

Probabilistic Dimensional Reduction with the Gaussian Process Latent Variable Model

An Overview of the GP-LVM and its extensions with some state
of the art applications

Neil Lawrence
Machine Learning Group
Department of Computer Science
University of Sheffield, U.K.

11th July 2006

Outline

1 Motivation

- High Dimensional Data
- Smooth Low Dimensional Embedded Spaces
- Existing Methodologies

2 Mathematical Foundations

- Probabilistic Linear Dimensionality Reduction
- Gaussian Processes
- A Non-linear Latent Variable Model

3 Examples

- Oil Flow Data
- Motion Capture Data
- Graphics and Vision Applications

4 Extensions

- Back Constraints
- Dynamics



Online Resources

All source code and slides are available online

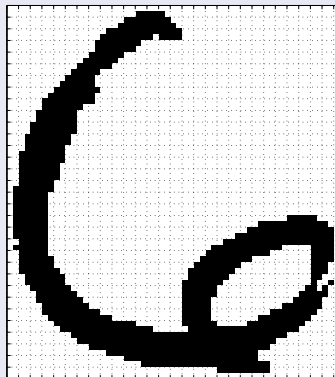
- This talk available from my home page (see talks link on left hand side).
- MATLAB examples in the 'oxford' toolbox (vrs 0.13),
demGplvmTalk.
 - <http://www.dcs.shef.ac.uk/~neil/oxford/>.
- And the 'fgplvm' toolbox (vrs 0.132).
 - <http://www.dcs.shef.ac.uk/~neil/fgplvm/>.
- MATLAB commands used for examples given in typewriter font.



High Dimensional Data

USPS Data Set Handwritten Digit

- 3648 Dimensions
 - 64 rows by 57 columns
- Space contains more than just this digit.
- Even if we sample every nanosecond from now until the end of the universe, you won't see the original six!



High Dimensional Data

USPS Data Set Handwritten Digit

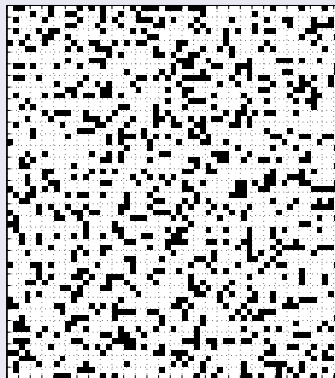
- 3648 Dimensions
 - 64 rows by 57 columns
- Space contains more than just this digit.
- Even if we sample every nanosecond from now until the end of the universe, you won't see the original six!



High Dimensional Data

USPS Data Set Handwritten Digit

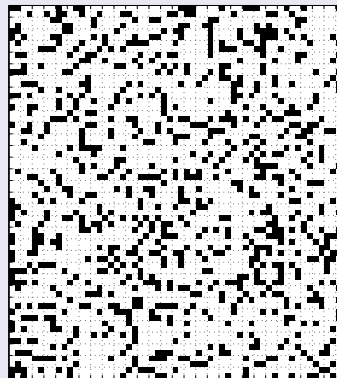
- 3648 Dimensions
 - 64 rows by 57 columns
- Space contains more than just this digit.
- Even if we sample every nanosecond from now until the end of the universe, you won't see the original six!



High Dimensional Data

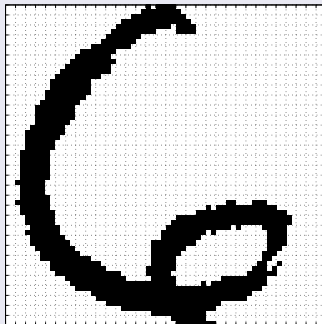
USPS Data Set Handwritten Digit

- 3648 Dimensions
 - 64 rows by 57 columns
- Space contains more than just this digit.
- Even if we sample every nanosecond from now until the end of the universe, you won't see the original six!



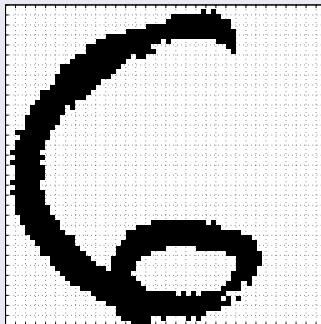
Simple Model of Digit

Rotate a 'Prototype'



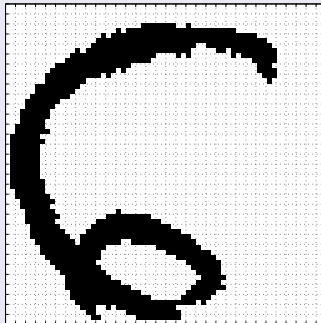
Simple Model of Digit

Rotate a 'Prototype'



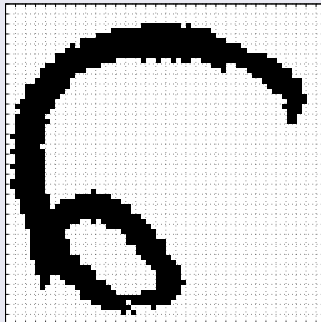
Simple Model of Digit

Rotate a 'Prototype'



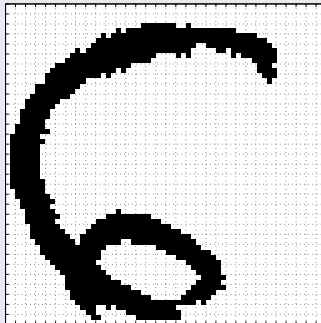
Simple Model of Digit

Rotate a 'Prototype'



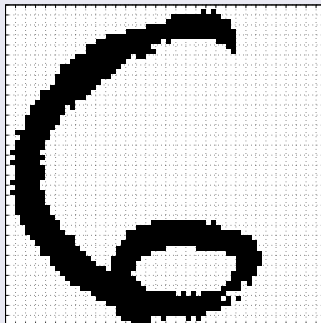
Simple Model of Digit

Rotate a 'Prototype'



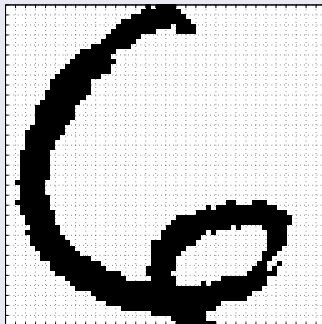
Simple Model of Digit

Rotate a 'Prototype'



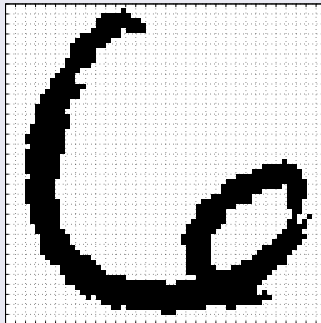
Simple Model of Digit

Rotate a 'Prototype'



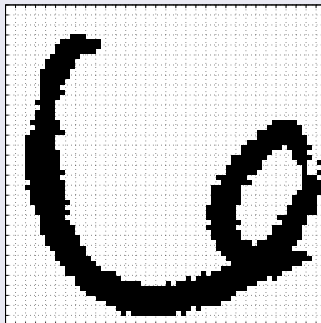
Simple Model of Digit

Rotate a 'Prototype'



Simple Model of Digit

Rotate a 'Prototype'

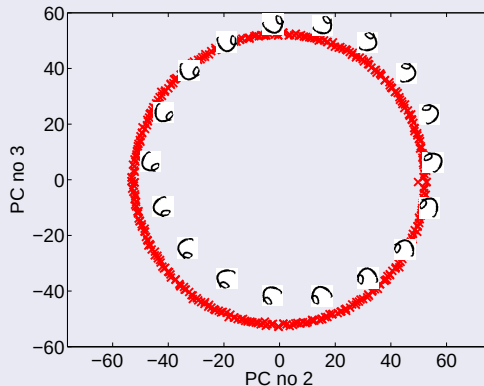


MATLAB Demo

```
demDigitsManifold[2 3], 'all')
```

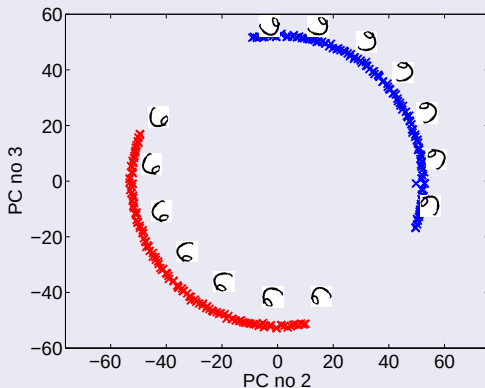
MATLAB Demo

```
demDigitsManifold[2 3], 'all')
```



MATLAB Demo

```
demDigitsManifold([2 3], 'sixnine')
```



Low Dimensional Manifolds

Pure Rotation is too Simple

- In practice the data may undergo several distortions.
 - e.g. digits undergo 'thinning', translation and rotation.
- For data with 'structure':
 - we expect fewer distortions than dimensions;
 - we therefore expect the data to live on a lower dimensional manifold.
- Conclusion: deal with high dimensional data by looking for lower dimensional non-linear embedding.



