Gaussian Processes and Probabilistic Models for Dimensionality Reduction

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Outline

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Notation

q— dimension of latent/embedded space
p— dimension of data space
n— number of data points

centred data, $\mathbf{Y} = [\mathbf{y}_{1,:}, \dots, \mathbf{y}_{n,:}]^\top = [\mathbf{y}_{:,1}, \dots, \mathbf{y}_{:,p}] \in \Re^{n \times p}$
latent variables, $\mathbf{X} = [\mathbf{x}_{1,:}, \dots, \mathbf{x}_{n,:}]^\top = [\mathbf{x}_{:,1}, \dots, \mathbf{x}_{:,q}] \in \Re^{n \times q}$
mapping matrix, $\mathbf{W} \in \Re^{p \times q}$

$\mathbf{a}_{i,:}$ is a vector from the ith row of a given matrix $\mathbf{A}$
$\mathbf{a}_{:,j}$ is a vector from the jth row of a given matrix $\mathbf{A}$

Reading Notation

$\mathbf{X}$ and $\mathbf{Y}$ are *design matrices*

- Covariance given by $n^{-1}\mathbf{Y}^\top\mathbf{Y}$.
- Inner product matrix given by $\mathbf{Y}\mathbf{Y}^\top$.

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 $\mathbf{D}$.

Isomap

- MDS finds geometric configuration preserving distances.
- MDS applied to Manifold distance.
- Geodesic Distance = Manifold Distance.
- Cannot compute geodesic distance without knowing manifold.
- Idea: compute distance via shortest path between point-pairs Tenenbaum et al. (2000).

Isomap

- Isomap: define neighbors and compute distances between neighbors.
- Geodesic distance approximated by shortest path through adjacency matrix.

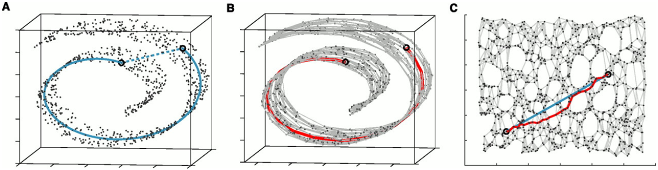
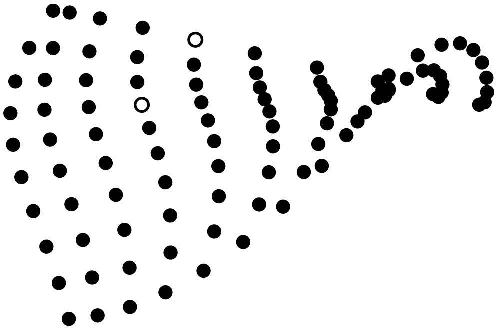


Figure: A: true geodesic distance. B: Approximate distance on graph. C: comparison of true and approximate distances. Image from Tenenbaum et al. (2000).

Isomap Neighborhood

- Compute nearest k neighbors for each point.
- Construct a graph linking data points through neighbors.



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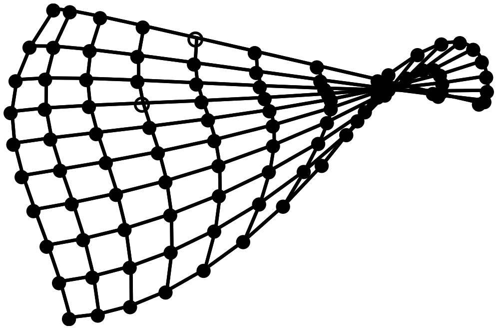

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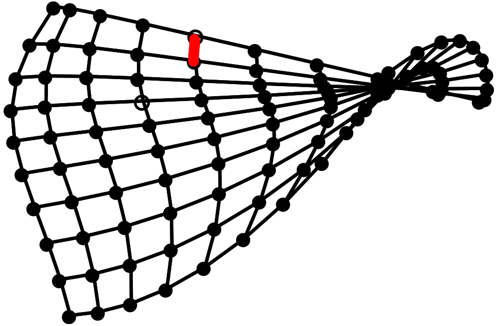

