# Probabilistic Dimensionality Reduction 

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## Outline

Probabilistic Linear Dimensionality Reduction

Non Linear Probabilistic Dimensionality Reduction

Examples

Conclusions

## Notation

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

$$
\begin{gathered}
\text { data, } \mathbf{Y}=\left[\mathbf{y}_{1,:}, \ldots, \mathbf{y}_{n,:}\right]^{\top}=\left[\mathbf{y}_{:, 1}, \ldots, \mathbf{y}_{:, p}\right] \in \mathfrak{R}^{n \times p} \\
\text { centred data, } \hat{\mathbf{Y}}=\left[\hat{\mathbf{y}}_{1,:,}, \ldots, \hat{\mathbf{y}}_{n,:}\right]^{\top}=\left[\hat{\mathbf{y}}_{:, 1}, \ldots, \hat{\mathbf{y}}_{:, p}\right] \in \mathfrak{R}^{n \times p}, \\
\hat{\mathbf{y}}_{i,:}=\mathbf{y}_{i,:}-\boldsymbol{\mu} \\
\text { latent variables, } \mathbf{X}=\left[\mathbf{x}_{1, i,}, \ldots, \mathbf{x}_{n,}\right]^{\top}=\left[\mathbf{x}_{:, 1}, \ldots, \mathbf{x}_{:, q}\right] \in \mathfrak{R}^{n \times q} \\
\text { mapping matrix, } \mathbf{W} \in \mathfrak{R}^{p \times q}
\end{gathered}
$$

$\mathbf{a}_{i, \text { : }}$ 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

- Data covariance given by $\frac{1}{n} \hat{\mathbf{Y}}^{\top} \hat{\mathbf{Y}}$

$$
\operatorname{cov}(\mathbf{Y})=\frac{1}{n} \sum_{i=1}^{n} \hat{\mathbf{y}}_{i,:} \hat{\mathbf{y}}_{i,:}^{\top}=\frac{1}{n} \hat{\mathbf{Y}}^{\top} \hat{\mathbf{Y}}=\mathbf{S} .
$$

- Inner product matrix given by $\mathbf{Y} \mathbf{Y}^{\top}$

$$
\mathbf{K}=\left(k_{i, j}\right)_{i, j}, \quad k_{i, j}=\mathbf{y}_{i,:}^{\top} \mathbf{y}_{j,:}
$$

## Linear Dimensionality Reduction

- Find a lower dimensional plane embedded in a higher dimensional space.
- The plane is described by the matrix $\mathbf{W} \in \mathfrak{R}^{p \times q}$.

$$
\mathbf{y}=\xrightarrow{\mathbf{W x}}+\mu
$$

$x_{1}$


Figure: Mapping a two dimensional plane to a higher dimensional space in a linear way. Data are generated by corrupting points on the plane with noise.

## 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

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

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(\mathbf{Y} \mid \mathbf{X}, \mathbf{W})=\prod_{i=1}^{n} \mathcal{N}\left(\mathbf{y}_{i,:} \mid \mathbf{W} \mathbf{x}_{i,:}, \sigma^{2} \mathbf{I}\right)
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## Linear Latent Variable Model

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- Define linear-Gaussian relationship between latent variables and data.
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variable approach:

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p(\mathbf{Y} \mid \mathbf{X}, \mathbf{W})=\prod_{i=1}^{n} \mathcal{N}\left(\mathbf{y}_{i, j} \mid \mathbf{W} \mathbf{x}_{i, i}, \sigma^{2} \mathbf{I}\right)
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- Define linear-Gaussian relationship between latent variables and data.

- Standard Latent variable approach:
- Define Gaussian prior over latent space, $\mathbf{X}$.

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## 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.

$$
\begin{aligned}
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p(\mathbf{X}) & =\prod_{i=1}^{n} \mathcal{N}\left(\mathbf{x}_{i,:} \mid \mathbf{0}, \mathbf{I}\right)
\end{aligned}
$$

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

## Computation of the Marginal Likelihood

$$
\mathbf{y}_{i,:}=\mathbf{W} \mathbf{x}_{i,:}+\boldsymbol{\epsilon}_{i, i} \quad \mathbf{x}_{i,:} \sim \mathcal{N}(\mathbf{0}, \mathbf{I}), \quad \epsilon_{i,:} \sim \mathcal{N}\left(\mathbf{0}, \sigma^{2} \mathbf{I}\right)
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## Linear Latent Variable Model II

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



$$
p(\mathbf{Y} \mid \mathbf{W})=\prod_{i=1}^{n} \mathcal{N}\left(\mathbf{y}_{i,:} \mid \mathbf{0}, \mathbf{W} \mathbf{W}^{\top}+\sigma^{2} \mathbf{I}\right)
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If $\mathbf{U}_{q}$ are first $q$ principal eigenvectors of $n^{-1} \mathbf{Y}^{\top} \mathbf{Y}$ and the corresponding eigenvalues are $\boldsymbol{\Lambda}_{q}$,