Existing Methods

Spectral Approaches

- Classical Multidimensional Scaling (MDS) [Mardia et al., 1979].
 - Uses eigenvectors of similarity matrix.
 - Isomap [Tenenbaum et al., 2000] is MDS with a particular proximity measure.
 - Kernel PCA [Schölkopf et al., 1998]
 - Provides a low dimensional representation and a mapping.
 - Mapping is implied through the use of a kernel function as a similarity matrix.
 - Locally Linear Embedding [Roweis and Saul, 2000].
 - Looks to preserve locally linear relationships in a low dimensional space.



Existing Methods II

Iterative Methods

- Multidimensional Scaling (MDS)
 - Iterative optimisation of a stress function [Kruskal, 1964].
 - Sammon Mappings [Sammon, 1969].
 - Strictly speaking not a mapping — similar to iterative MDS.
- NeuroScale [Lowe and Tipping, 1997]
 - Augmentation of iterative MDS methods with a mapping.



Existing Methods III

Probabilistic Approaches

- Probabilistic PCA [Tipping and Bishop, 1999, Roweis, 1998]
 - A linear method.
- Density Networks [MacKay, 1995]
 - Use importance sampling and a multi-layer perceptron.
- Generative Topographic Mapping (GTM) [Bishop et al., 1998]
 - Uses a grid based sample and an RBF network.



Existing Methods III

Probabilistic Approaches

- Probabilistic PCA [Tipping and Bishop, 1999, Roweis, 1998]
 - A linear method.
- Density Networks [MacKay, 1995]
 - Use importance sampling and a multi-layer perceptron.
- Generative Topographic Mapping (GTM) [Bishop et al., 1998]
 - Uses a grid based sample and an RBF network.



Existing Methods III

Probabilistic Approaches

- Probabilistic PCA [Tipping and Bishop, 1999, Roweis, 1998]
 - A linear method.
- Density Networks [MacKay, 1995]
 - Use importance sampling and a multi-layer perceptron.
- Generative Topographic Mapping (GTM) [Bishop et al., 1998]
 - Uses a grid based sample and an RBF network.



Existing Methods III

Probabilistic Approaches

- Probabilistic PCA [Tipping and Bishop, 1999, Roweis, 1998]
 - A linear method.
- Density Networks [MacKay, 1995]
 - Use importance sampling and a multi-layer perceptron.
- Generative Topographic Mapping (GTM) [Bishop et al., 1998]
 - Uses a grid based sample and an RBF network.

Difficulty for Probabilistic Approaches

Propagate a probability distribution through a non-linear mapping.



The New Model

A Probabilistic Non-linear PCA

- PCA has a probabilistic interpretation [Tipping and Bishop, 1999].
- It is difficult to 'non-linearise'.

Dual Probabilistic PCA

- We present a new probabilistic interpretation of PCA [Lawrence, 2005].
- This interpretation can be made non-linear.
- The result is non-linear probabilistic PCA.



Notation

q — dimension of latent/embedded space

d — dimension of data space

n — number of data points

centred data, $\mathbf{Y} = [\mathbf{y}_{1,:}, \dots, \mathbf{y}_{n,:}]^T = [\mathbf{y}_{:,1}, \dots, \mathbf{y}_{:,d}] \in \mathbb{R}^{n \times d}$

latent variables, $\mathbf{X} = [\mathbf{x}_{1,:}, \dots, \mathbf{x}_{n,:}]^T = [\mathbf{x}_{:,1}, \dots, \mathbf{x}_{:,q}] \in \mathbb{R}^{n \times q}$

mapping matrix, $\mathbf{W} \in \mathbb{R}^{d \times q}$

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

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



Reading Notation

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

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



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

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

where

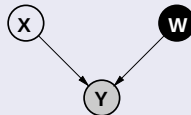
$$\boldsymbol{\eta}_{i,:} \sim N(\mathbf{0}, \sigma^2 \mathbf{I}).$$



Linear Latent Variable Model

Probabilistic PCA

- Define *linear-Gaussian relationship* between latent variables and data.
- **Standard** Latent variable approach:
 - Define Gaussian prior over latent space, $\mathbf{X}$.
 - Integrate out latent variables.



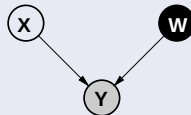
$$p(\mathbf{Y}|\mathbf{X}, \mathbf{W}) = \prod_{i=1}^n N(\mathbf{y}_{i,:} | \mathbf{W}\mathbf{x}_{i,:}, \sigma^2 \mathbf{I})$$



Linear Latent Variable Model

Probabilistic PCA

- Define *linear-Gaussian relationship* between latent variables and data.
- **Standard** Latent variable approach:
 - Define Gaussian prior over *latent space*, $\mathbf{X}$.
 - Integrate out *latent variables*.



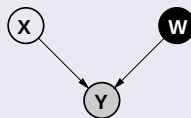
$$p(\mathbf{Y}|\mathbf{X}, \mathbf{W}) = \prod_{i=1}^n N(\mathbf{y}_{i,:} | \mathbf{W}\mathbf{x}_{i,:}, \sigma^2 \mathbf{I})$$



Linear Latent Variable Model

Probabilistic PCA

- Define *linear-Gaussian relationship* between latent variables and data.
- **Standard** Latent variable approach:
 - Define Gaussian prior over *latent space*, $\mathbf{X}$.
 - Integrate out *latent variables*.



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

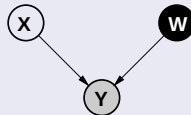
$$p(\mathbf{X}) = \prod_{i=1}^n N(\mathbf{x}_{i,:} | \mathbf{0}, \mathbf{I})$$



Linear Latent Variable Model

Probabilistic PCA

- Define *linear-Gaussian relationship* between latent variables and data.
- **Standard** Latent variable approach:
 - Define Gaussian prior over *latent space*, $\mathbf{X}$.
 - Integrate out *latent variables*.



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

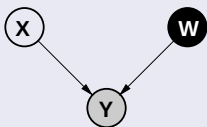
$$p(\mathbf{X}) = \prod_{i=1}^n N(\mathbf{x}_{i,:} | \mathbf{0}, \mathbf{I})$$

$$p(\mathbf{Y}|\mathbf{W}) = \prod_{i=1}^n N(\mathbf{y}_{i,:} | \mathbf{0}, \mathbf{W}\mathbf{W}^T + \sigma^2 \mathbf{I})$$



Linear Latent Variable Model II

Probabilistic PCA Max. Likelihood Soln [Tipping and Bishop, 1999]



$$p(\mathbf{Y}|\mathbf{W}) = \prod_{i=1}^n \mathcal{N}(\mathbf{y}_{i,:} | \mathbf{0}, \mathbf{W}\mathbf{W}^T + \sigma^2 \mathbf{I})$$



Linear Latent Variable Model II

Probabilistic PCA Max. Likelihood Soln [Tipping and Bishop, 1999]

$$p(\mathbf{Y}|\mathbf{W}) = \prod_{i=1}^n N(\mathbf{y}_{i,:}|\mathbf{0}, \mathbf{C}), \quad \mathbf{C} = \mathbf{W}\mathbf{W}^T + \sigma^2\mathbf{I}$$

$$\log p(\mathbf{Y}|\mathbf{W}) = -\frac{n}{2} \log |\mathbf{C}| - \frac{1}{2} \text{tr}(\mathbf{C}^{-1}\mathbf{Y}^T\mathbf{Y}) + \text{const.}$$

If $\mathbf{U}_q$ are first q principal eigenvectors of $n^{-1}\mathbf{Y}^T\mathbf{Y}$ and the corresponding eigenvalues are Λ_q ,

$$\mathbf{W} = \mathbf{U}_q \mathbf{L} \mathbf{V}^T, \quad \mathbf{L} = (\Lambda_q - \sigma^2 \mathbf{I})^{\frac{1}{2}}$$

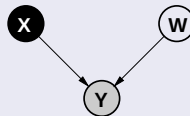
where $\mathbf{V}$ is an arbitrary rotation matrix.



