Machine Learning

Lecture. 12.

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PCA

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- Principal Component Analysis

PCA

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- Principal Component Analysis
- Feature Extraction

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- Dimensionality Reduction

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- Data Compression

PCA

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- Feature Extraction
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- Data Compression
- Data Visualisation

Image Representation

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- 64×64 grey-scale images with $64^2 = 4096$ pixels

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- Pixel representation very powerful - overfitting almost certain

Classification

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- As $\mathbf{w}$ has dimension $M = 4096 \times 1$ with only 400 available samples overfitting is highly likely
- Alleviate problem by extracting a smaller number of informative features

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- Shape of face, lighting, ...
- Variability in images due to a small number (smaller than 256^{4096}) of degrees of freedom

Linear Subspace

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- In other words the data lies in a lower-dimensional feature space which accounts for all of the information or variability in the images
- By extracting these features from original representation it may be possible to overcome potential generalisation problems
- Images of faces may be described by a subspace of the 4096 dimensional pixel space

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Linear Subspace

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- Assume M dimensional data actually lies within a P dimensional subspace where $P << M$
- Further assume that the subspace is linear
- Orthonormal basis vectors (coordinates) span subspace i.e. $\{\boldsymbol{\beta}_1 \cdots \boldsymbol{\beta}_P\}$ where each $\boldsymbol{\beta}_p \in \mathbb{R}^D$
- Data point $\mathbf{x}$ approximated by linear combination of basis vectors

$$\mathbf{x}_n \approx \sum_{p=1}^{P} u_{np}\boldsymbol{\beta}_p = \mathbf{B}\mathbf{u}_n$$

where $D \times P$ dimensional matrix $\mathbf{B} = [\boldsymbol{\beta}_1 \cdots \boldsymbol{\beta}_P]$ and $\mathbf{u}_n$ is a $P \times 1$ dimensional vector.

PCA Derivation

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- Squared reconstruction error incurred by approximation $\mathbf{x}_n = u_{1n}\boldsymbol{\beta}_1$ defined as

$$\mathcal{E} = \frac{1}{N}\sum_{n=1}^{N}(\mathbf{x}_n - u_{1n}\boldsymbol{\beta}_1)^2$$

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$$\mathcal{E} = \frac{1}{N}\sum_{n=1}^{N}(\mathbf{x}_n - u_{1n}\boldsymbol{\beta}_1)^2$$

- Taking derivatives with respect to each u_{1n} and setting to zero gives

$$\frac{\partial \mathcal{E}}{\partial u_{1n}} = -\frac{2}{N}(\boldsymbol{\beta}_1^{\mathsf{T}}\mathbf{x}_n - u_{1n}) = 0 \Rightarrow u_{1n} = \boldsymbol{\beta}_1^{\mathsf{T}}\mathbf{x}_n$$

PCA Derivation

- Plugging this value back into the expression for $\mathcal{E}$ yields

$$\begin{aligned}
\mathcal{E} &= \frac{1}{N}\sum_{n=1}^{N}(\mathbf{x}_n - u_{1n}\boldsymbol{\beta}_1)^2 \\
&= \frac{1}{N}\sum_{n=1}^{N}\mathbf{x}_n^{\mathsf{T}}\mathbf{x}_n - 2u_{1n}\boldsymbol{\beta}_1^{\mathsf{T}}\mathbf{x}_n + u_{1n}^2\boldsymbol{\beta}_1^{\mathsf{T}}\boldsymbol{\beta}_1 \\
&= \frac{1}{N}\sum_{n=1}^{N}\mathbf{x}_n^{\mathsf{T}}\mathbf{x}_n - 2u_{1n}^2 + u_{1n}^2\boldsymbol{\beta}_1^{\mathsf{T}}\boldsymbol{\beta}_1 \\
&= \frac{1}{N}\sum_{n=1}^{N}\mathbf{x}_n^{\mathsf{T}}\mathbf{x}_n - u_{1n}^2 = \frac{1}{N}\sum_{n=1}^{N}\mathbf{x}_n^{\mathsf{T}}\mathbf{x}_n - \boldsymbol{\beta}_1^{\mathsf{T}}\mathbf{x}_n\mathbf{x}_n^{\mathsf{T}}\boldsymbol{\beta}_1
\end{aligned}$$

PCA Derivation

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- So to minimise our reconstruction error we require to maximise

$$\frac{1}{N}\sum_{n=1}^{N}\boldsymbol{\beta}_1^{\mathsf{T}}\mathbf{x}_n\mathbf{x}_n^{\mathsf{T}}\boldsymbol{\beta}_1 = \frac{1}{N}\boldsymbol{\beta}_1^{\mathsf{T}}\mathbf{X}^{\mathsf{T}}\mathbf{X}\boldsymbol{\beta}_1 = \boldsymbol{\beta}_1^{\mathsf{T}}\widehat{\mathbf{C}}\boldsymbol{\beta}_1$$

PCA Derivation

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- Subject to $\boldsymbol{\beta}_1^{\mathsf{T}}\boldsymbol{\beta}_1 = 1$ where the sample covariance matrix is denoted as $\widehat{\mathbf{C}}$ (remember that each $\mathbf{X}$ is zero mean).