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If $\mathbf{U}_{q}$ are first $q$ principal eigenvectors of $n^{-1} \mathbf{Y}^{\top} \mathbf{Y}$ and the corresponding eigenvalues are $\boldsymbol{\Lambda}_{q}$,

$$
\mathbf{W}=\mathbf{U}_{q} \mathbf{L R}^{\top}, \quad \mathbf{L}=\left(\boldsymbol{\Lambda}_{q}-\sigma^{2} \mathbf{I}\right)^{\frac{1}{2}}
$$

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

## Linear Latent Variable Model

Factor Analysis

- Linear-Gaussian relationship between latent variables and data,

$\mathbf{y}_{i,:}=\mathbf{W} \mathbf{x}_{i,:}+\boldsymbol{\mu}+\boldsymbol{\eta}_{i,:}$.
- Now each $\eta_{i, j} \sim \mathcal{N}\left(0, \sigma_{j}^{2}\right)$ has a separate variance.

1. Optimize likelihood wrt W.

$$
p(\mathbf{X})=\prod_{i=1}^{n} \mathcal{N}\left(\mathbf{x}_{i, j} \mid \mathbf{0}, \mathbf{I}\right)
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## Linear Latent Variable Model

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- Linear-Gaussian relationship between latent variables and data,

$\mathbf{y}_{i,:}=\mathbf{W} \mathbf{x}_{i,:}+\boldsymbol{\mu}+\boldsymbol{\eta}_{i,:}$.
- Now each $\eta_{i, j} \sim \mathcal{N}\left(0, \sigma_{j}^{2}\right)$
$p(\hat{\mathbf{Y}} \mid \mathbf{W})=\prod_{i=1}^{n} \mathcal{N}\left(\hat{\mathbf{y}}_{i, i} \mid \mathbf{0}, \mathbf{W W}^{\top}+\mathbf{D}\right)$ has a separate variance.

1. Optimize likelihood wrt W.
where $\mathbf{D}$ is diagonal with elements given by $\sigma_{j}^{2}$.

## Factor Analysis Optimization

- Optimization is more difficult: no longer an eigenvalue problem.


## Linear Latent Variable Model

## Independent Component

 Analysis- Linear-Gaussian relationship between latent variables and data,

$\mathbf{y}_{i,:}=\mathbf{W} \mathbf{x}_{i,:}+\boldsymbol{\mu}+\boldsymbol{\eta}_{i,:}$.
- Now latent variables are independent and non-Gaussian:

$$
x_{i,:} \sim \prod_{j=1}^{q} p\left(x_{i, j}\right)
$$

1. Optimize likelihood

$$
p(\mathbf{X})=\prod_{i=1}^{n} \prod_{j=1}^{p} p\left(x_{i, j}\right)
$$

## Independent Component Analysis Samples

- Rotational symmetry of Gaussian is removed.


Figure: Independent variables which are Gaussian.

## Independent Component Analysis Samples

- Rotational symmetry of Gaussian is removed.


Figure: Independent variables which are super-Gaussian.

## Independent Component Analysis Samples

- Rotational symmetry of Gaussian is removed.


Figure: Independent variables which are sub-Gaussian.

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## Motivation for Non-Linear Dimensionality Reduction

## USPS Data Set Handwritten Digit

- 3648 Dimensions
- 64 rows by 57 columns



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- Space contains more than just this digit.



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USPS Data Set Handwritten Digit

- 3648 Dimensions
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- 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!


## Motivation for Non-Linear Dimensionality Reduction

USPS Data Set Handwritten Digit

- 3648 Dimensions
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- Space contains more than just this digit.
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## Simple Model of Digit

Rotate a 'Prototype'


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MATLAB Demo
demDigitsManifold([1 2], 'all')

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demDigitsManifold([1 2], 'all')


## MATLAB Demo

demDigitsManifold([1 2], '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.


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- Define Gaussian prior over latent space, $\mathbf{X}$.