Linear Latent Variable Model III

Dual Probabilistic PCA

- Define *linear-Gaussian relationship* between latent variables and data.
- **Novel** Latent variable approach:
 - Define Gaussian prior over *parameters*, $\mathbf{W}$.
 - Integrate out *parameters*.



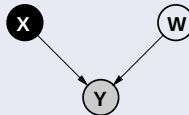
$$p(\mathbf{Y}|\mathbf{X}, \mathbf{W}) = \prod_{i=1}^n N(\mathbf{y}_{i,:} | \mathbf{W}\mathbf{x}_{i,:}, \sigma^2 \mathbf{I})$$



Linear Latent Variable Model III

Dual Probabilistic PCA

- Define *linear-Gaussian relationship* between latent variables and data.
- **Novel** Latent variable approach:
 - Define Gaussian prior over *parameters*, $\mathbf{W}$.
 - Integrate out *parameters*.



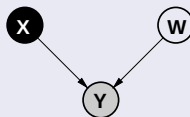
$$p(\mathbf{Y}|\mathbf{X}, \mathbf{W}) = \prod_{i=1}^n N(\mathbf{y}_{i,:} | \mathbf{W}\mathbf{x}_{i,:}, \sigma^2 \mathbf{I})$$



Linear Latent Variable Model III

Dual Probabilistic PCA

- Define *linear-Gaussian relationship* between latent variables and data.
- **Novel** Latent variable approach:
 - Define Gaussian prior over *parameters*, $\mathbf{W}$.
 - Integrate out *parameters*.



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

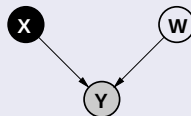
$$p(\mathbf{W}) = \prod_{i=1}^d N(\mathbf{w}_{i,:} | \mathbf{0}, \mathbf{I})$$



Linear Latent Variable Model III

Dual Probabilistic PCA

- Define *linear-Gaussian relationship* between latent variables and data.
- **Novel** Latent variable approach:
 - Define Gaussian prior over *parameters*, $\mathbf{W}$.
 - Integrate out *parameters*.



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

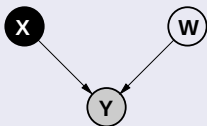
$$p(\mathbf{W}) = \prod_{i=1}^d N(\mathbf{w}_{i,:} | \mathbf{0}, \mathbf{I})$$

$$p(\mathbf{Y}|\mathbf{X}) = \prod_{j=1}^d N(\mathbf{y}_{:,j} | \mathbf{0}, \mathbf{X}\mathbf{X}^T + \sigma^2 \mathbf{I})$$



Linear Latent Variable Model IV

Dual Probabilistic PCA Max. Likelihood Soln [Lawrence, 2004]



$$p(\mathbf{Y}|\mathbf{X}) = \prod_{j=1}^d N(\mathbf{y}_{:,j} | \mathbf{0}, \mathbf{X}\mathbf{X}^T + \sigma^2 \mathbf{I})$$



Linear Latent Variable Model IV

Dual Probabilistic PCA Max. Likelihood Soln [Lawrence, 2004]

$$p(\mathbf{Y}|\mathbf{X}) = \prod_{j=1}^d N(\mathbf{y}_{:,j} | \mathbf{0}, \mathbf{K}), \quad \mathbf{K} = \mathbf{X}\mathbf{X}^T + \sigma^2 \mathbf{I}$$

$$\log p(\mathbf{Y}|\mathbf{X}) = -\frac{d}{2} \log |\mathbf{K}| - \frac{1}{2} \text{tr}(\mathbf{K}^{-1} \mathbf{Y}\mathbf{Y}^T) + \text{const.}$$

If $\mathbf{U}'_q$ are first q principal eigenvectors of $d^{-1} \mathbf{Y}\mathbf{Y}^T$ and the corresponding eigenvalues are Λ_q ,

$$\mathbf{X} = \mathbf{U}'_q \mathbf{L} \mathbf{V}^T, \quad \mathbf{L} = (\Lambda_q - \sigma^2 \mathbf{I})^{\frac{1}{2}}$$

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



Linear Latent Variable Model IV

Probabilistic PCA Max. Likelihood Soln [Tipping and Bishop, 1999]

$$p(\mathbf{Y}|\mathbf{W}) = \prod_{i=1}^n N(\mathbf{y}_{i,:}|\mathbf{0}, \mathbf{C}), \quad \mathbf{C} = \mathbf{W}\mathbf{W}^T + \sigma^2\mathbf{I}$$

$$\log p(\mathbf{Y}|\mathbf{W}) = -\frac{n}{2} \log |\mathbf{C}| - \frac{1}{2} \text{tr}(\mathbf{C}^{-1}\mathbf{Y}^T\mathbf{Y}) + \text{const.}$$

If $\mathbf{U}_q$ are first q principal eigenvectors of $n^{-1}\mathbf{Y}^T\mathbf{Y}$ and the corresponding eigenvalues are Λ_q ,

$$\mathbf{W} = \mathbf{U}_q \mathbf{L} \mathbf{V}^T, \quad \mathbf{L} = (\Lambda_q - \sigma^2 \mathbf{I})^{\frac{1}{2}}$$

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



Equivalence of Formulations

The Eigenvalue Problems are equivalent

- Solution for Probabilistic PCA (solves for the mapping)

$$\mathbf{Y}^T \mathbf{Y} \mathbf{U}_q = \mathbf{U}_q \Lambda_q \quad \mathbf{W} = \mathbf{U}_q \mathbf{L} \mathbf{V}^T$$

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

$$\mathbf{Y} \mathbf{Y}^T \mathbf{U}'_q = \mathbf{U}'_q \Lambda_q \quad \mathbf{X} = \mathbf{U}'_q \mathbf{L} \mathbf{V}^T$$

- Equivalence is from

$$\mathbf{U}_q = \mathbf{Y}^T \mathbf{U}'_q \Lambda_q^{-\frac{1}{2}}$$



Gaussian Process (GP)

Prior for Functions

- Probability Distribution over Functions
 - Functions are infinite dimensional.
 - Prior distribution over *instantiations* of the function: finite dimensional objects.
- Can prove by induction that GP is 'consistent'.
- Mean and Covariance Functions
 - Instead of mean and covariance matrix, GP is defined by mean function and covariance function.
 - Mean function often taken to be zero or constant.
 - Covariance function must be *positive definite*.
 - Class of valid covariance functions is the same as the class of *Mercer kernels*.



Gaussian Processes II

Zero mean Gaussian Process

- A (zero mean) Gaussian process likelihood is of the form

$$p(\mathbf{y}|\mathbf{X}) = N(\mathbf{y}|\mathbf{0}, \mathbf{K}),$$

where $\mathbf{K}$ is the covariance function or *kernel*.

- The *linear kernel* with noise has the form

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

- Priors over non-linear functions are also possible.
 - To see what functions look like, we can sample from the prior process.