Variance Maximisation

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- Note that minimisation of reconstruction error by maximisation of

$$\frac{1}{N}\sum_{n=1}^{N}\boldsymbol{\beta}_1^{\mathsf{T}}\mathbf{x}_n\mathbf{x}_n^{\mathsf{T}}\boldsymbol{\beta}_1 = \frac{1}{N}\sum_{n=1}^{N}u_{1n}^2$$

provides projections which have maximum variance so are maximally informative.

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  provides projections which have maximum variance so are maximally informative.

- Minimisation of reconstruction error requires to find projection which maximises variance of projection - retain as much information as possible.

Variance Maximisation

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- Remember that we are restricting each basis-vector to have unit norm in which case we require to create the Langrangian (Refer to the Week 5 notes)

$$\boldsymbol{\beta}_1^{\mathsf{T}} \widehat{\mathbf{C}} \boldsymbol{\beta}_1 - \lambda_1 \boldsymbol{\beta}_1^{\mathsf{T}} \boldsymbol{\beta}_1$$

and maximise with respect to $\boldsymbol{\beta}_1$.

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  and maximise with respect to $\boldsymbol{\beta}_1$.

- The corresponding vector of partial derivatives gives

$$\frac{\partial}{\partial\boldsymbol{\beta}_1} = \widehat{\mathbf{C}}\boldsymbol{\beta}_1 - \lambda_1\boldsymbol{\beta}_1$$

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$$\frac{\partial}{\partial \boldsymbol{\beta}_1} = \widehat{\mathbf{C}} \boldsymbol{\beta}_1 - \lambda_1 \boldsymbol{\beta}_1$$

- Setting to zero obtain an eigenvalue problem

$$\widehat{\mathbf{C}} \boldsymbol{\beta}_1 = \lambda_1 \boldsymbol{\beta}_1$$

Variance Maximisation

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- As the variance of the projection is defined $\boldsymbol{\beta}_1^{\mathsf{T}} \widehat{\mathbf{C}} \boldsymbol{\beta}_1$ then for $\boldsymbol{\beta}_1^{\mathsf{T}} \boldsymbol{\beta}_1 = 1$ it should be clear that the variance of the projection is equal to λ_1 the associated eigenvalue.

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- We have now found the direction $\boldsymbol{\beta}_1$ which maximises the variance of the projection $\boldsymbol{\beta}_1^\mathsf{T}\mathbf{x}$ and correspondingly minimises the reconstruction error

$$\mathcal{E} = \frac{1}{N}\sum_{n=1}^{N}(\mathbf{x}_n - u_{1n}\boldsymbol{\beta}_1)^2$$

This is referred to as the First Principal Direction and the projections of the data in this direction are the Principal Components in this direction.

Finding Additional Directions

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- Now we want to find another direction vector $\boldsymbol{\beta}_2$ which will satisfy $\boldsymbol{\beta}_1^{\mathsf{T}}\boldsymbol{\beta}_2 = 0$ and $\boldsymbol{\beta}_2^{\mathsf{T}}\boldsymbol{\beta}_2 = 1$

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- Reconstruction error is

$$\mathcal{E} = \frac{1}{N}\sum_{n=1}^{N}(\mathbf{x}_n - u_{1n}\boldsymbol{\beta}_1 - u_{2n}\boldsymbol{\beta}_2)^2$$

it is straightforward to see that $u_{2n} = \boldsymbol{\beta}_2^\mathsf{T}\mathbf{x}_n$

Finding Additional Directions

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- The reconstruction error can obtained as the following where the orthonormal characteristics of both directions has been exploited

$$\frac{1}{N}\sum_{n=1}^{N}\mathbf{x}_n^{\mathsf{T}}\mathbf{x}_n - \boldsymbol{\beta}_1^{\mathsf{T}}\mathbf{x}_n\mathbf{x}_n^{\mathsf{T}}\boldsymbol{\beta}_1 - \boldsymbol{\beta}_2^{\mathsf{T}}\mathbf{x}_n\mathbf{x}_n^{\mathsf{T}}\boldsymbol{\beta}_2$$

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- It is clear that given $\boldsymbol{\beta}_1$ then we require to obtain a solution for

$$\widehat{\mathbf{C}}\boldsymbol{\beta}_2 = \lambda_2\boldsymbol{\beta}_2$$

subject to the orthonormal constraints imposed.