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$$
p(\mathbf{Y} \mid \mathbf{W})=\prod_{i=1}^{n} \mathcal{N}\left(\mathbf{y}_{i,:}, \mathbf{0}, \mathbf{W} \mathbf{W}^{\top}+\sigma^{2} \mathbf{I}\right)
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$$
\mathbf{y}_{i,:}=\mathbf{W} \mathbf{x}_{i,:}+\boldsymbol{\epsilon}_{i, i} \quad \mathbf{x}_{i,:} \sim \mathcal{N}(\mathbf{0}, \mathbf{I}), \quad \epsilon_{i,:} \sim \mathcal{N}\left(\mathbf{0}, \sigma^{2} \mathbf{I}\right)
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## Linear Latent Variable Model II

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



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\mathbf{W}=\mathbf{U}_{q} \mathbf{L R}^{\top}, \quad \mathbf{L}=\left(\boldsymbol{\Lambda}_{q}-\sigma^{2} \mathbf{I}\right)^{\frac{1}{2}}
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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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p(\mathbf{Y} \mid \mathbf{X}, \mathbf{W})=\prod_{i=1}^{n} \mathcal{N}\left(\mathbf{y}_{i, \mid} \mid \mathbf{W} \mathbf{x}_{i, .}, \sigma^{2} \mathbf{I}\right)
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## Dual Probabilistic PCA

- Define linear-Gaussian relationship between latent variables and data.
- Novel Latent variable approach:


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## 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, W.

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p(\mathbf{W}) & =\prod_{i=1}^{p} \mathcal{N}\left(\mathbf{w}_{i, \mid} \mid \mathbf{0}, \mathbf{I}\right)
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## Dual Probabilistic PCA

- Define linear-Gaussian relationship between latent variables and
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p(\mathbf{Y} \mid \mathbf{X}, \mathbf{W})=\prod_{i=1}^{n} \mathcal{N}\left(\mathbf{y}_{i, \mid} \mid \mathbf{W} \mathbf{x}_{i_{i},}, \sigma^{2} \mathbf{I}\right) \\
p(\mathbf{W})=\prod_{i=1}^{p} \mathcal{N}\left(\mathbf{w}_{i, i} \mid \mathbf{0}, \mathbf{I}\right) \\
p(\mathbf{Y} \mid \mathbf{X})=\prod_{j=1}^{p} \mathcal{N}\left(\mathbf{y}_{: j, j} \mid \mathbf{0}, \mathbf{X} \mathbf{X}^{\top}+\sigma^{2} \mathbf{I}\right)
\end{gathered}
$$

## Computation of the Marginal Likelihood

$$
\mathbf{y}_{:, j}=\mathbf{X w}_{:, j}+\epsilon_{i, j}, \quad \mathbf{w}_{:, j} \sim \mathcal{N}(\mathbf{0}, \mathbf{I}), \quad \epsilon_{i,:} \sim \mathcal{N}\left(\mathbf{0}, \sigma^{2} \mathbf{I}\right)
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\end{aligned}
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Dual Probabilistic PCA Max. Likelihood Soln (Lawrence, 2004, 2005)


$$
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p(\mathbf{Y} \mid \mathbf{X})=\prod_{j=1}^{p} \mathcal{N}\left(\mathbf{y}_{:, j} \mid \mathbf{0}, \mathbf{K}\right), \quad \mathbf{K}=\mathbf{X X}^{\top}+\sigma^{2} \mathbf{I}
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$$
\log p(\mathbf{Y} \mid \mathbf{X})=-\frac{p}{2} \log |\mathbf{K}|-\frac{1}{2} \operatorname{tr}\left(\mathbf{K}^{-1} \mathbf{Y} \mathbf{Y}^{\top}\right)+\text { const. }
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## PPCA Max. Likelihood Soln

$$
p(\mathbf{Y} \mid \mathbf{X})=\prod_{j=1}^{p} \mathcal{N}\left(\mathbf{y}_{: j} ; \mathbf{0}, \mathbf{K}\right), \quad \mathbf{K}=\mathbf{X X}^{\top}+\sigma^{2} \mathbf{I}
$$

$$
\log p(\mathbf{Y} \mid \mathbf{X})=-\frac{p}{2} \log |\mathbf{K}|-\frac{1}{2} \operatorname{tr}\left(\mathbf{K}^{-1} \mathbf{Y} \mathbf{Y}^{\top}\right)+\text { const. }
$$

If $\mathbf{U}_{q}^{\prime}$ are first $q$ principal eigenvectors of $p^{-1} \mathbf{Y} \mathbf{Y}^{\top}$ and the corresponding eigenvalues are $\boldsymbol{\Lambda}_{q}$,

## Linear Latent Variable Model IV

## PPCA Max. Likelihood Soln

$$
p(\mathbf{Y} \mid \mathbf{X})=\prod_{j=1}^{p} \mathcal{N}\left(\mathbf{y}_{: j} ; \mathbf{0}, \mathbf{K}\right), \quad \mathbf{K}=\mathbf{X X}^{\top}+\sigma^{2} \mathbf{I}
$$

$$
\log p(\mathbf{Y} \mid \mathbf{X})=-\frac{p}{2} \log |\mathbf{K}|-\frac{1}{2} \operatorname{tr}\left(\mathbf{K}^{-1} \mathbf{Y} \mathbf{Y}^{\top}\right)+\text { const. }
$$