Covariance Samples

demCovFuncSample

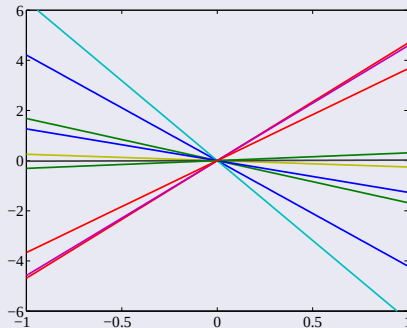


Figure: linear kernel, $\mathbf{K} = \mathbf{XX}^T$



Covariance Samples

demCovFuncSample

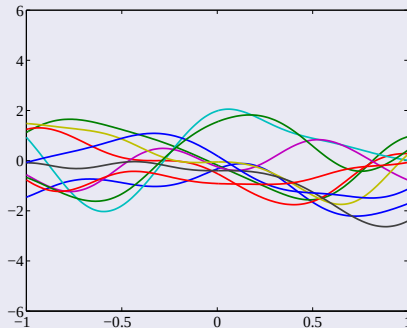


Figure: RBF kernel with $\gamma = 10$, $\alpha = 1$



Covariance Samples

demCovFuncSample

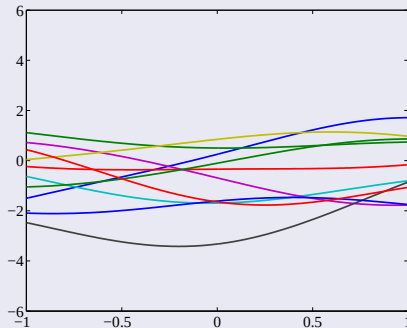


Figure: RBF kernel with $l = 1$, $\alpha = 1$



Covariance Samples

demCovFuncSample

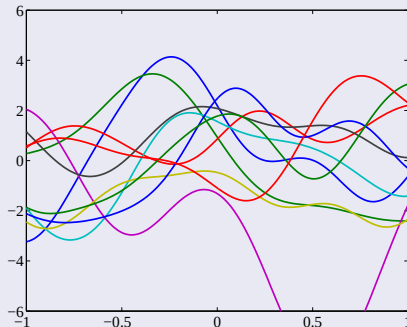


Figure: RBF kernel with $l = 0.3$, $\alpha = 4$



Covariance Samples

demCovFuncSample

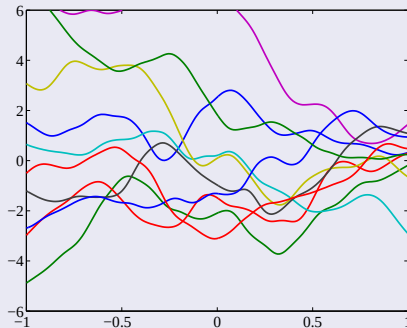


Figure: MLP kernel with $\alpha = 8$, $w = 100$ and $b = 100$



Covariance Samples

demCovFuncSample

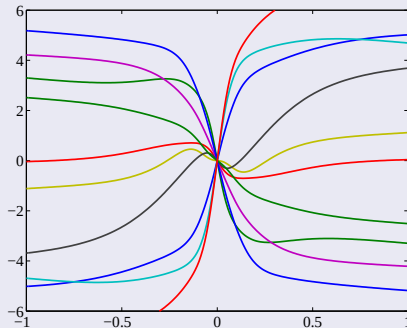


Figure: MLP kernel with $\alpha = 8$, $b = 0$ and $w = 100$



Covariance Samples

demCovFuncSample

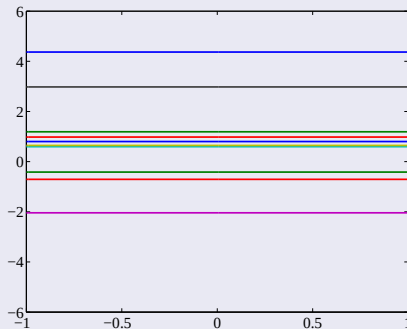


Figure: bias kernel with $\alpha = 1$ and



Covariance Samples

demCovFuncSample

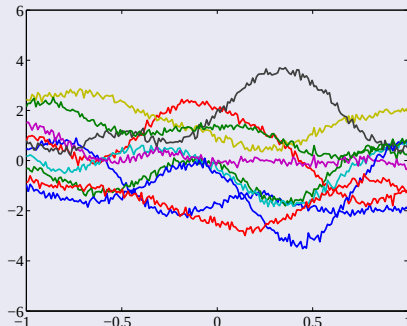


Figure: summed combination of: RBF kernel, $\alpha = 1$, $l = 0.3$; bias kernel, $\alpha = 1$; and white noise kernel, $\beta = 100$



Gaussian Process Regression

Posterior Distribution over Functions

- Gaussian processes are often used for regression.
- We are given a known inputs $\mathbf{X}$ and targets $\mathbf{Y}$.
- We assume a prior distribution over functions by selecting a kernel.
- Combine the prior with data to get a *posterior* distribution over functions.



Gaussian Process Regression

demRegression

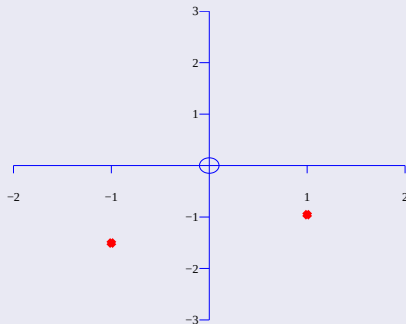


Figure: Examples include WiFi localization, C14 calibration curve.



Gaussian Process Regression

demRegression

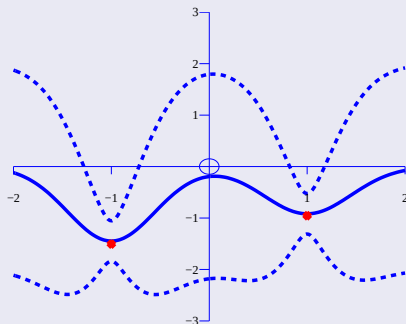


Figure: Examples include WiFi localization, C14 calibration curve.



Gaussian Process Regression

demRegression

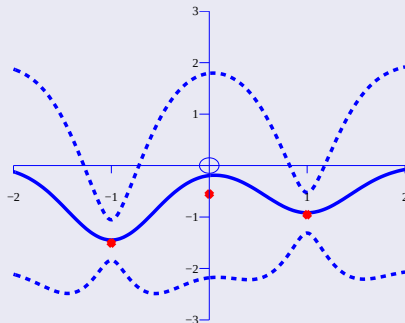


Figure: Examples include WiFi localization, C14 calibration curve.



Gaussian Process Regression

demRegression

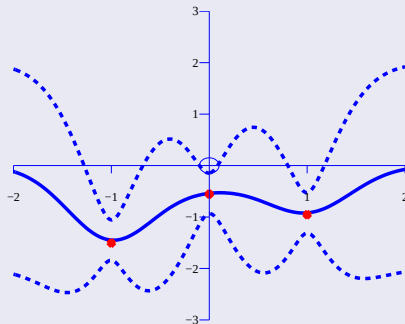


Figure: Examples include WiFi localization, C14 calibration curve.



Gaussian Process Regression

demRegression

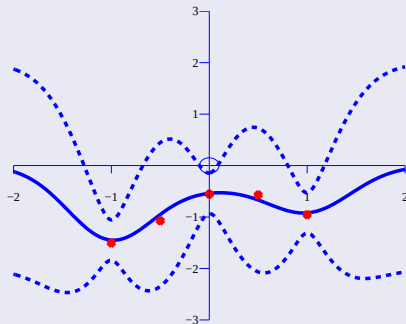


Figure: Examples include WiFi localization, C14 calibration curve.



Gaussian Process Regression

demRegression

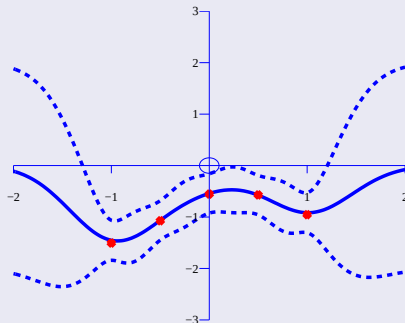


Figure: Examples include WiFi localization, C14 calibration curve.



Gaussian Process Regression

demRegression

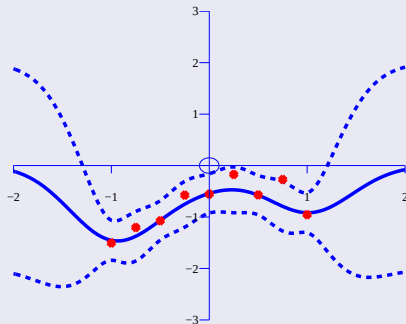


Figure: Examples include WiFi localization, C14 calibration curve.



Gaussian Process Regression

demRegression

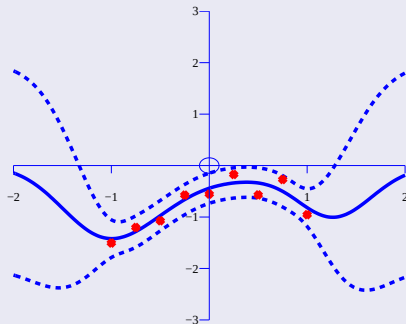


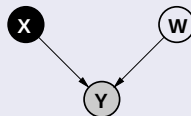
Figure: Examples include WiFi localization, C14 calibration curve.



Non-Linear Latent Variable Model

Dual Probabilistic PCA

- Define *linear-Gaussian relationship* between latent variables and data.
- **Novel** Latent variable approach:
 - Define Gaussian prior over *parameters*, $\mathbf{W}$.
 - Integrate out *parameters*.



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

$$p(\mathbf{W}) = \prod_{i=1}^d N(\mathbf{w}_{i,:} | \mathbf{0}, \mathbf{I})$$

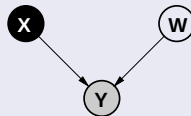
$$p(\mathbf{Y}|\mathbf{X}) = \prod_{j=1}^d N(\mathbf{y}_{:,j} | \mathbf{0}, \mathbf{X}\mathbf{X}^T + \sigma^2 \mathbf{I})$$



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).