Projection and Deflation

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- If $\boldsymbol{\beta}_1$ and $\boldsymbol{\beta}_2$ are orthonormal then

$$\begin{aligned}\mathbf{x} &= u_1\boldsymbol{\beta}_1 + u_2\boldsymbol{\beta}_2 \\ &= (\mathbf{x}^{\mathsf{T}}\boldsymbol{\beta}_1)\boldsymbol{\beta}_1 + (\mathbf{x}^{\mathsf{T}}\boldsymbol{\beta}_2)\boldsymbol{\beta}_2\end{aligned}$$

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- Where $(\mathbf{x}^{\mathsf{T}}\boldsymbol{\beta}_2)\boldsymbol{\beta}_2$ is the projection orthogonal to $(\mathbf{x}^{\mathsf{T}}\boldsymbol{\beta}_1)\boldsymbol{\beta}_1$ so projection orthogonal to first principal direction is

$$(\mathbf{x}^{\mathsf{T}}\boldsymbol{\beta}_2)\boldsymbol{\beta}_2 = (\mathbf{I} - \boldsymbol{\beta}_1\boldsymbol{\beta}_1^{\mathsf{T}})\mathbf{x}$$

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$$(\mathbf{x}^\mathsf{T}\boldsymbol{\beta}_2)\boldsymbol{\beta}_2 = (\mathbf{I} - \boldsymbol{\beta}_1\boldsymbol{\beta}_1^\mathsf{T})\mathbf{x}$$

- Applying this to all of the data gives

$$\mathbf{X}(\mathbf{I} - \boldsymbol{\beta}_1\boldsymbol{\beta}_1^\mathsf{T})^\mathsf{T} = \mathbf{X}(\mathbf{I} - \boldsymbol{\beta}_1\boldsymbol{\beta}_1^\mathsf{T})$$

Projection and Deflation

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- We can think of this operation as removing from the D-dimensional data the component that lies in the direction of the first principal direction. In other words we are deflating the matrix $\mathbf{X}$ and thus reducing its rank from D to $D-1$ i.e. removing one direction component, the principal direction.

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- Consider then the covariance of this deflated data matrix $\widetilde{\mathbf{X}} = \mathbf{X}(\mathbf{I} - \boldsymbol{\beta}_1\boldsymbol{\beta}_1^\mathsf{T})$ i.e. $\frac{1}{N}\widetilde{\mathbf{X}}^\mathsf{T}\widetilde{\mathbf{X}}$

$$
\begin{aligned}
&= \frac{1}{N}(\mathbf{I} - \boldsymbol{\beta}_1\boldsymbol{\beta}_1^\mathsf{T})\widetilde{\mathbf{X}}^\mathsf{T}\widetilde{\mathbf{X}}(\mathbf{I} - \boldsymbol{\beta}_1\boldsymbol{\beta}_1^\mathsf{T}) \\
&= \frac{1}{N}\Big(\mathbf{X}^\mathsf{T}\mathbf{X} - \boldsymbol{\beta}_1\boldsymbol{\beta}_1^\mathsf{T}\mathbf{X}^\mathsf{T}\mathbf{X} - \mathbf{X}^\mathsf{T}\mathbf{X}\boldsymbol{\beta}_1\boldsymbol{\beta}_1^\mathsf{T} + \boldsymbol{\beta}_1\boldsymbol{\beta}_1^\mathsf{T}\mathbf{X}^\mathsf{T}\mathbf{X}\boldsymbol{\beta}_1\boldsymbol{\beta}
\end{aligned}
$$

Projection and Deflation

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- Taking this expression term by term we see that the right hand term can be written as

$$\boldsymbol{\beta}_1 \left(\boldsymbol{\beta}_1^{\mathsf{T}} \mathbf{X}^{\mathsf{T}} \mathbf{X} \boldsymbol{\beta}_1 \right) \boldsymbol{\beta}_1^{\mathsf{T}} = \boldsymbol{\beta}_1 \left(N \lambda_1 \right) \boldsymbol{\beta}_1^{\mathsf{T}} = N \lambda_1 \boldsymbol{\beta}_1 \boldsymbol{\beta}_1^{\mathsf{T}}$$

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- and

$$\mathbf{X}^{\mathsf{T}} \mathbf{X} \boldsymbol{\beta}_1 \boldsymbol{\beta}_1^{\mathsf{T}} = N\lambda_1 \boldsymbol{\beta}_1 \boldsymbol{\beta}_1^{\mathsf{T}}$$

