Latent Variable Models

Neil Lawrence

GPRS
14th February 2014

Outline

Outline

Motivation

Motivation for Non-Linear Dimensionality Reduction

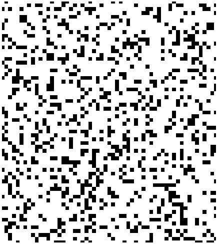
USPS Data Set Handwritten Digit

- 3648 Dimensions
  - 64 rows by 57 columns

Motivation for Non-Linear Dimensionality Reduction

USPS Data Set Handwritten Digit

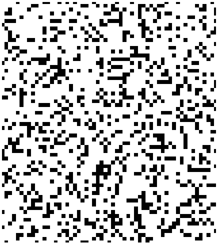
- 3648 Dimensions
  - 64 rows by 57 columns
  - Space contains more than just this digit.



Motivation for Non-Linear Dimensionality Reduction

USPS Data Set Handwritten Digit

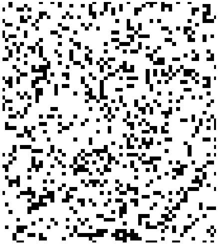
- 3648 Dimensions
  - 64 rows by 57 columns
  - Space contains more than just this digit.
  - Even if we sample every nanosecond from now until the end of the universe, you won't see the original six!



Motivation for Non-Linear Dimensionality Reduction

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'

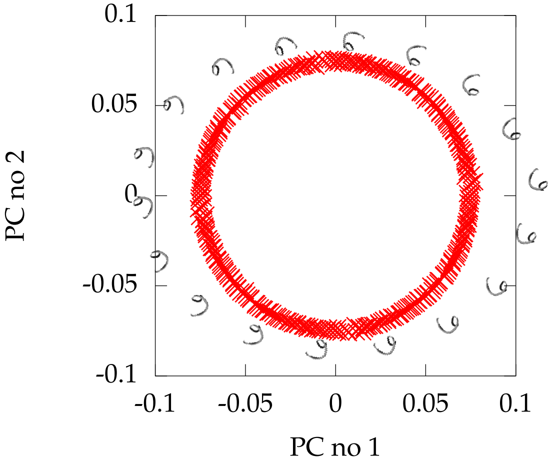
Rotate a 'Prototype'