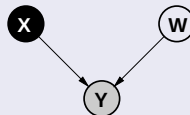
$$p(\mathbf{Y}|\mathbf{X}) = \prod_{j=1}^d N(\mathbf{y}_{:,j} | \mathbf{0}, \mathbf{X}\mathbf{X}^T + \sigma^2 \mathbf{I})$$



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).



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

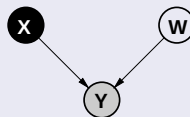
$$\mathbf{K} = \mathbf{X}\mathbf{X}^T + \sigma^2\mathbf{I}$$



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).



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

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

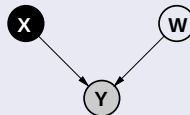
This is a product of Gaussian processes with linear kernels.



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).



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

$$\mathbf{K} = ?$$

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



Non-linear Latent Variable Models

RBF Kernel

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

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

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



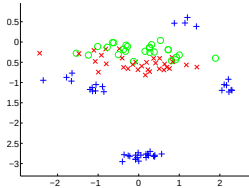
Oil Data I

Example Data set

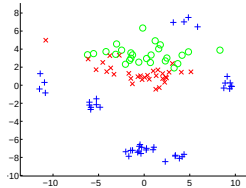
- Oil flow data [Bishop and James, 1993].
- Three phases of flow (stratified, annular, homogenous).
- Twelve measurement probes.
- 1000 data points.
- We sub-sampled to 100 data points
- Compare, with KPCA, MDS, Sammon mappings, PCA and GTM.



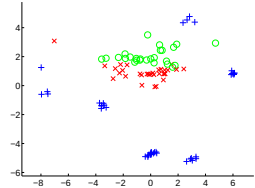
Oil Data II



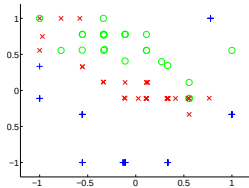
(a) PCA



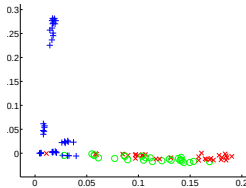
(b) Non-metric MDS



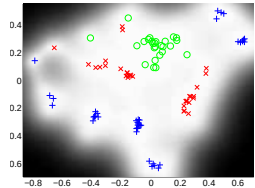
(c) Sammon Mapping



(d) GTM



(e) Kernel PCA



(f) GP-LVM



Oil Data III

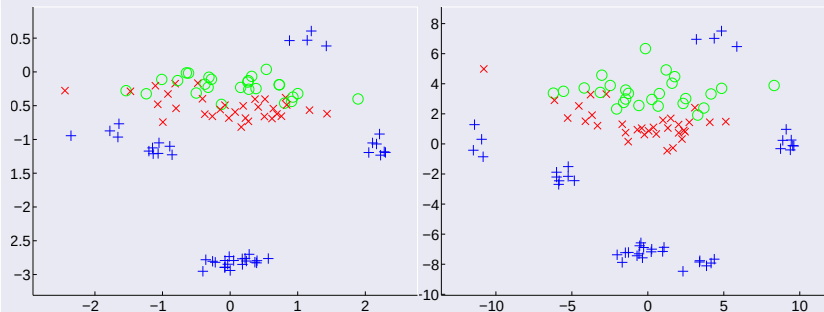


Figure: *Left PCA, right Non-metric MDS*



Oil Data III

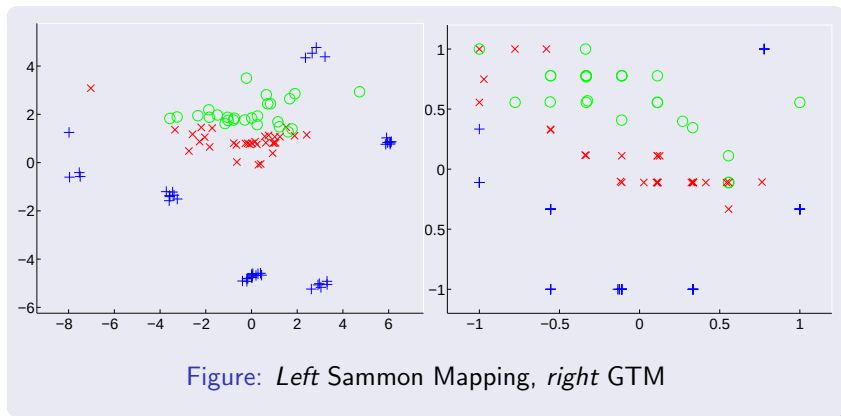


Figure: *Left* Sammon Mapping, *right* GTM



Oil Data III

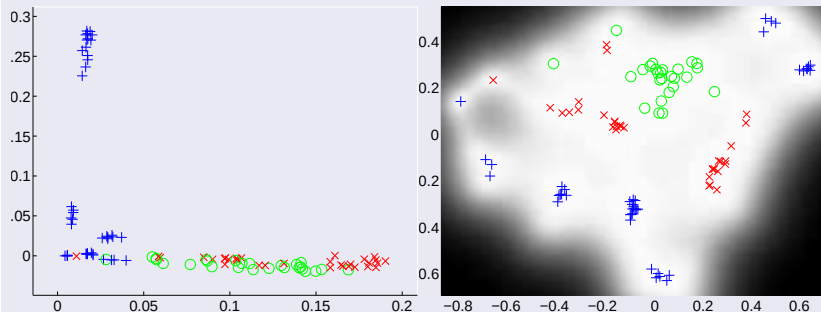


Figure: *Left* Kernel PCA, *right* GP-LVM



Oil Data IV

Nearest neighbour errors in $\mathbf{X}$ space

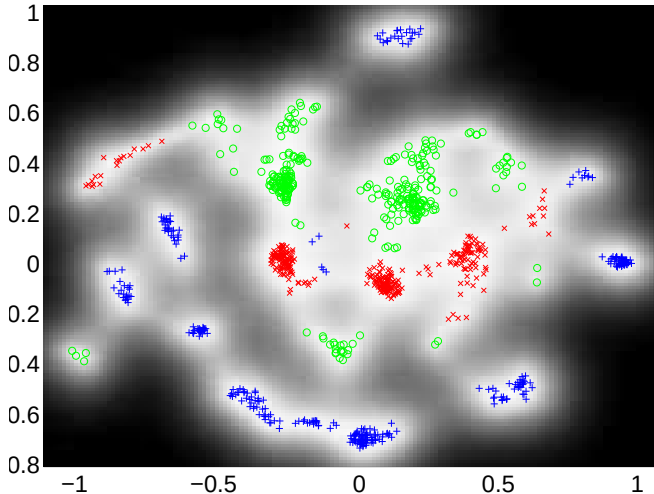
- Nearest neighbour classification in latent space.

Method	PCA	Non-metric MDS	Sammon Mapping
Errors	20	13	6
Method	GTM*	Kernel PCA*	GP-LVM
Errors	7	13	4

* These models require parameter selection.



Full Oil Data Set I



Full Oil Data Set II

Nearest Neighbour error in $\mathbf{X}$

- Nearest neighbour classification in latent space.

Method	PCA	GTM	GP-LVM
Errors	162	11	1

cf 2 errors in data space.



Stick Man

Generalization with less Data than Dimensions

- Powerful uncertainty handling of GPs leads to surprising 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

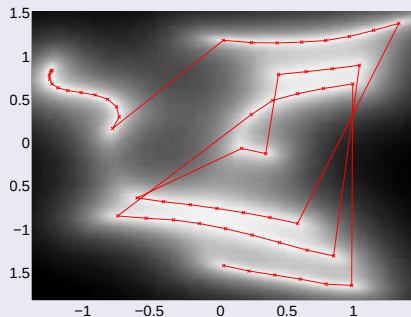


Figure: The latent space for the stick man motion capture data.



Applications

Style Based Inverse Kinematics

Facilitating animation through modelling 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]

Face Animation

Modelling facial motion capture data for synthesis of emotion and speech.



Back Constraints I

Local Distance Preservation [Lawrence and Quiñero Candela, 2006]

- Most dimensional reduction techniques preserve local distances.
- The GP-LVM does not.
- GP-LVM maps smoothly from latent to data space.
 - Points close in latent space are close in data space.
 - This does not imply points close in data space are close in latent space.
- Kernel PCA maps smoothly from data to latent space.
 - Points close in data space are close in latent space.
 - This does not imply points close in latent space are close in data space.