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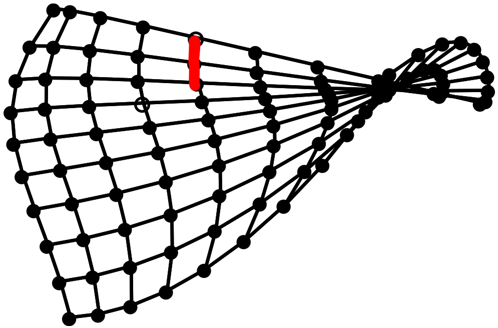

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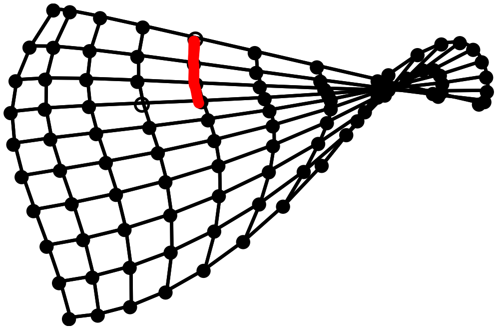

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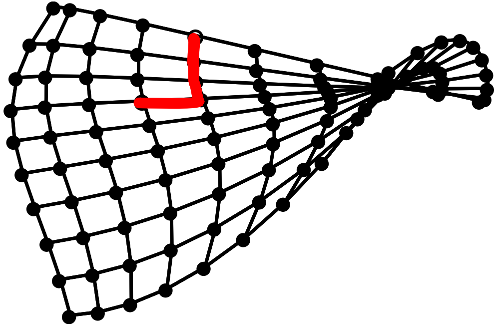

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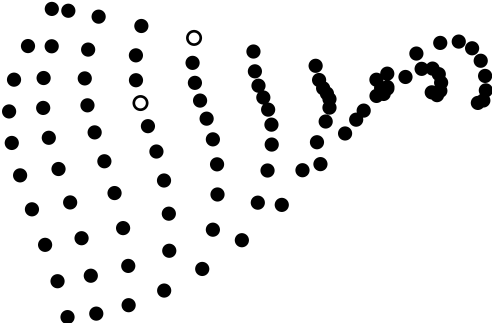

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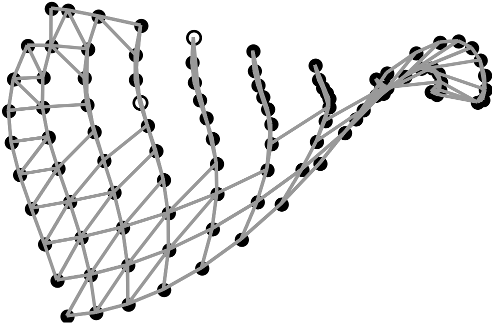

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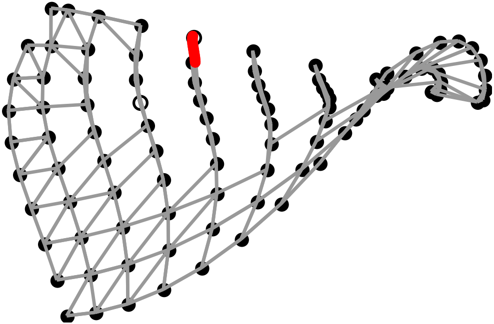

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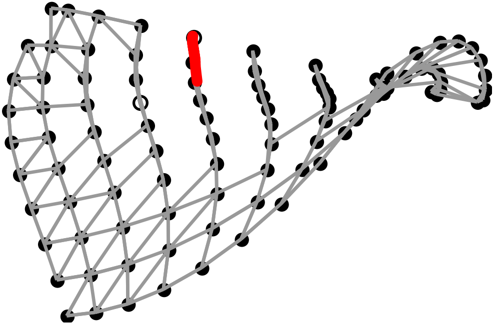