If $\mathbf{U}_{q}^{\prime}$ are first $q$ principal eigenvectors of $p^{-1} \mathbf{Y} \mathbf{Y}^{\top}$ and the corresponding eigenvalues are $\boldsymbol{\Lambda}_{q}$,

$$
\mathbf{X}=\mathbf{U}_{q}^{\prime} \mathbf{L} \mathbf{R}^{\top}, \quad \mathbf{L}=\left(\boldsymbol{\Lambda}_{q}-\sigma^{2} \mathbf{I}\right)^{\frac{1}{2}}
$$

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

## Linear Latent Variable Model IV

Dual PPCA Max. Likelihood Soln (Lawrence, 2004, 2005)

$$
p(\mathbf{Y} \mid \mathbf{X})=\prod_{j=1}^{p} \mathcal{N}\left(\mathbf{y}_{:, j} \mid \mathbf{0}, \mathbf{K}\right), \quad \mathbf{K}=\mathbf{X X}^{\top}+\sigma^{2} \mathbf{I}
$$

$$
\log p(\mathbf{Y} \mid \mathbf{X})=-\frac{p}{2} \log |\mathbf{K}|-\frac{1}{2} \operatorname{tr}\left(\mathbf{K}^{-1} \mathbf{Y} \mathbf{Y}^{\top}\right)+\text { const. }
$$

If $\mathbf{U}_{q}^{\prime}$ are first $q$ principal eigenvectors of $p^{-1} \mathbf{Y} \mathbf{Y}^{\top}$ and the corresponding eigenvalues are $\boldsymbol{\Lambda}_{q}$,

$$
\mathbf{X}=\mathbf{U}_{q}^{\prime} \mathbf{L} \mathbf{R}^{\top}, \quad \mathbf{L}=\left(\boldsymbol{\Lambda}_{q}-\sigma^{2} \mathbf{I}\right)^{\frac{1}{2}}
$$

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

## Linear Latent Variable Model IV

PPCA Max. Likelihood Soln (Tipping and Bishop, 1999)

$$
\begin{gathered}
p(\mathbf{Y} \mid \mathbf{W})=\prod_{i=1}^{n} \mathcal{N}\left(\mathbf{y}_{i,:} \mid \mathbf{0}, \mathbf{C}\right), \quad \mathbf{C}=\mathbf{W} \mathbf{W}^{\top}+\sigma^{2} \mathbf{I} \\
\log p(\mathbf{Y} \mid \mathbf{W})=-\frac{n}{2} \log |\mathbf{C}|-\frac{1}{2} \operatorname{tr}\left(\mathbf{C}^{-1} \mathbf{Y}^{\top} \mathbf{Y}\right)+\text { const. }
\end{gathered}
$$

If $\mathbf{U}_{q}$ are first $q$ principal eigenvectors of $n^{-1} \mathbf{Y}^{\top} \mathbf{Y}$ and the corresponding eigenvalues are $\boldsymbol{\Lambda}_{q}$,

$$
\mathbf{W}=\mathbf{U}_{q} \mathbf{L} \mathbf{R}^{\top}, \quad \mathbf{L}=\left(\boldsymbol{\Lambda}_{q}-\sigma^{2} \mathbf{I}\right)^{\frac{1}{2}}
$$

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

## Equivalence of Formulations

## The Eigenvalue Problems are equivalent

- Solution for Probabilistic PCA (solves for the mapping)

$$
\mathbf{Y}^{\top} \mathbf{Y} \mathbf{U}_{q}=\mathbf{U}_{q} \mathbf{\Lambda}_{q} \quad \mathbf{W}=\mathbf{U}_{q} \mathbf{L} \mathbf{R}^{\top}
$$

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

$$
\mathbf{Y} \mathbf{Y}^{\top} \mathbf{U}_{q}^{\prime}=\mathbf{U}_{q}^{\prime} \boldsymbol{\Lambda}_{q} \quad \mathbf{X}=\mathbf{U}_{q}^{\prime} \mathbf{L R ^ { \top }}
$$

- Equivalence is from

$$
\mathbf{U}_{q}=\mathbf{Y}^{\top} \mathbf{U}_{q}^{\prime} \boldsymbol{\Lambda}_{q}^{-\frac{1}{2}}
$$