MATLAB Demo

```
demDigitsManifold([1 2], 'all')
```

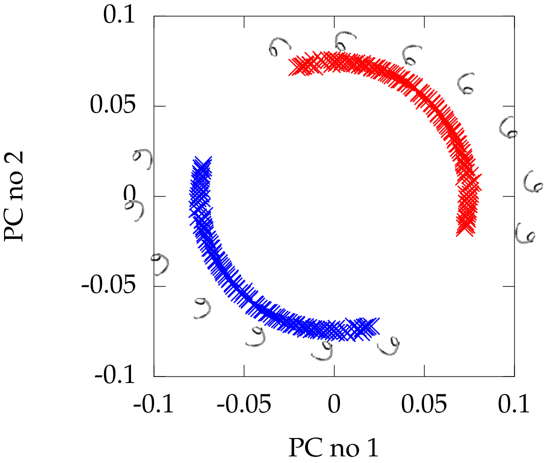
MATLAB Demo

```
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.

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 representation and a mapping — dimensional expansion.
    - Mapping is implied throught he 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.

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.

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; Roweis, 1998).
- 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
p— dimension of data space
n— number of data points

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

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

X and Y are *design matrices*

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

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

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

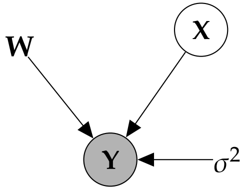
  where

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

Linear Latent Variable Model

Probabilistic PCA

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

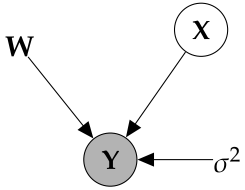


$$p\left(\mathbf{Y}|\mathbf{X},\mathbf{W}\right)=\prod_{i=1}^{n}\mathcal{N}\left(\mathbf{y}_{i,:}|\mathbf{W}\mathbf{x}_{i,:},\sigma^2\mathbf{I}\right)$$

Linear Latent Variable Model

Probabilistic PCA

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

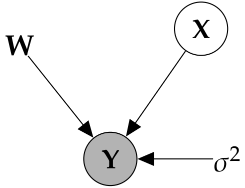


$$p(\mathbf{Y}|\mathbf{X}, \mathbf{W}) = \prod_{i=1}^{n} \mathcal{N}\left(\mathbf{y}_{i,:}|\mathbf{W}\mathbf{x}_{i,:}, \sigma^2\mathbf{I}\right)$$

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*, $\mathbf{X}$.



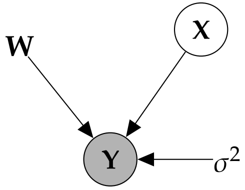
$$p(\mathbf{Y}|\mathbf{X}, \mathbf{W}) = \prod_{i=1}^{n} \mathcal{N}\left(\mathbf{y}_{i,:}|\mathbf{W}\mathbf{x}_{i,:}, \sigma^2\mathbf{I}\right)$$

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

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*, **X**.
  - Integrate out *latent variables*.



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

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

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

Computation of the Marginal Likelihood

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

Computation of the Marginal Likelihood

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

$$\mathbf{W}\mathbf{x}_{i,:} \sim \mathcal{N}\left(\mathbf{0}, \mathbf{W}\mathbf{W}^\top\right),$$

Computation of the Marginal Likelihood

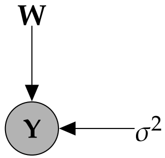
$$\mathbf{y}_{i,:} = \mathbf{W}\mathbf{x}_{i,:} + \boldsymbol{\epsilon}_{i,:}, \quad \mathbf{x}_{i,:} \sim \mathcal{N}(\mathbf{0}, \mathbf{I}), \quad \boldsymbol{\epsilon}_{i,:} \sim \mathcal{N}\left(\mathbf{0}, \sigma^2\mathbf{I}\right)$$

$$\mathbf{W}\mathbf{x}_{i,:} \sim \mathcal{N}\left(\mathbf{0}, \mathbf{W}\mathbf{W}^\top\right),$$

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

Linear Latent Variable Model II

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



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

Linear Latent Variable Model II

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

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

Linear Latent Variable Model II

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

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

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

Linear Latent Variable Model II

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

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

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

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

Linear Latent Variable Model II

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

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

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

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

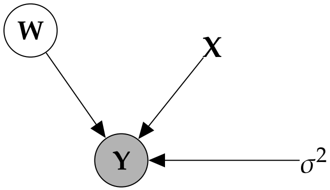
$$\mathbf{W} = \mathbf{U}_q\mathbf{L}\mathbf{R}^{\top}, \quad \mathbf{L} = \left(\boldsymbol{\Lambda}_q - \sigma^2\mathbf{I}\right)^{\frac{1}{2}}$$

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

Linear Latent Variable Model III

Dual Probabilistic PCA

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

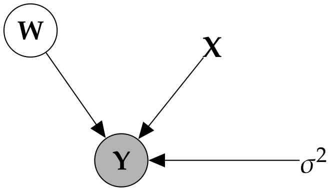


$$p(\mathbf{Y}|\mathbf{X},\mathbf{W}) = \prod_{i=1}^{n} \mathcal{N}\left(\mathbf{y}_{i,:}|\mathbf{W}\mathbf{x}_{i,:},\sigma^2\mathbf{I}\right)$$

Linear Latent Variable Model III

Dual Probabilistic PCA

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

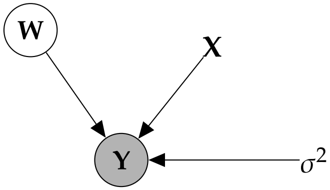


$$p(\mathbf{Y}|\mathbf{X},\mathbf{W}) = \prod_{i=1}^{n} \mathcal{N}\left(\mathbf{y}_{i,:}|\mathbf{W}\mathbf{x}_{i,:},\sigma^2\mathbf{I}\right)$$

Linear Latent Variable Model III

Dual Probabilistic PCA

