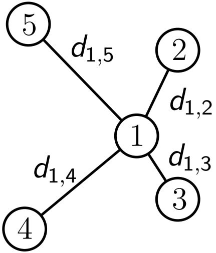

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$$d_{i,j} = k_{i,i} - 2k_{i,j} + k_{j,j}$$

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 ($\mathbf{L1} = \mathbf{0}$).

Outline

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

$$\mathbf{K} = \mathbf{U}\boldsymbol{\Lambda}\mathbf{U}^\top$$

- Eigendecomposition of the Laplacian is

$$\mathbf{L} = \mathbf{U}\left(\boldsymbol{\Lambda}^{-1} - \gamma\mathbf{I}\right)\mathbf{U}^\top$$

- 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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Outline

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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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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Second Point

- Pseudolikelihood approximation (see e.g. Koller and Friedman, 2009, pg 970): product of the conditional densities:

$$p(\mathbf{Y}) \approx \prod_{i=1}^{n} p(\mathbf{y}_{i,:}|\mathbf{Y}_{\backslash i}),$$

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Conditionals

- Factors in the GRF are the conditionals,

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- Maximizing each conditional is equivalent to optimizing LLE objective.
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- LLE is an approximation to maximum likelihood.
- Laplacian has factorized form.
- Pseudolikelihood also allows for relatively quick parameter estimation.
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- Interestingly, as we increase the neighborhood size to $K = n - 1$ we do not recover PCA.
- But PCA is the "optimal" linear embedding!!
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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

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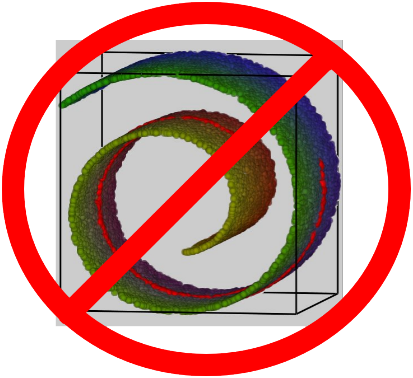
Campaign for Real Data

Say NO to the Swiss Roll



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.
- The higher the likelihood the better the embedding.

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- 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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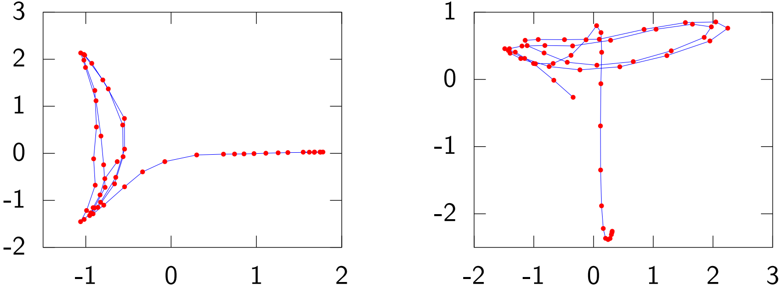
Laplacian Eigenmaps and LLE



(a) Laplacian Eigenmaps (b) Locally Linear Embedding

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

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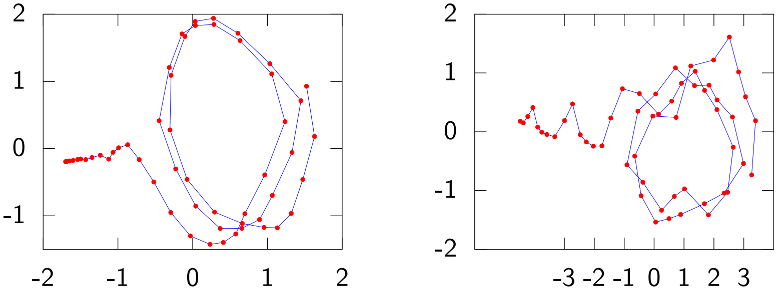

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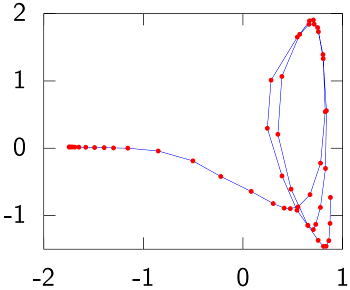

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Motion Capture: Model Scores

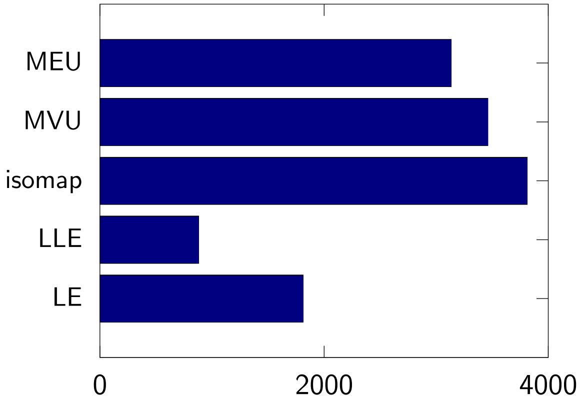

Figure: Model score for the different spectral approaches.