## Gaussian Processes: Extremely Short Overview



## Gaussian Processes: Extremely Short Overview



## Gaussian Processes: Extremely Short Overview



## Gaussian Processes: Extremely Short Overview




## 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 parameteters, $\mathbf{W}$.
- Integrate out parameters.

$$
\begin{gathered}
p(\mathbf{Y} \mid \mathbf{X}, \mathbf{W})=\prod_{i=1}^{n} \mathcal{N}\left(\mathbf{y}_{i, /} \mid \mathbf{W} \mathbf{x}_{i, i}, \sigma^{2} \mathbf{I}\right) \\
p(\mathbf{W})=\prod_{i=1}^{p} \mathcal{N}\left(\mathbf{w}_{i, \mid} \mid \mathbf{0}, \mathbf{I}\right) \\
p(\mathbf{Y} \mid \mathbf{X})=\prod_{j=1}^{p} \mathcal{N}\left(\mathbf{y}_{: j, j} \mid \mathbf{0}, \mathbf{X} \mathbf{X}^{\top}+\sigma^{2} \mathbf{I}\right)
\end{gathered}
$$

## Non-Linear Latent Variable Model

## Dual Probabilistic PCA

- Inspection of the marginal likelihood shows ...


$$
p(\mathbf{Y} \mid \mathbf{X})=\prod_{j=1}^{p} \mathcal{N}\left(\mathbf{y}_{:, j} \mid \mathbf{0}, \mathbf{X} \mathbf{X}^{\top}+\sigma^{2} \mathbf{I}\right)
$$

## Non-Linear Latent Variable Model

## Dual Probabilistic PCA

- Inspection of the marginal likelihood shows ...
- The covariance matrix is a covariance function.


$$
\begin{aligned}
p(\mathbf{Y} \mid \mathbf{X}) & =\prod_{j=1}^{p} \mathcal{N}\left(\mathbf{y}_{:, j} \mid \mathbf{0}, \mathbf{K}\right) \\
\mathbf{K} & =\mathbf{X X}^{\top}+\sigma^{2} \mathbf{I}
\end{aligned}
$$

## 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'.


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

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

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).


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

$$
\mathbf{K}=\text { ? }
$$

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

## Non-linear Latent Variable Models

## Exponentiated Quadratic (EQ) Covariance

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

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

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


## Outline

Probabilistic Linear Dimensionality Reduction<br>Non Linear Probabilistic Dimensionality Reduction

## Examples

Conclusions

## Applications

## Style Based Inverse Kinematics

- Facilitating animation through modeling human motion (Grochow et al., 2004)


## Tracking

- Tracking using human motion models (Urtasun et al., 2005, 2006)


## Assisted Animation

- Generalizing drawings for animation (Baxter and Anjyo, 2006)


## Shape Models

- Inferring shape (e.g. pose from silhouette). (Ek et al., 2008b,a; Priacuriu and Reid, 2011a,b)


## Example: Latent Doodle Space

(Baxter and Anjyo, 2006)

## Example: Latent Doodle Space

(Baxter and Anjyo, 2006)

## Generalization with much less Data than Dimensions

- Powerful uncertainly handling of GPs leads to surprising properties.
- Non-linear models can be used where there are fewer data points than dimensions without overfitting.


## Prior for Supervised Learning

(Urtasun and Darrell, 2007)

- We introduce a prior that is based on the Fisher criteria

$$
p(\mathbf{X}) \propto \exp \left\{-\frac{1}{\sigma_{d}^{2}} \operatorname{tr}\left(\mathbf{S}_{w}^{-1} \mathbf{S}_{b}\right)\right\},
$$

with $\mathbf{S}_{b}$ the between class matrix and $\mathbf{S}_{w}$ the within class matrix


## Prior for Supervised Learning

(Urtasun and Darrell, 2007)

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p(\mathbf{X}) \propto \exp \left\{-\frac{1}{\sigma_{d}^{2}} \operatorname{tr}\left(\mathbf{S}_{w}^{-1} \mathbf{S}_{b}\right)\right\}
$$

with $\mathbf{S}_{b}$ the between class matrix and $\mathbf{S}_{w}$ the within class matrix


$$
\mathbf{S}_{w}=\sum_{i=1}^{L} \frac{n_{i}}{n}\left(\mathbf{M}_{i}-\mathbf{M}_{0}\right)\left(\mathbf{M}_{i}-\mathbf{M}_{0}\right)^{\top}
$$

where $\mathbf{X}^{(i)}=\left[\mathbf{x}_{1}^{(i)}, \cdots, \mathbf{x}_{n_{i}}^{(i)}\right]$ are the $n_{i}$ training points of class $i, \mathbf{M}_{i}$ is the mean of the elements of class $i$, and $\mathbf{M}_{0}$ is the mean of all the training points of all classes.