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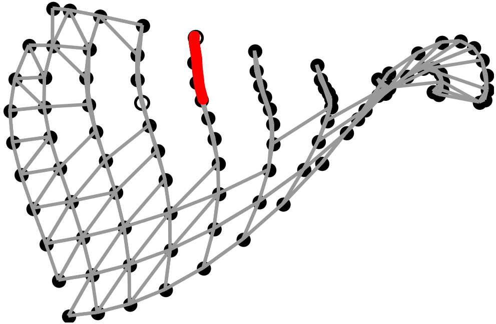

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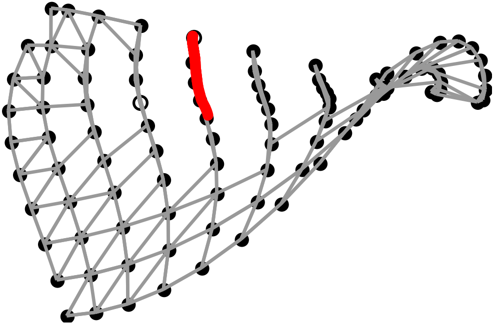

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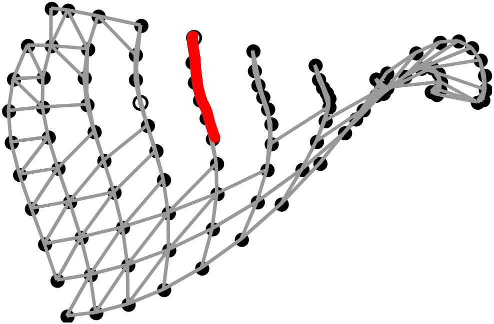

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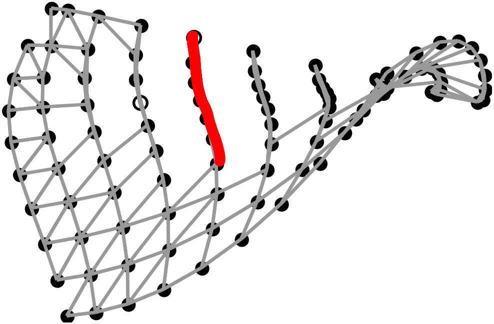

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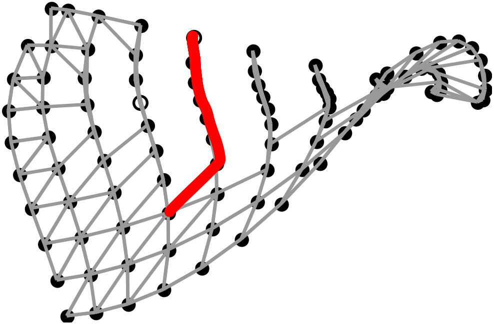

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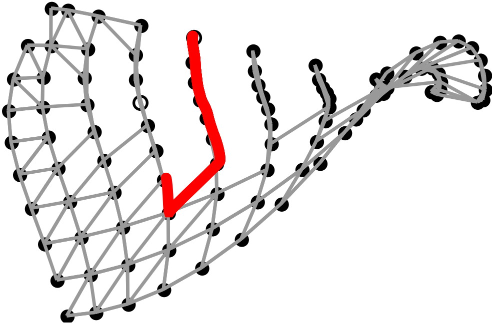

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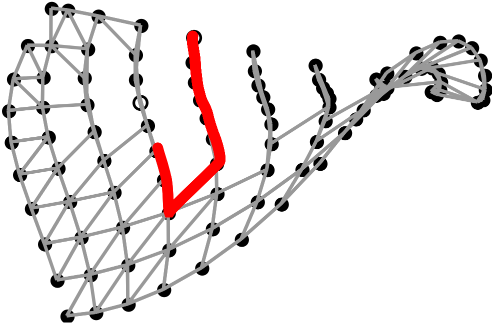

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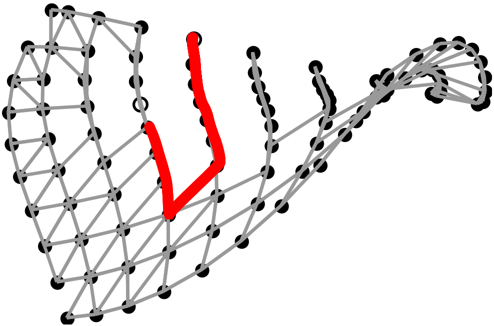