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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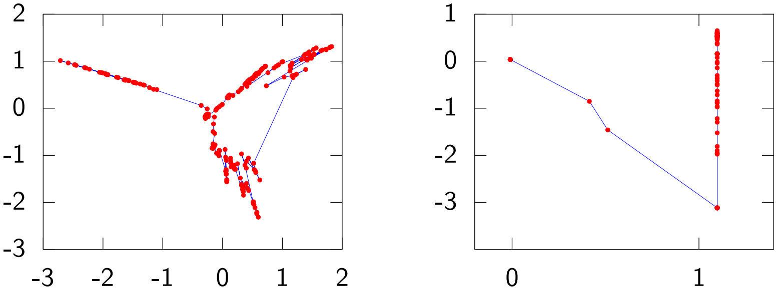

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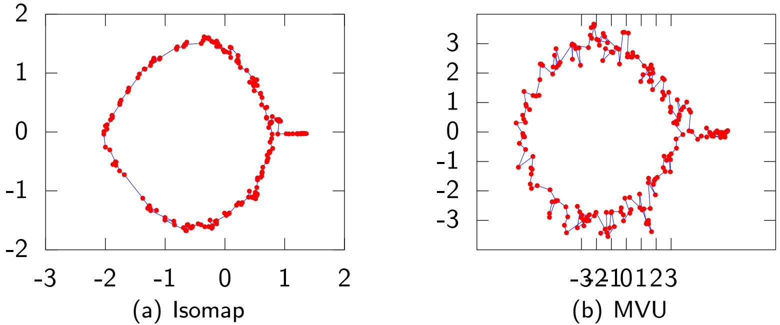

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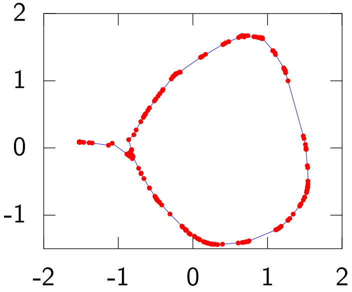

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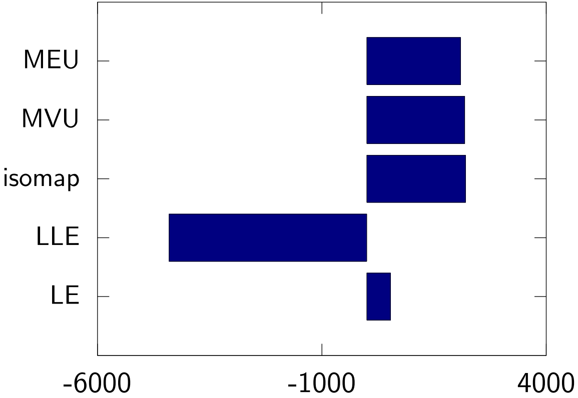

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- Each step is somewhat orthogonal.
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Acknowledgements

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References I

M. Belkin and P. Niyogi. Laplacian eigenmaps for dimensionality reduction and data representation. *Neural Computation*, 15(6):1373–1396, 2003. [DOI].

B. D. Ferris, D. Fox, and N. D. Lawrence. WiFi-SLAM using Gaussian process latent variable models. In M. M. Veloso, editor, *Proceedings of the 20th International Joint Conference on Artificial Intelligence (IJCAI 2007)*, pages 2480–2485, 2007. [PDF].

R. Greiner and D. Schuurmans, editors. *Proceedings of the International Conference in Machine Learning*, volume 21, 2004. Omnipress.

J. Ham, D. D. Lee, S. Mika, and B. Schölkopf. A kernel view of dimensionality reduction of manifolds. In Greiner and Schuurmans (2004). [PDF].