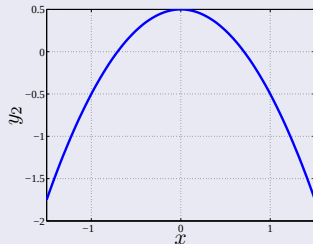
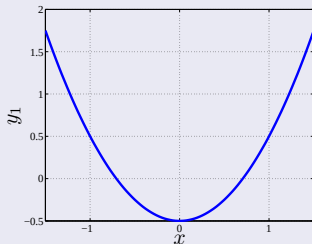


Back Constraints II

Forward Mapping (demBackMapping in oxford toolbox)

- Mapping from 1-D latent space to 2-D data space.

$$y_1 = x^2 - 0.5, \quad y_2 = -x^2 + 0.5$$

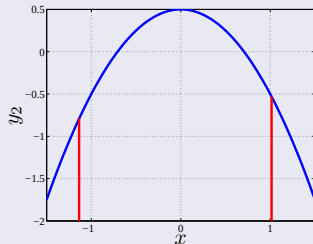
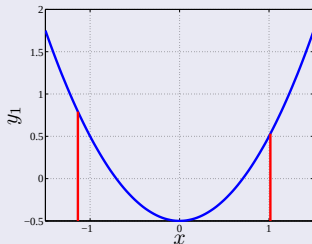


Back Constraints II

Forward Mapping (demBackMapping in oxford toolbox)

- Mapping from 1-D latent space to 2-D data space.

$$y_1 = x^2 - 0.5, \quad y_2 = -x^2 + 0.5$$

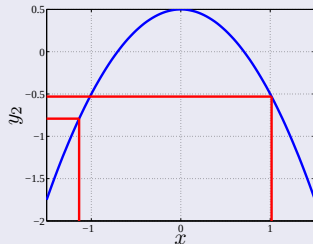
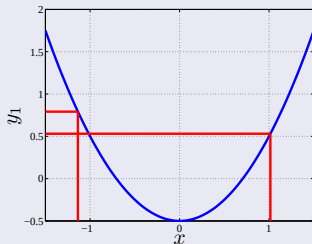


Back Constraints II

Forward Mapping (demBackMapping in oxford toolbox)

- Mapping from 1-D latent space to 2-D data space.

$$y_1 = x^2 - 0.5, \quad y_2 = -x^2 + 0.5$$

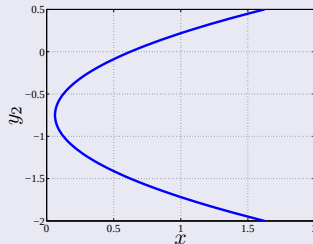
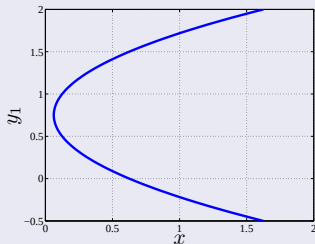


Back Constraints II

Backward Mapping (demBackMapping in oxford toolbox)

- Mapping from 2-D data space to 1-D latent.

$$x = 0.5 (y_1^2 + y_2^2 + 1)$$

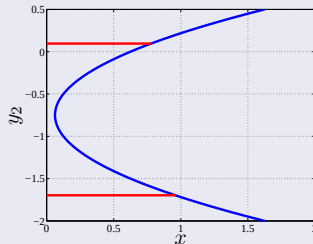
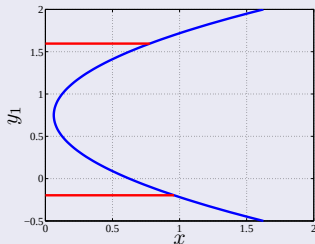


Back Constraints II

Backward Mapping (demBackMapping in oxford toolbox)

- Mapping from 2-D data space to 1-D latent.

$$x = 0.5 (y_1^2 + y_2^2 + 1)$$

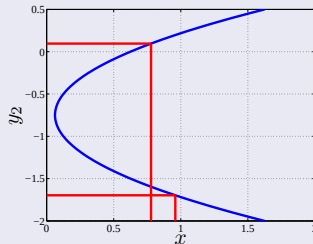
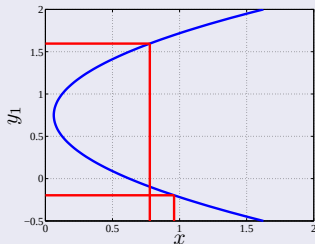


Back Constraints II

Backward Mapping (demBackMapping in oxford toolbox)

- Mapping from 2-D data space to 1-D latent.

$$x = 0.5 (y_1^2 + y_2^2 + 1)$$



NeuroScale

Multi-Dimensional Scaling with a Mapping

- Lowe and Tipping [1997] made latent positions a function of the data.

$$x_{ij} = f_j(\mathbf{y}_i; \mathbf{w})$$

- Function was either multi-layer perceptron or a radial basis function network.
- Their motivation was different from ours:
 - They wanted to add the advantages of a true mapping to multi-dimensional scaling.



Back Constraints in the GP-LVM

Back Constraints

- We can use the same idea to force the GP-LVM to respect local distances.
 - By constraining each $\mathbf{x}_i$ to be a 'smooth' mapping from $\mathbf{y}_i$ local distances can be respected.
- This works because in the GP-LVM we maximise wrt latent variables, we don't integrate out.
- Can use any 'smooth' function:
 - 1 Neural network.
 - 2 RBF Network.
 - 3 Kernel based mapping.



Optimising BC-GPLVM

Computing Gradients

- GP-LVM normally proceeds by optimising

$$L(\mathbf{X}) = \log p(\mathbf{Y}|\mathbf{X})$$

with respect to $\mathbf{X}$ using $\frac{dL}{d\mathbf{X}}$.

- The back constraints are of the form

$$x_{ij} = f_j(\mathbf{y}_{i,:}; \mathbf{B})$$

where $\mathbf{B}$ are parameters.

- We can compute $\frac{dL}{d\mathbf{B}}$ via chain rule and optimise parameters of mapping.

Motion Capture Results

demStick1 and demStick3

Figure: The latent space for the motion capture data with (*right*) and without (*left*) dynamics. The dynamics use a Gaussian process with an RBF kernel.



Motion Capture Results

demStick1 and demStick3

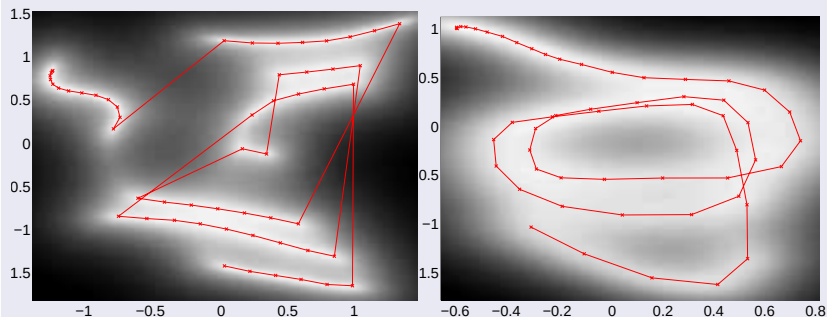
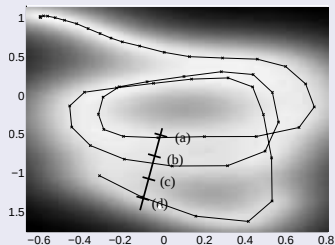


Figure: The latent space for the motion capture data with (*right*) and without (*left*) dynamics. The dynamics use a Gaussian process with an RBF kernel.



Stick Man Results

demStickResults



Projection into data space from four points in the latent space. The inclination of the runner changes becoming more upright.

Vowel Data

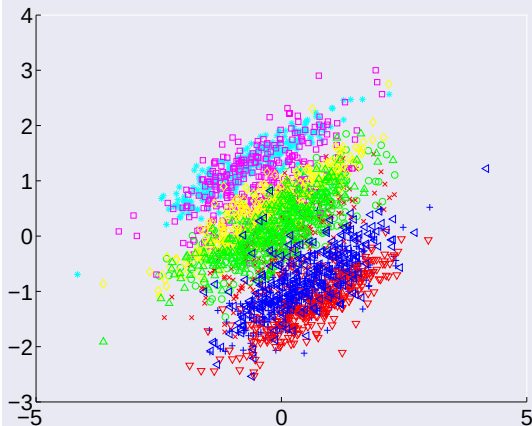
Vocal Joystick Data

- Vowel sounds from a vocal joystick system [Bilmes et al., 2006].
 - <http://ssli.ee.washington.edu/vj>
- Vowels are from a single speaker and represented as:
 - cepstral coefficients (12 dimensions) and
 - 'deltas' (further 12 dimensions).
- 2700 data points in total (300 for each vowel).