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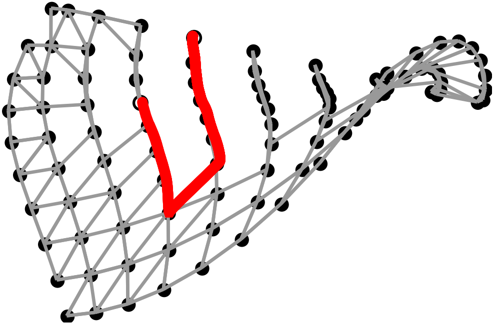

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- Spectral approaches in machine learning give a *nonlinear* relationship between the data and the distances.
- This is done by not computing $\mathbf{D}$ directly in the space of $\mathbf{Y}$.
- This is very clear for kernel PCA, where $\mathbf{D}$ is computed in a feature space derived from $\mathbf{Y}$.

Kernel PCA

- Kernel PCA squared distance is defined through a kernel:

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

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- $k(\cdot, \cdot)$ 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*.

Classical MDS and KPCA

- CMDS procedure performs eigenvalue problem on

$$\mathbf{B} = \mathbf{HKH}.$$

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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,

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

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

---

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Maximum Variance Unfolding

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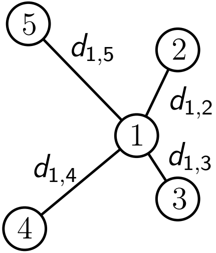
- Preserve only *local* proximity relationships in the data.
  - Take a set of neighbors.
  - Construct a kernel matrix where only distances between neighbors match data distances.

Maximum Variance Unfolding

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



- 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

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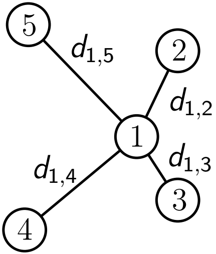
- Each spectral approach approximates MEU in some way.

Maximum Entropy Unfolding

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



- MEU constraints are on expected distances between neighbors.

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

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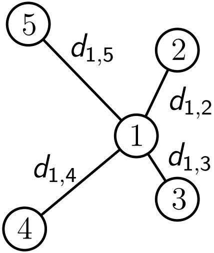

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which can be written in terms of the covariance.

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 ($\mathbf{L}\mathbf{1} = \mathbf{0}$).

Data Feature Independence

- The GRF specifying independence across data *features*.
- Most applications of Gaussian models are applied independently across data *points*.
  - Notable exceptions include Zhu et al. (2003); Lawrence (2004, 2005); Kemp and Tenenbaum (2008).
- Maximum likelihood in this model is equivalent maximizing entropy under distance constraints.

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- There is a "Blessing of Dimensionality" in this model.

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  - i.e. $m_{i,i} = -\sum_{j \in \mathcal{N}(i)} m_{j,i}$
  - Set $m_{j,i} = 0$ if $j \notin \mathcal{N}(i)$.

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  1. The diagonal sums, $m_{i,i}$, are further constrained to unity.
  2. Model parameters found by maximizing *pseudolikelihood* of the data.

Point One

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

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Conditionals

- Factors in the GRF are the conditionals,

$$p(\mathbf{y}_{i,:}|\mathbf{Y}_{\backslash i}) = \left(\frac{m_{i,i}^2}{2\pi}\right)^{\frac{p}{2}} \exp\left(-\frac{m_{i,i}^2}{2}\left\|\mathbf{y}_{i,:} - \sum_{j\in\mathcal{N}(i)} \frac{w_{j,i}}{m_{i,i}}\mathbf{y}_{j,:}\right\|_2^2\right).$$

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- In LLE a *further* constraint is imposed $m_{i,i} = 1$.

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- LLE is an approximation to maximum likelihood.
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- Pseudolikelihood also allows for relatively quick parameter estimation.
  - ignoring the partition function removes the need to invert to recover the covariance matrix.
  - LLE can be applied to larger data sets than MEU or MVU.