S. Harmeling. Exploring model selection techniques for nonlinear dimensionality reduction. Technical Report EDI-INF-RR-0960, University of Edinburgh,

E. T. Jaynes. Bayesian methods: General background. In J. H. Justice, editor, *Maximum Entropy and Bayesian Methods in Applied Statistics*, pages 1–25. Cambridge University Press, 1986.

D. Koller and N. Friedman. *Probabilistic Graphical Models: Principles and Techniques*. MIT Press, 2009. [Google Books] .

N. D. Lawrence. Probabilistic non-linear principal component analysis with Gaussian process latent variable models. *Journal of Machine Learning Research*, 6:1783–1816, 11 2005.

K. V. Mardia, J. T. Kent, and J. M. Bibby. *Multivariate analysis*. Academic Press, London, 1979. [Google Books] .

S. T. Roweis and L. K. Saul. Nonlinear dimensionality reduction by locally linear embedding. *Science*, 290(5500): 2323–2326, 2000. [DOI].

B. Schölkopf, A. Smola, and K.-R. Müller. Nonlinear component analysis as a kernel eigenvalue problem. *Neural Computation*, 10:1299–1319, 1998. [DOI].

B. Schölkopf and A. J. Smola. *Learning with Kernels*. MIT Press, Cambridge, MA, 2001.

J. B. Tenenbaum, V. de Silva, and J. C. Langford. A global geometric framework for nonlinear dimensionality reduction. *Science*, 290(5500):2319–2323, 2000. [DOI].

K. Q. Weinberger, F. Sha, and L. K. Saul. Learning a kernel matrix for nonlinear dimensionality reduction. In Greiner and Schuurmans (2004), pages 839–846.

C. K. I. Williams. On a connection between kernel PCA and metric multidimensional scaling. In T. K. Leen, T. G. Dietterich, and V. Tresp, editors, *Advances in Neural Information Processing Systems*, volume 13, pages 675–681, Cambridge, MA, 2001. MIT Press.

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

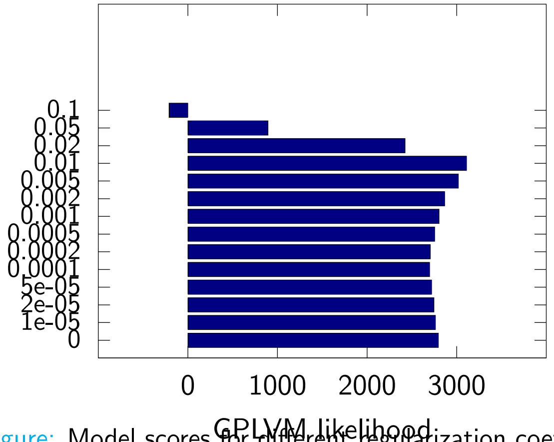

Figure: Model scores for different regularization coefficients.

Structure Learning from Neighborhood of 20

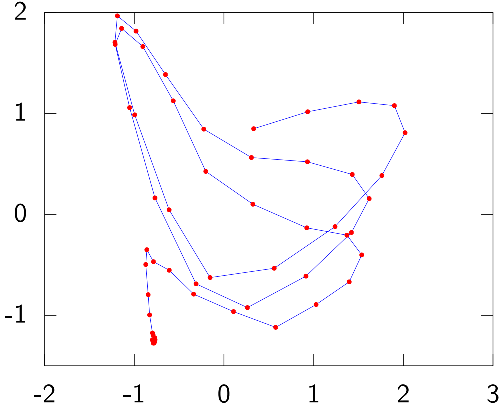

Figure: Visualization associated with highest model score.

Full Structure Learning

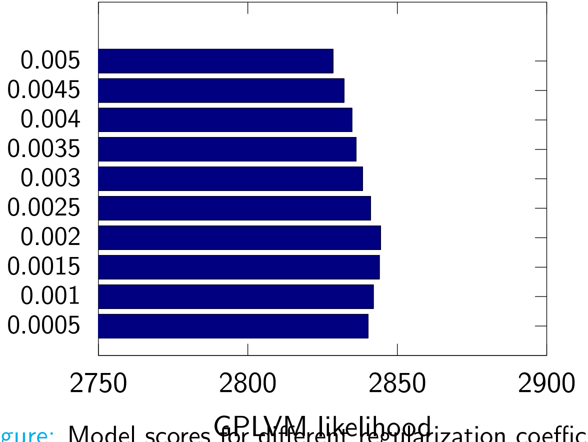

Figure: Model scores for different regularization coefficients.