PCA Results

PCA (used as initialisation for GP-LVM)

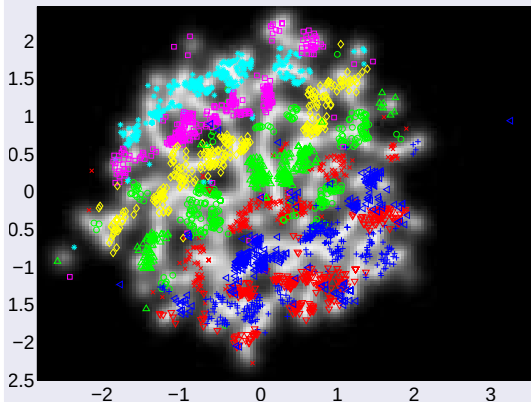


The different vowels are shown as follows: /a/ red cross /ae/ green circle /ao/ blue plus /e/ cyan asterisk /i/ pink square /ibar/ yellow diamond /o/ red down triangle /schwa/ green up triangle and /u/ blue left triangle.



GP-LVM Results

demVowels2

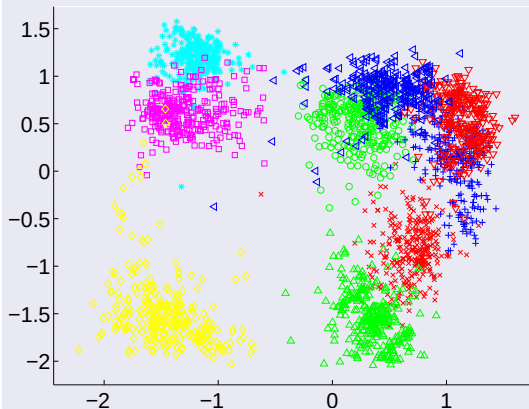


The different vowels are shown as follows: /a/ red cross /ae/ green circle /ao/ blue plus /e/ cyan asterix /i/ pink square /ibar/ yellow diamond /o/ red down triangle /schwa/ green up triangle and /u/ blue left triangle.



Isomap Results

demVowelsIsomap

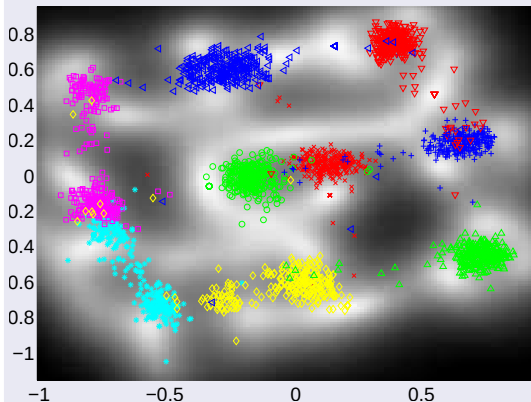


The different vowels are shown as follows: $/a/$ red cross $/ae/$ green circle $/ao/$ blue plus $/e/$ cyan asterisk $/i/$ pink square $/ibar/$ yellow diamond $/o/$ red down triangle $/schwa/$ green up triangle and $/u/$ blue left triangle.



BC-GPLVM Results

demVowels3



The different vowels are shown as follows: /a/ red cross /ae/ green circle /ao/ blue plus /e/ cyan asterisk /i/ pink square /ibar/ yellow diamond /o/ red down triangle /schwa/ green up triangle and /u/ blue left triangle.



1-Nearest Neighbour in $\mathbf{X}$

Comparison of the Approaches

- Nearest neighbour classification in latent space.

Method	GP-LVM	Isomap	BC-GP-LVM
Errors	226	458	155

cf 24 errors in data space.



Adding Dynamics

MAP Solutions for Dynamics Models

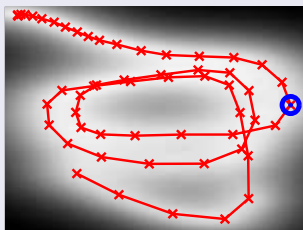
- Data often has a temporal ordering.
- Markov-based dynamics are often used.
- For the GP-LVM
 - Marginalising such dynamics is intractable.
 - But: MAP solutions are trivial to implement.
- Many choices: Kalman filter, Markov chains *etc.*.
- Wang et al. [2006] suggest using a Gaussian Process.



Gaussian Process Dynamics

GP-LVM with Dynamics

- Gaussian process mapping in latent space between time points.



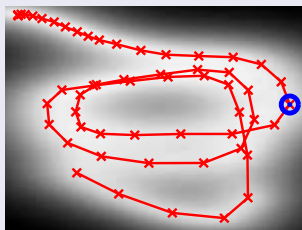
t



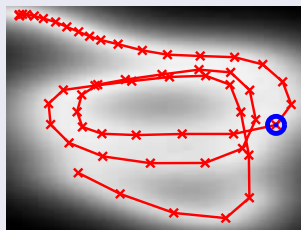
Gaussian Process Dynamics

GP-LVM with Dynamics

- Gaussian process mapping in latent space between time points.



t



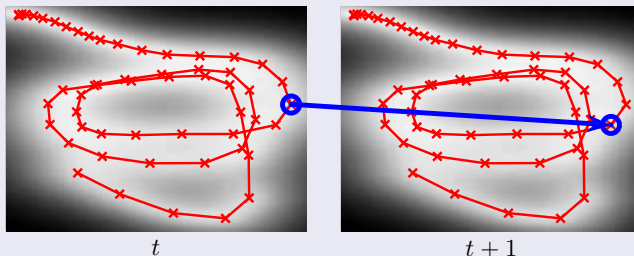
$t + 1$



Gaussian Process Dynamics

GP-LVM with Dynamics

- Gaussian process mapping in latent space between time points.



Motion Capture Results

demStick1 and demStick2

Figure: The latent space for the motion capture data with (*right*) and without (*left*) back constraints based on an RBF kernel.



Motion Capture Results

demStick1 and demStick2

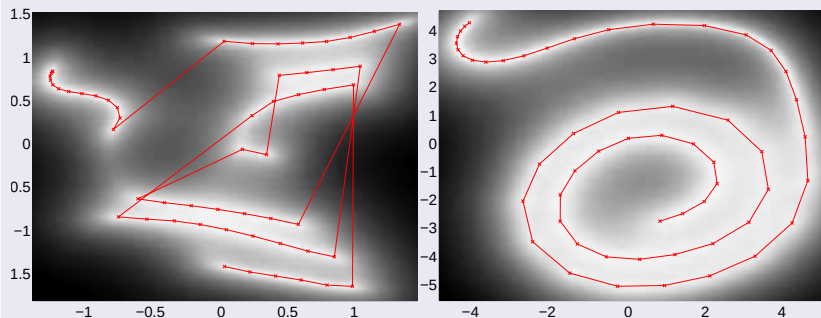


Figure: The latent space for the motion capture data with (*right*) and without (*left*) back constraints based on an RBF kernel.



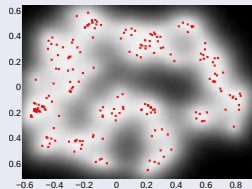
Robot SLAM I

Navigating by WiFi

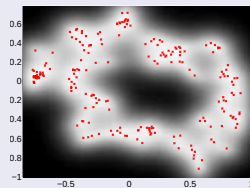
- Wireless access point signal strengths measured by robot moving around building.
 - 215 separate signal strength readings.
 - 30 separate access points.
- Robot moves in two dimensions so we expect data to be inherently 2-D.
- Learn GP-LVM, GP-LVM with Dynamics, back constrained GP-LVM and back constrained GP-LVM with dynamics.



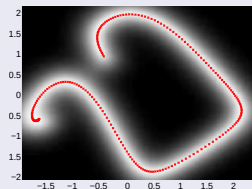
Robot SLAM II



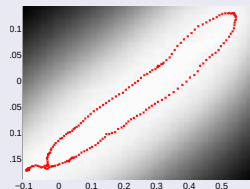
(a) Standard GP-LVM



(b) Standard GP-LVM



(c) Standard GP-LVM



(d) Standard GP-LVM



Summary

- GP-LVM is a Probabilistic Non-Linear Generalisation of PCA.
- Works Effectively as a Probabilistic Model in High Dimensional Spaces.
- Back constraints can be introduced to force local distance preservation.
- Dynamics can be introduced for modelling data with a temporal structure.
- And finally ...



Acknowledgements

Collaborators:

- Vocal Joystick
 - Jeff Bilmes and John Malkin
- Other ongoing work with (PASCAL EU FP6 Network Funded)
 - Phil Torr, Carl Henrik Ek and Raquel Urtasun
- Face Animation.
 - Manuel Sanchez (now at EA).
- Robotics
 - Brian Ferris and Dieter Fox.