## Prior for Supervised Learning

(Urtasun and Darrell, 2007)

- We introduce a prior that is based on the Fisher criteria

$$
p(\mathbf{X}) \propto \exp \left\{-\frac{1}{\sigma_{d}^{2}} \operatorname{tr}\left(\mathbf{S}_{w}^{-1} \mathbf{S}_{b}\right)\right\}
$$

with $\mathbf{S}_{b}$ the between class matrix and $\mathbf{S}_{w}$ the within class matrix


$$
\begin{gathered}
\mathbf{S}_{w}=\sum_{i=1}^{L} \frac{n_{i}}{n}\left(\mathbf{M}_{i}-\mathbf{M}_{0}\right)\left(\mathbf{M}_{i}-\mathbf{M}_{0}\right)^{\top} \\
\mathbf{S}_{b}=\sum_{i=1}^{L} \frac{n_{i}}{n}\left[\frac{1}{n_{i}} \sum_{k=1}^{n_{i}}\left(\mathbf{x}_{k}^{(i)}-\mathbf{M}_{i}\right)\left(\mathbf{x}_{k}^{(i)}-\mathbf{M}_{i}\right)^{\top}\right]
\end{gathered}
$$

where $\mathbf{X}^{(i)}=\left[\mathbf{x}_{1}^{(i)}, \cdots, \mathbf{x}_{n_{i}}^{(i)}\right]$ are the $n_{i}$ training points of class
$i$ M.ic tho moan of tho olomonte of clacc $i$ and Moic tho

## Prior for Supervised Learning

(Urtasun and Darrell, 2007)

- We introduce a prior that is based on the Fisher criteria

$$
p(\mathbf{X}) \propto \exp \left\{-\frac{1}{\sigma_{d}^{2}} \operatorname{tr}\left(\mathbf{S}_{w}^{-1} \mathbf{S}_{b}\right)\right\}
$$

with $\mathbf{S}_{b}$ the between class matrix and $\mathbf{S}_{w}$ the within class matrix




## GaussianFace

(Lu and Tang, 2014)

- First system to surpass human performance on cropped Learning Faces in Wild Data.


## http://tinyurl.com/nkt9a38

- Lots of feature engineering, followed by a Discriminative GP-LVM.


Figure 4: The ROC curve on LFW. Our method achieves the best performance, beating human-level performance.


Figure 5: The two rows present examples of matched anc mismatched pairs respectively from LFW that were incorrectly classified by the GaussianFace model.

Conclusion and Future Work

## Continuous Character Control

(Levine et al., 2012)

- Graph diffusion prior for enforcing connectivity between motions.

$$
\log p(\mathbf{X})=w_{c} \sum_{i, j} \log K_{i j}^{d}
$$

with the graph diffusion kernel $\mathbf{K}^{d}$ obtain from

$$
K_{i j}^{d}=\exp (\beta \mathbf{H}) \quad \text { with } \quad \mathbf{H}=-\mathbf{T}^{-1 / 2} \mathbf{L} \mathbf{T}^{-1 / 2}
$$

the graph Laplacian, and $\mathbf{T}$ is a diagonal matrix with $T_{i i}=\sum_{j} w\left(\mathbf{x}_{i}, \mathbf{x}_{j}\right)$,

$$
L_{i j}= \begin{cases}\sum_{k} w\left(\mathbf{x}_{i}, \mathbf{x}_{k}\right) & \text { if } i=j \\ -w\left(\mathbf{x}_{i}, \mathbf{x}_{j}\right) & \text { otherwise } .\end{cases}
$$

and $w\left(\mathbf{x}_{i}, \mathbf{x}_{j}\right)=\left\|\mathbf{x}_{i}-\mathbf{x}_{j}\right\|^{-p}$ measures similarity.

## Character Control: Results

## GPLVM for Character Animation

- Learn a GPLVM from a small mocap sequence
- Pose synthesis by solving an optimization problem

$$
\begin{array}{r}
\arg \min \mathbf{x}, \mathbf{y}-\log p(\mathbf{y} \mid \mathbf{x}) \\
\text { such that } C(\mathbf{y})=0
\end{array}
$$

- These handle constraints may come from a user in an interactive session, or from a mocap system.
- Smooth the latent space by adding noise in order to reduce the number of local minima.
- Optimization in an annealed fashion over different anneal version of the latent space.


## Application: Replay same motion

## Application: Keyframing joint trajectories

(Grochow et al., 2004)

## Application: Deal with missing data in mocap

(Grochow et al., 2004)

## Application: Style Interpolation

## Shape Priors in Level Set Segmentation

- Represent contours with elliptic Fourier descriptors

- Learn a GPLVM on the parameters of those descriptors
- We can now generate close contours from the latent space
- Segmentation is done by non-linear minimization of an image-driven energy which is a function of the latent space


## GPLVM on Contours

[ V. Prisacariu and I. Reid, ICCV 2011]


## Segmentation Results

[ V. Prisacariu and I. Reid, ICCV 2011]