Note: The sparsity pattern in the Laplacian for LLE will not match that used in the Laplacian for the other algorithms due to the factorized representation.

LLE and PCA

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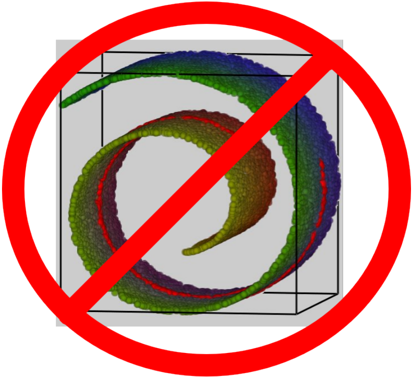
- But PCA is the "optimal" linear embedding!!
- LLE is optimizing a pseudolikelihood: in contrast the MEU algorithm, which LLE approximates, does recover PCA when $K = n - 1$.

Campaign for Real Data

Say NO to the Swiss Roll



Simple Experiments

- Simple motion capture data example.
- Changing incline of run of human captured with 34 markers (102 dimensions).
- 55 frames in the data.
- Follow the suggestion of Harmeling. (Harmeling, 2007) and use the GPLVM likelihood (Lawrence, 2005) for embedding quality.

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- The higher the likelihood the better the embedding.

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- The two dominant eigenvectors are visualized in following figures.

Stick Man Data

- Visualize data.

PCA on Stick Man

- First two principal components of stick man data.

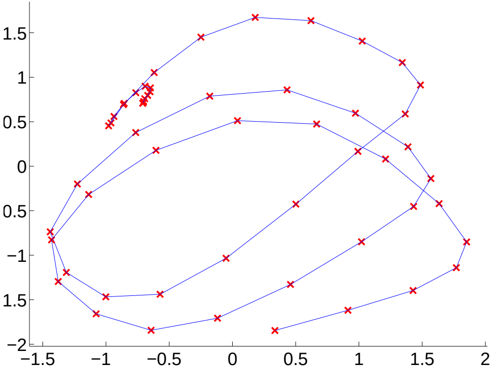


Figure: Stick man data projected onto their first two principal components. `demStickPpca1`.

Laplacian Eigenmaps and LLE

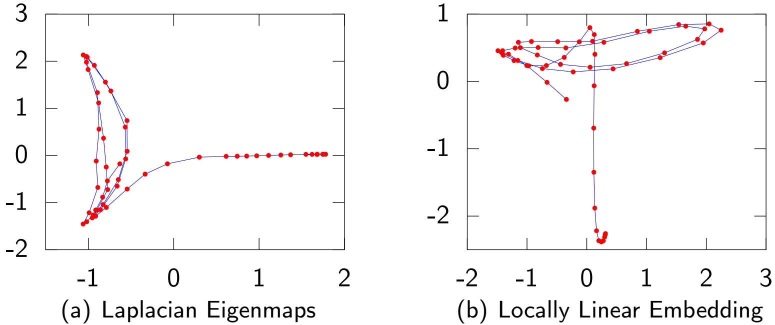
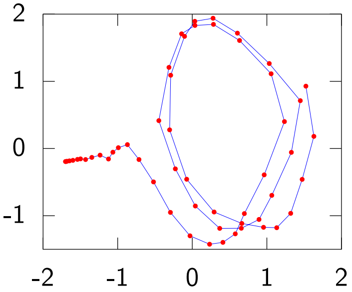
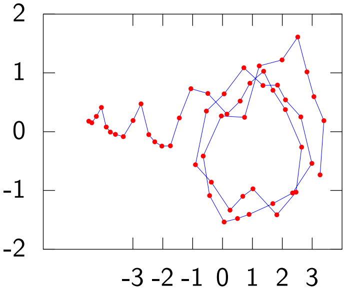


Figure: Models capture either the cyclic structure or the structure associated with the start of the run or both parts.