Initialisation

'Swiss Roll'

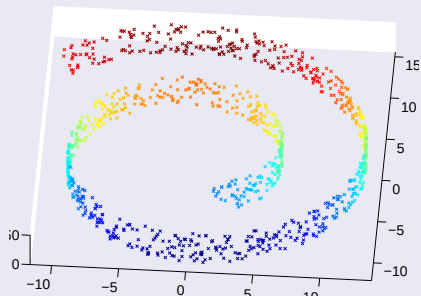


Figure: The 'Swiss Roll' data set is data in three dimensions that is inherently two dimensional.



Initialisation II

Quality of solution is Initialisation Dependent

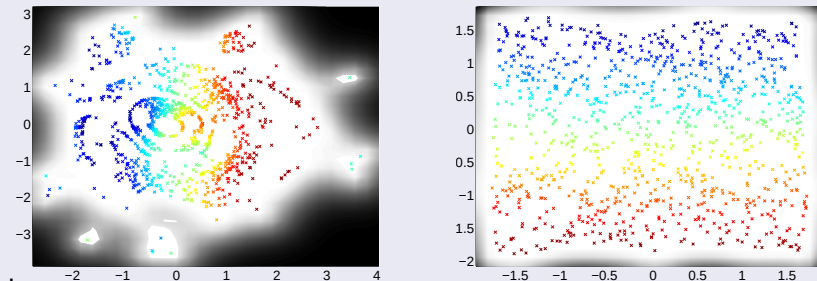


Figure: *Left:* Swiss roll solution initialised by PCA. *Right:* Swiss roll solution initialised by Isomap.



Linear Back Constraints I

- Special case of back constraints is a *linear* back constraint.

$$\mathbf{X} = \mathbf{YB}$$

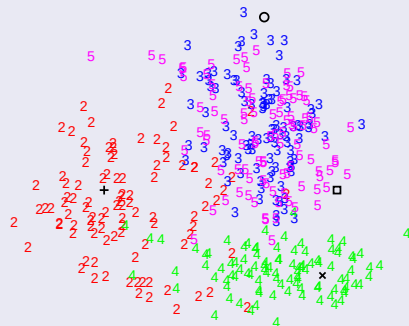
where $\mathbf{B} \in \mathbb{R}^{d \times q}$.

- Maximise the likelihood with respect to the projection matrix $\mathbf{B}$.
- Seems strange to sacrifice the ‘non-linearity’ of the model in this way.
- Motivate this through a digits data set.



Linear Back Constraints II

Digits Model with Linear Back Constraints



Linear Back Constraints III

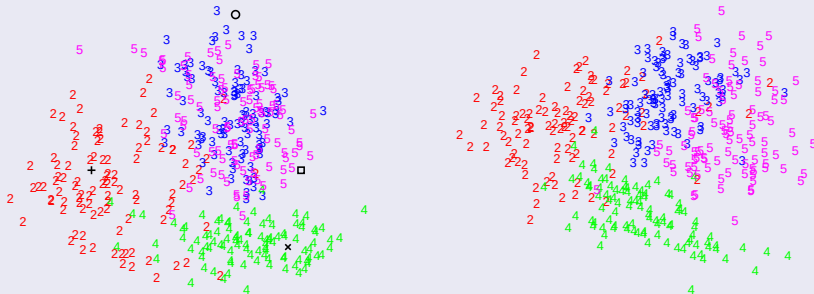


Figure: Linear projections from PCA (*left*) and linear back constrained GP-LVM (*right*)



1-Nearest Neighbour in $\mathbf{X}$

Comparison for increasing latent dimensionality

q	2	3	4
PCA Errors	131	115	47
Linear constrained GP-LVM Errors	79	60	39

c.f. 24 errors in data space



Non-Gaussian Data

Modelling Binary Data

- A common form of non-Gaussian data is *binary data*.
 - Can use Assumed Density Filtering to model binary data.
 - This can also easily be extended to the Expectation Propagation Algorithm Minka [2001].
- Practical consequences:
 - d times slower.
 - requires d times more storage.



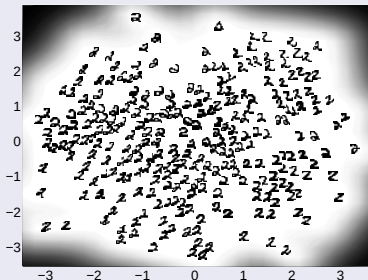
Modelling Binary Twos

Cedar CD ROM digits

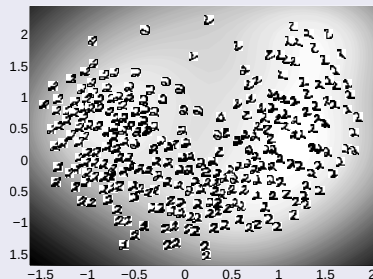
- We model 700 examples of binary 8×8 handwritten twos.
- Use a standard GP-LVM (a Gaussian noise assumption).
- Compare with ADF approximation for the Bernoulli noise model.



Two Results I



(a) Gaussian Noise Model



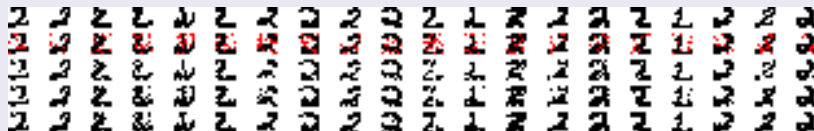
(b) Bernoulli Noise Model

Figure:



Two Results II

Reconstruction of Deleted Pixels



Reconstruction Method	Pixel Error Rate
GP-LVM Bernoulli noise	23.5%
GP-LVM Gaussian noise	35.9%
Missing pixels 'not ink'	51.5%



References

- J. Bilmes, J. Malkin, X. Li, S. Harada, K. Kilanski, K. Kirchhoff, R. Wright, A. Subramanya, J. Landay, P. Dowden, and H. Chizeck. The vocal joystick. In *Proceedings of the IEEE Conference on Acoustics, Speech and Signal Processing*. IEEE, May 2006. To appear.
- C. M. Bishop and G. D. James. Analysis of multiphase flows using dual-energy gamma densitometry and neural networks. *Nuclear Instruments and Methods in Physics Research*, A327:580–593, 1993.
- C. M. Bishop, M. Svensén, and C. K. I. Williams. GTM: the Generative Topographic Mapping. *Neural Computation*, 10(1):215–234, 1998.
- K. Grochow, S. L. Martin, A. Hertzmann, and Z. Popovic. Style-based inverse kinematics. In *ACM Transactions on Graphics (SIGGRAPH 2004)*, 2004.
- J. B. Kruskal. Multidimensional scaling by optimizing goodness-of-fit to a nonmetric hypothesis. *Psychometrika*, 29(1):1–28, 1964.
- N. D. Lawrence. Gaussian process models for visualisation of high dimensional data. In S. Thrun, L. Saul, and B. Schölkopf, editors, *Advances in Neural Information Processing Systems*, volume 16, pages 329–336, Cambridge, MA, 2004. MIT Press.
- N. D. Lawrence. Probabilistic non-linear principal component analysis with Gaussian process latent variable models. *Journal of Machine Learning Research*, 6:1783–1816, Nov 2005.
- N. D. Lawrence and J. Quiñero Candela. Local distance preservation in the GP-LVM through back constraints. In W. Cohen and A. Moore, editors, *Proceedings of the International Conference in Machine Learning*, volume 23, pages 513–520. Omnipress, 2006. ISBN 1-59593-383-2. Accepted for ICML 2006.
- D. Lowe and M. E. Tipping. Neuroscale: Novel topographic feature extraction with radial basis function networks. In M. C. Mozer, M. I. Jordan, and T. Petsche, editors, *Advances in Neural Information Processing Systems*, volume 9, pages 543–549, Cambridge, MA, 1997. MIT Press.
- D. J. C. MacKay. Bayesian neural networks and density networks. *Nuclear Instruments and Methods in Physics Research*, A, 354(1):73–80, 1995.
- K. V. Mardia, J. T. Kent, and J. M. Bibby. *Multivariate analysis*. Academic Press, London, 1979.
- T. P. Minka. Expectation propagation for approximate Bayesian inference. In J. S. Breese and D. Koller, editors, *Uncertainty in Artificial Intelligence*, volume 14, San Francisco, CA, 2001. Morgan Kauffman.
- S. T. Roweis. EM algorithms for PCA and SPCA. In M. I. Jordan, M. J. Kearns, and S. A. Solla, editors, *Advances in Neural Information Processing Systems*, volume 10, pages 626–632, Cambridge, MA, 1998. MIT Press.