## 5) Style Content Separation and Multi-linear models

Multiple aspects that affect the input signal, interesting to factorize them


## Multilinear models

- Style-Content Separation (Tenenbaum and Freeman, 2000)

$$
\mathbf{y}=\sum_{i, j} w_{i, j} a_{i} b_{j}+\epsilon
$$

- Multi-linear analysis (Vasilescu and Terzopoulos, 2002)

$$
\mathbf{y}=\sum_{i, j, k, \cdots} w_{i, j, k, \ldots} a_{i} b_{j} c_{k} \cdots+\epsilon
$$

- Non-linear basis functions (Elgammal and Lee, 2004)

$$
\mathbf{y}=\sum_{i, j} w_{i, j} a_{i} \phi_{j}(b)+\epsilon
$$

## Multi (non)-linear models with GPs

- In the GPLVM

$$
\mathbf{y}=\sum_{j} w_{j} \phi_{j}(\mathbf{x})+\epsilon=\mathbf{w}^{\top} \Phi(\mathbf{x})+\epsilon
$$

with

$$
E\left[\mathbf{y}, \mathbf{y}^{\prime}\right]=\Phi(\mathbf{x})^{\top} \Phi(\mathbf{y})+\beta^{-1} \delta=k\left(\mathbf{x}, \mathbf{x}^{\prime}\right)+\beta^{-1} \delta
$$

- Multifactor Gaussian process

$$
\mathbf{y}=\sum_{i, j, k, \cdots} w_{i j k \ldots} \phi_{i}^{(1)} \phi_{j}^{(1)} \phi_{k}^{(1)} \cdots+\epsilon
$$

with

$$
E\left[\mathbf{y}, \mathbf{y}^{\prime}\right]=\prod_{i} \Phi^{(i)^{\top}} \Phi^{(i)}+\beta^{-1} \delta=\prod_{i} k_{i}\left(\mathbf{x}^{(i)}, \mathbf{x}^{(i)^{\prime}}\right)+\beta^{-1} \delta
$$

- Learning in this model is the same, just the kernel changes.


## Training Data

Each training motion is a collection of poses, sharing the same combination of subject (s) and gait (g).

## Stylistic factors

$$
\begin{array}{lll}
\text { subject } 1 & \text { subject } 2 & \text { subject } 3
\end{array}
$$

stride

run

walk


## Character Animation

(Wang et al., 2007)

Training data, 6 sequences, 314 frames in total

## Generating new styles for a subject

## Interpolating Gaits

## Generating Different Styles

## Other Topics

- Dynamical models Details
- Hierarchical models © Details
- Bayesian GP-LVM Details
- Deep GPs - Details


## Hierarchical GP-LVM

(Lawrence and Moore, 2007)

## Stacking Gaussian Processes

- Regressive dynamics provides a simple hierarchy.
- The input space of the GP is governed by another GP.
- By stacking GPs we can consider more complex hierarchies.
- Ideally we should marginalise latent spaces
- In practice we seek MAP solutions.


## Two Correlated Subjects

(Lawrence and Moore, 2007)


Figure: Hierarchical model of a 'high five'.

## Within Subject Hierarchy

(Lawrence and Moore, 2007)

## Decomposition of Body



Figure: Decomposition of a subject.

## Single Subject Run/Walk

(Lawrence and Moore, 2007)


Figure: Hierarchical model of a walk and a run.

## Selecting Data Dimensionality

- GP-LVM Provides probabilistic non-linear dimensionality reduction.
- How to select the dimensionality?
- Need to estimate marginal likelihood.
- In standard GP-LVM it increases with increasing $q$.


## Integrate Mapping Function and Latent Variables

## Bayesian GP-LVM

- Start with a standard GP-LVM.


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

## 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, $\mathbf{X}$.

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


## 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.

$$
\begin{aligned}
& p(\mathbf{Y} \mid \mathbf{X})=\prod_{j=1}^{p} \mathcal{N}\left(\mathbf{y}_{: ; j} \mid \mathbf{0}, \mathbf{K}\right) \\
& p(\mathbf{X})=\prod_{j=1}^{q} \mathcal{N}\left(\mathbf{x}_{; ; j} \mathbf{0}, \alpha_{i}^{-2} \mathbf{I}\right)
\end{aligned}
$$

## 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.

$$
\begin{aligned}
& p(\mathbf{Y} \mid \mathbf{X})=\prod_{j=1}^{p} \mathcal{N}\left(\mathbf{y}_{:, j} \mid \mathbf{0}, \mathbf{K}\right) \\
& p(\mathbf{X})=\prod_{j=1}^{q} \mathcal{N}\left(\mathbf{x}_{:, j} \mid \mathbf{0}, \alpha_{i}^{-2} \mathbf{I}\right) \\
& p(\mathbf{Y} \mid \boldsymbol{\alpha})=? ?
\end{aligned}
$$

- Unfortunately integration is intractable.