Isomap and MVU



(a) Isomap



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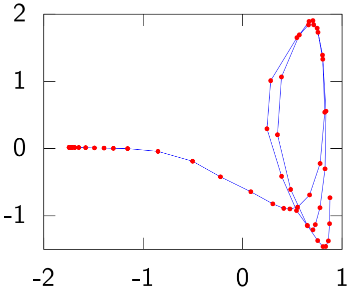
MEU



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Motion Capture: Model Scores

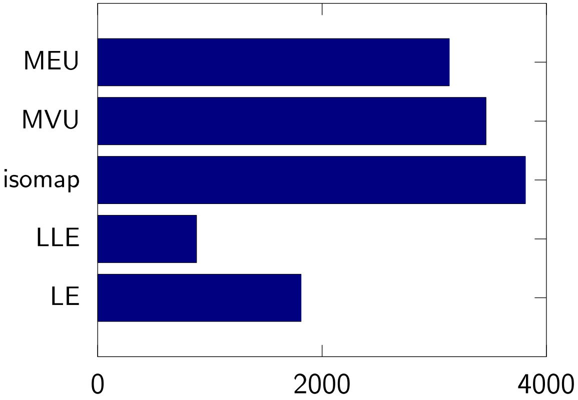


Figure: Model score for the different spectral approaches.

Outline

Linear Dimensionality Reduction

Linear Latent Variable Model

- Represent data, $\mathbf{Y}$, with a lower dimensional set of latent variables $\mathbf{X}$.
- Assume a linear relationship of the form

$$\mathbf{y}_{i,:} = \mathbf{W}\mathbf{x}_{i,:} + \boldsymbol{\epsilon}_{i,:},$$

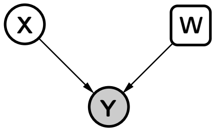
where

$$\boldsymbol{\epsilon}_{i,:} \sim \mathcal{N}\left(\mathbf{0}, \sigma^2\mathbf{I}\right).$$

Linear Latent Variable Model

Probabilistic PCA

- Define *linear-Gaussian relationship* between latent variables and data.



$$p\left(\mathbf{Y}|\mathbf{X},\mathbf{W}\right)=\prod_{i=1}^{n}\mathcal{N}\left(\mathbf{y}_{i,:}|\mathbf{W}\mathbf{x}_{i,:},\sigma^2\mathbf{I}\right)$$

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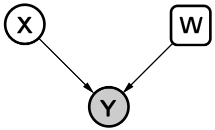

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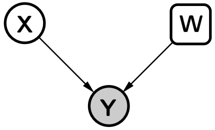

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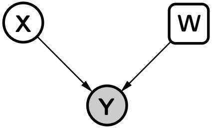

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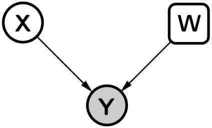
Probabilistic PCA Max. Likelihood Soln (Tipping and Bishop, 1999)



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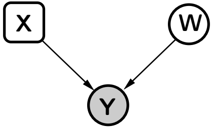
where $\mathbf{R}$ is an arbitrary rotation matrix.

Linear Latent Variable Model III

Dual Probabilistic PCA

- Define *linear-Gaussian relationship* between latent variables and data.



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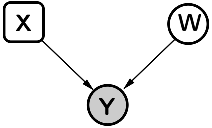

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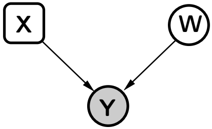

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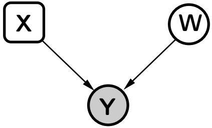

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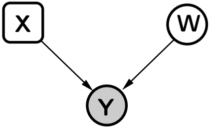
Linear Latent Variable Model IV

Dual Probabilistic PCA Max. Likelihood Soln (Lawrence, 2004)



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Equivalence of Formulations

The Eigenvalue Problems are equivalent

- Solution for Probabilistic PCA (solves for the mapping)

$$\mathbf{Y}^{\top}\mathbf{Y}\mathbf{U}_q = \mathbf{U}_q\boldsymbol{\Lambda}_q \qquad \mathbf{W} = \mathbf{U}_q\mathbf{L}\mathbf{R}^{\top}$$