Full Structure Learning

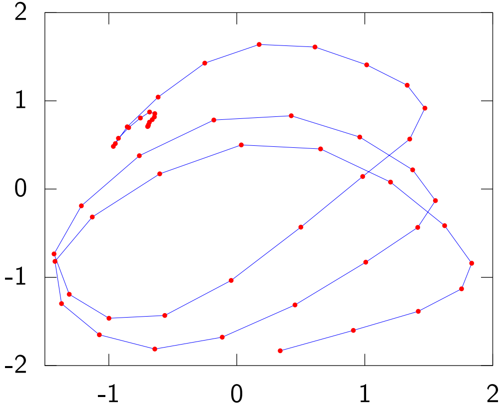

Figure: Visualization associated with highest model score.

Different Neighborhood Scores

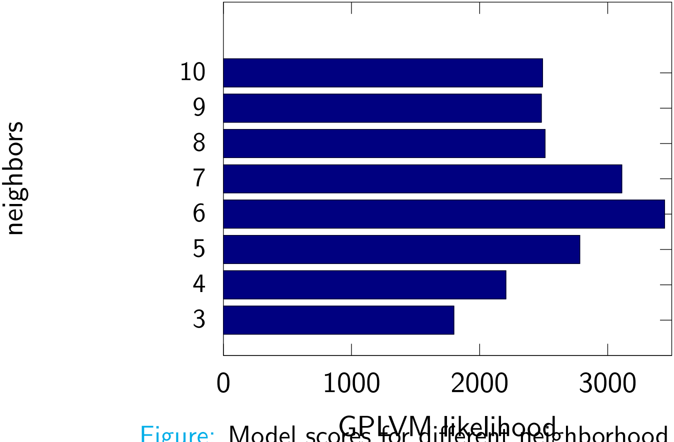

Figure: Model scores for different neighborhood sizes.

Different Neighborhood Scores

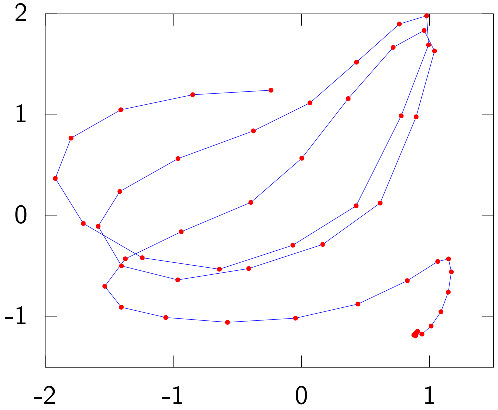

Figure: Visualization associated with highest model score.

Structure Learning from Neighborhood of 6

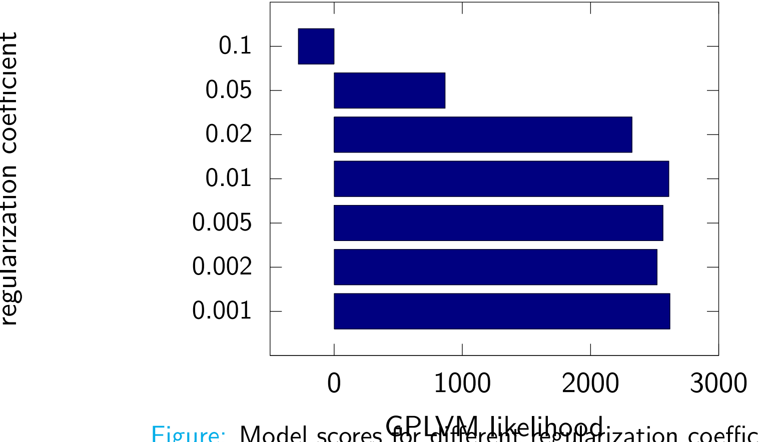

Figure: Model scores for different regularization coefficients.

Structure Learning from Neighborhood of 6

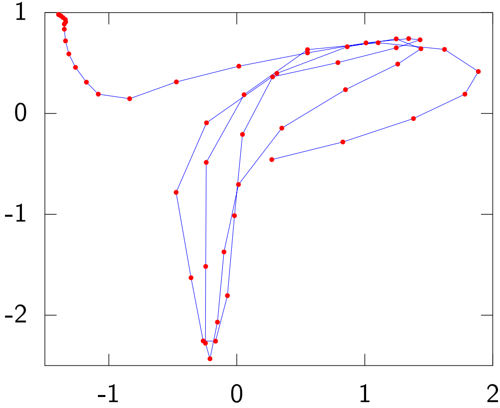

Figure: Visualization associated with highest model score.