## Priors for Latent Space

Titsias and Lawrence (2010)

- Variational marginalization of $\mathbf{X}$ allows us to learn parameters of $p(\mathbf{X})$.
- Standard GP-LVM where $\mathbf{X}$ learnt by MAP, this is not possible (see e.g. Wang et al., 2008).
- First example: learn the dimensionality of latent space.


## Graphical Representations of GP-LVM



## Graphical Representations of GP-LVM



## Graphical Representations of GP-LVM



## Graphical Representations of GP-LVM



## Graphical Representations of GP-LVM



## Graphical Representations of GP-LVM



## Graphical Representations of GP-LVM



$$
\begin{gathered}
\mathbf{w} \sim \mathcal{N}(\mathbf{0}, \mathbf{I}) \quad x_{i} \sim \mathcal{N}\left(0, \alpha_{i}\right) \\
y \sim \mathcal{N}\left(\mathbf{x}^{\top} \mathbf{w}, \sigma^{2}\right)
\end{gathered}
$$

## Graphical Representations of GP-LVM



## Non-linear $f(\mathbf{x})$

- In linear case equivalence because $f(\mathbf{x})=\mathbf{w}^{\top} \mathbf{x}$

$$
p\left(w_{i}\right) \sim \mathcal{N}\left(\mathbf{0}, \alpha_{i}\right)
$$

- In non linear case, need to scale columns of $\mathbf{X}$ in prior for $f(\mathbf{x})$.
- This implies scaling columns of $\mathbf{X}$ in covariance function

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

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

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

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


## Automatic dimensionality detection

- Achieved by employing an Automatic Relevance Determination (ARD) covariance function for the prior on the GP mapping
- $f \sim G P\left(\mathbf{0}, k_{f}\right)$ with

$$
k_{f}\left(\mathbf{x}_{i}, \mathbf{x}_{j}\right)=\sigma^{2} \exp \left(-\frac{1}{2} \sum_{q=1}^{Q} w_{q}\left(x_{i, q}-x_{j, q}\right)^{2}\right)
$$

- Example




## Gaussian Process Dynamical Systems

(Damianou et al., 2011)


## Gaussian Process over Latent Space

- Assume a GP prior for $p(\mathbf{X})$.
- Input to the process is time, $p(\mathbf{X} \mid t)$.


## Interpolation of HD Video

## Modeling Multiple 'Views'

- Single space to model correlations between two different data sources, e.g., images \& text, image \& pose.
- Shared latent spaces: (Shon et al., 2006; Navaratnam et al., 2007; Ek et al., 2008b)

- Effective when the 'views' are correlated.
- But not all information is shared between both 'views'.
- PCA applied to concatenated data vs CCA applied to data.


## Shared-Private Factorization

- In real scenarios, the 'views' are neither fully independent, nor fully correlated.
- Shared models
- either allow information relevant to a single view to be mixed in the shared signal,
- or are unable to model such private information.
- Solution: Model shared and private information (Virtanen et al., 2011; Ek et al., 2008a; Leen and Fyfe, 2006; Klami and Kaski, 2007, 2008; Tucker, 1958)

- Probabilistic CCA is case when dimensionality of $\mathbf{Z}$ matches $\mathbf{Y}^{(i)}$ (cf Inter Battery Factor Analysis (Tucker, 1958)).


## Manifold Relevance Determination

## Pox

Damianou et al. (2012)


## Shared GP-LVM



Separate ARD parameters for mappings to $\mathbf{Y}^{(1)}$ and $\mathbf{Y}^{(2)}$.

## Example: Yale faces



- Dataset Y: 3 persons under all illumination conditions
- Dataset Z: As above for 3 different persons
- Align datapoints $\mathbf{x}_{n}$ and $\mathbf{z}_{n}$ only based on the lighting direction


## Results

- Latent space X initialised with 14 dimensions
-Weights define a segmentation of $X$
-Video / demo...



## Potential applications..?



Manifold Relevance Determination

## Deep Neural Network



## Deep Neural Network



## Outline

Probabilistic Linear Dimensionality Reduction<br>Non Linear Probabilistic Dimensionality Reduction<br>Examples

Conclusions

## Summary

- We've advocated Dimenstionality Reduction as a good way of modeling in high dimensions.
- Spectral techniques lead to convex algorithms.
- Probabilistic techniques map the "correct way" around.
- This leads to problems with local minima.
- Have shown ability of probabilistic techniques to deal with high dimensional data.


## Summary

- We've advocated Dimenstionality Reduction as a good way of probabilistic modelling in high dimensions.
- Probabilistic techniques map the "correct way" around.
- This leads to problems with local minima.
- Probabilistic dimensionality reduction is useful in practice.
- There are still many open problems to be overcome.


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