- Solution for Dual Probabilistic PCA (solves for the latent positions)

$$\mathbf{Y}\mathbf{Y}^{\top}\mathbf{U}_q' = \mathbf{U}_q'\boldsymbol{\Lambda}_q \qquad \mathbf{X} = \mathbf{U}_q'\mathbf{L}\mathbf{R}^{\top}$$

- Equivalence is from

$$\mathbf{U}_q = \mathbf{Y}^{\top}\mathbf{U}_q'\boldsymbol{\Lambda}_q^{-\frac{1}{2}}$$

Non-Linear Latent Variable Model

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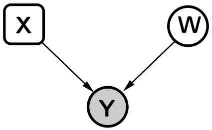

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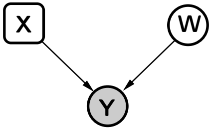
- Inspection of the marginal likelihood shows ...



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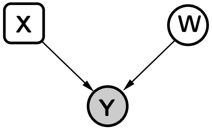

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Dual Probabilistic PCA

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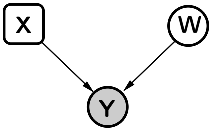
  - We recognise it as the 'linear kernel'.



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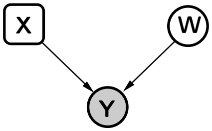
$$\mathbf{K} = \mathbf{X}\mathbf{X}^{\top} + \sigma^2\mathbf{I}$$

This is a product of Gaussian processes with linear kernels.

Non-Linear Latent Variable Model

Dual Probabilistic PCA

- Inspection of the marginal likelihood shows ...
  - The covariance matrix is a covariance function.
  - We recognise it as the 'linear kernel'.
  - We call this the Gaussian Process Latent Variable model (GP-LVM).



$$p(\mathbf{Y}|\mathbf{X}) = \prod_{j=1}^{p} \mathcal{N}\left(\mathbf{y}_{:,j}|\mathbf{0}, \mathbf{K}\right)$$

$$\mathbf{K} = ?$$

Replace linear kernel with non-linear kernel for non-linear model.

RBF Kernel

- The RBF kernel has the form $k_{i,j} = k\left(\mathbf{x}_{i,:}, \mathbf{x}_{j,:}\right)$, where

$$k\left(\mathbf{x}_{i,:}, \mathbf{x}_{j,:}\right) = \alpha \exp\left(-\frac{\left(\mathbf{x}_{i,:} - \mathbf{x}_{j,:}\right)^{\top}\left(\mathbf{x}_{i,:} - \mathbf{x}_{j,:}\right)}{2\ell^{2}}\right).$$

- No longer possible to optimise wrt $\mathbf{X}$ via an eigenvalue problem.
- Instead find gradients with respect to $\mathbf{X}, \alpha, \ell$ and σ^2 and optimise using conjugate gradients.

Applications

Style Based Inverse Kinematics

- Facilitating animation through modeling human motion with the GP-LVM (Grochow et al., 2004)

Tracking

- Tracking using models of human motion learnt with the GP-LVM (Urtasun et al., 2005, 2006)

Stick Man

Generalization with less Data than Dimensions

- Powerful uncertainly handling of GPs leads to suprising properties.
- Non-linear models can be used where there are fewer data points than dimensions *without overfitting*.
- Example: Modelling a stick man in 102 dimensions with 55 data points!

Stick Man II

`demStick1`

Figure: The latent space for the stick man motion capture data.

Stick Man II

`demStick1`

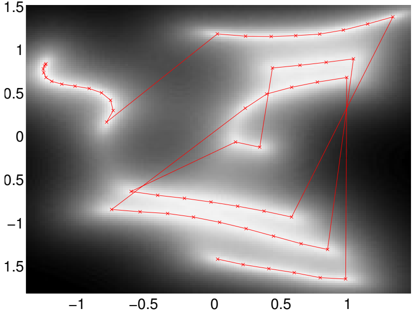


Figure: The latent space for the stick man motion capture data.

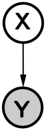
Selecting Data Dimensionality

- GP-LVM Provides probabilistic non-linear dimensionality reduction.
- How to select the dimensionality?
- Bayesian approach to model selection (Titsias and Lawrence, 2010).