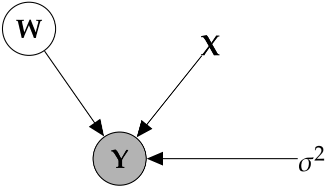
- Define *linear-Gaussian relationship* between latent variables and data.
- **Novel** Latent variable approach:
  - Define Gaussian prior over *parameters*, $\mathbf{W}$.



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

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

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*.

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

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

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

Computation of the Marginal Likelihood

$$\mathbf{y}_{:,j} = \mathbf{X}\mathbf{w}_{:,j} + \boldsymbol{\epsilon}_{:,j}, \quad \mathbf{w}_{:,j} \sim \mathcal{N}\left(\mathbf{0}, \mathbf{I}\right), \quad \boldsymbol{\epsilon}_{i,:} \sim \mathcal{N}\left(\mathbf{0}, \sigma^2\mathbf{I}\right)$$

Computation of the Marginal Likelihood

$$\mathbf{y}_{:,j} = \mathbf{X}\mathbf{w}_{:,j} + \boldsymbol{\epsilon}_{:,j}, \quad \mathbf{w}_{:,j} \sim \mathcal{N}\left(\mathbf{0}, \mathbf{I}\right), \quad \boldsymbol{\epsilon}_{i,:} \sim \mathcal{N}\left(\mathbf{0}, \sigma^2\mathbf{I}\right)$$

$$\mathbf{X}\mathbf{w}_{:,j} \sim \mathcal{N}\left(\mathbf{0}, \mathbf{X}\mathbf{X}^\top\right),$$

Computation of the Marginal Likelihood

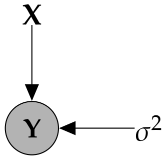
$$\mathbf{y}_{:,j} = \mathbf{X}\mathbf{w}_{:,j} + \boldsymbol{\epsilon}_{:,j}, \quad \mathbf{w}_{:,j} \sim \mathcal{N}\left(\mathbf{0}, \mathbf{I}\right), \quad \boldsymbol{\epsilon}_{i,:} \sim \mathcal{N}\left(\mathbf{0}, \sigma^2\mathbf{I}\right)$$

$$\mathbf{X}\mathbf{w}_{:,j} \sim \mathcal{N}\left(\mathbf{0}, \mathbf{X}\mathbf{X}^\top\right),$$

$$\mathbf{X}\mathbf{w}_{:,j} + \boldsymbol{\epsilon}_{:,j} \sim \mathcal{N}\left(\mathbf{0}, \mathbf{X}\mathbf{X}^\top + \sigma^2\mathbf{I}\right)$$

Linear Latent Variable Model IV

Dual Probabilistic PCA Max. Likelihood Soln (Lawrence, 2004, 2005)



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

Linear Latent Variable Model IV

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

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

Linear Latent Variable Model IV

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

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

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

Linear Latent Variable Model IV

PPCA Max. Likelihood Soln

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

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

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

Linear Latent Variable Model IV

PPCA Max. Likelihood Soln

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

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

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

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

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

Linear Latent Variable Model IV

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

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

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

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

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

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

Linear Latent Variable Model IV

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

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

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

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

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

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

Equivalence of Formulations

The Eigenvalue Problems are equivalent

- Solution for Probabilistic PCA (solves for the mapping)

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

- 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

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

References I

C. M. Bishop, M. Svensén, and C. K. I. Williams. GTM: the Generative Topographic Mapping. *Neural Computation*, 10(1):215–234, 1998. [DOI].

J. B. Kruskal. Multidimensional scaling by optimizing goodness-of-fit to a nonmetric hypothesis. *Psychometrika*, 29 (1):1–28, 1964. [DOI].

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, 11 2005.

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. [DOI].

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

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.

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

J. W. Sammon. A nonlinear mapping for data structure analysis. *IEEE Transactions on Computers*, C-18(5):401–409, 1969. [DOI].

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

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

M. E. Tipping and C. M. Bishop. Probabilistic principal component analysis. *Journal of the Royal Statistical Society, B*, 6 (3):611–622, 1999. [PDF]. [DOI].