Integrate Mapping Function and Latent Variables

Bayesian GP-LVM

- Start with a standard GP-LVM.

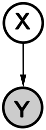


$$p(\mathbf{Y}|\mathbf{X}) = \prod_{j=1}^{p} \mathcal{N}\left(\mathbf{y}_{:,j}|\mathbf{0}, \mathbf{K}\right)$$

Integrate Mapping Function and Latent Variables

Bayesian GP-LVM

- Start with a standard GP-LVM.
- Apply standard latent variable approach:
  - Define Gaussian prior over *latent space*, $\mathbf{X}$.

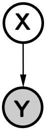


$$p(\mathbf{Y}|\mathbf{X}) = \prod_{j=1}^{p} \mathcal{N}\left(\mathbf{y}_{:,j}|\mathbf{0},\mathbf{K}\right)$$

Integrate Mapping Function and Latent Variables

Bayesian GP-LVM

- Start with a standard GP-LVM.
- Apply standard latent variable approach:
  - Define Gaussian prior over *latent space*, $\mathbf{X}$.
  - Integrate out *latent variables*.



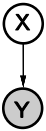
$$p(\mathbf{Y}|\mathbf{X}) = \prod_{j=1}^{p} \mathcal{N}\left(\mathbf{y}_{:,j}|\mathbf{0}, \mathbf{K}\right)$$

$$p(\mathbf{X}) = \prod_{j=1}^{q} \mathcal{N}\left(\mathbf{x}_{:,j}|\mathbf{0}, \alpha_i^{-2}\mathbf{I}\right)$$

Integrate Mapping Function and Latent Variables

Bayesian GP-LVM

- Start with a standard GP-LVM.
- Apply standard latent variable approach:
  - Define Gaussian prior over *latent space*, $\mathbf{X}$.
  - Integrate out *latent variables*.
  - Unfortunately integration is intractable. Use variational approximations (Titsias and Lawrence, 2010).



$$p(\mathbf{Y}|\mathbf{X}) = \prod_{j=1}^{p} \mathcal{N}\left(\mathbf{y}_{:,j}|\mathbf{0}, \mathbf{K}\right)$$

$$p(\mathbf{X}) = \prod_{j=1}^{q} \mathcal{N}\left(\mathbf{x}_{:,j}|\mathbf{0}, \alpha_i^{-2}\mathbf{I}\right)$$

$$p(\mathbf{Y}|\alpha) = ??$$

Learning Dimensionality: Automatic Relevance Determination

- Precision parameters, $\{\alpha_i\}_{i=1}^q$, softly switch off latent dimensions.

$$p(\mathbf{X}) = \prod_{j=1}^{q} \mathcal{N}\left(\mathbf{x}_{:,j}|\mathbf{0}, \alpha_i^{-2}\mathbf{I}\right)$$

- Equivalently, scale columns of $\mathbf{X}$ in the covariance function

$$k(\mathbf{x}_{i,:}, \mathbf{x}_{j,:}) = \exp\left(-\frac{1}{2}(\mathbf{x}_{:,i} - \mathbf{x}_{:,j})^\top \mathbf{A}^{-1}(\mathbf{x}_{:,i} - \mathbf{x}_{:,j})\right)$$

$\mathbf{A}$ is diagonal with elements α_i^2. Now keep prior spherical

$$p(\mathbf{X}) = \prod_{j=1}^{q} \mathcal{N}\left(\mathbf{x}_{:,j}|\mathbf{0}, \mathbf{I}\right)$$

- Covariance functions of this type are known as ARD (see e.g. Neal, 1996; MacKay, 2003; Rasmussen and Williams, 2006).

Summary

- Spectral approaches to dimensionality reduction have an underlying interpretation as a Gaussian random field.
- The probabilistic model is consistent as $p \to \infty$, not $n \to \infty$.
- Spectral approaches have the neighborhood pre-specified.
- The GP-LVM is also a Gaussian model of data with a generative interpretation.
- In the GP-LVM the "neighborhood" is learnt.
- The Bayesian GP-LVM allows the number of latent dimensions to be determined.

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