Projection and Deflation

- Plugging these into the expression for the covariance we obtain

$$
\begin{aligned}
\widetilde{\mathbf{C}} &= \frac{1}{N}\widetilde{\mathbf{X}}^{\mathsf{T}}\widetilde{\mathbf{X}} \\
&= \frac{1}{N}\mathbf{X}^{\mathsf{T}}\mathbf{X} - \lambda_1\boldsymbol{\beta}_1\boldsymbol{\beta}_1^{\mathsf{T}} = \widehat{\mathbf{C}} - \lambda_1\boldsymbol{\beta}_1\boldsymbol{\beta}_1^{\mathsf{T}}
\end{aligned}
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\end{aligned}
$$

- Find the principal direction of deflated covariance matrix $\widetilde{\mathbf{C}}$ by solving

$$\widetilde{\mathbf{C}}\boldsymbol{\beta}_2 = \lambda_2 \boldsymbol{\beta}_2$$

Projection and Deflation

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\end{aligned}
$$

- Find the principal direction of deflated covariance matrix $\widetilde{\mathbf{C}}$ by solving

$$\widetilde{\mathbf{C}}\boldsymbol{\beta}_2 = \lambda_2 \boldsymbol{\beta}_2$$

- Then $\boldsymbol{\beta}_2^{\mathsf{T}}\boldsymbol{\beta}_2 = 1$ and as $\widetilde{\mathbf{X}}$ resides in $D-1$ dimensional subspace orthogonal to the first principal direction $\boldsymbol{\beta}_1$ then $\boldsymbol{\beta}_1^{\mathsf{T}}\boldsymbol{\beta}_2 = 0$ must hold.

Projection and Deflation

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- We will see further on that continuing this joint matrix deflation and solving of the associated eigenvalue problems will provide a set of eigenvectors $\{\boldsymbol{\beta}_1 \cdots \boldsymbol{\beta}_D\}$ and associated eigenvalues $\{\lambda_1 \cdots \lambda_D\}$ which provide an orthonormal basis for the data which when truncated at $P << D$ will provide the minimum reconstruction error, in the least squares sense, of the data.

Reconstruction Error

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- The overall data reconstruction error can be written as

$$
\begin{aligned}
\mathcal{E} &= \frac{1}{N}\sum_{n=1}^{N}\left(\mathbf{x}_n - \sum_{p=1}^{P} u_{pn}\boldsymbol{\beta}_p\right)^2 \\
&= \frac{1}{N}\sum_{n=1}^{N}\left(\mathbf{x}_n^{\mathsf{T}}\mathbf{x}_n - \sum_{p=1}^{P}\boldsymbol{\beta}_p^{\mathsf{T}}\mathbf{x}_n\mathbf{x}_n^{\mathsf{T}}\boldsymbol{\beta}_p\right) \\
&= \frac{1}{N}\sum_{n=1}^{N}\mathbf{x}_n^{\mathsf{T}}\mathbf{x}_n - \sum_{p=1}^{P}\lambda_p
\end{aligned}
$$

Reconstruction Error

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- Now if there is no truncation and $P = D$ then $\mathcal{E}$ is clearly zero in which case

$$
\begin{aligned}
0 &= \frac{1}{N}\sum_{n=1}^{N}\mathbf{x}_n^{\mathsf{T}}\mathbf{x}_n - \sum_{p=1}^{P}\lambda_p - \sum_{p'=P+1}^{D}\lambda_{p'} \\
&= \mathcal{E} - \sum_{p'=P+1}^{D}\lambda_{p'} \\
\Rightarrow &\;\; \mathcal{E} = \sum_{p'=P+1}^{D}\lambda_{p'}
\end{aligned}
$$

Reconstruction Error

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- As the first principal component provides the largest reduction in error and the second principal component (PC) is obtained from the deflated covariance matrix $\widehat{\mathbf{C}} - \lambda_1 \boldsymbol{\beta}_1 \boldsymbol{\beta}_1^{\mathsf{T}}$ then the reduction in error obtained by the second PC will be smaller than that obtained from the first as such $\lambda_1 \geq \lambda_2 \geq \lambda_3 \cdots \geq \lambda_D$.

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- This means that by studying the distribution of the eigenvalues we can potentially identify the intrinsic dimension of the data by assessing which dimensions incur the main contributions to the overall reconstruction error.

Reconstruction Error

- If we define the $D \times D$ matrix $\mathbf{B}$ whose columns are $\boldsymbol{\beta}_p$ and the $D \times D$ diagonal matrix $\mathbf{D}$ whose elements are each λ_p then the covariance matrix can be represented in terms of the associated eigenvalues and eigenvectors as

$$\widehat{\mathbf{C}} = \mathbf{B}\mathbf{D}\mathbf{B}^{\mathsf{T}}$$

Illustrative Example

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- Consider 200 samples of 2-dimensional data denoted by the matrix $\mathbf{X}$.

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- Finally we set $\mathbf{Y} = \widetilde{\mathbf{Y}} + \boldsymbol{\epsilon}$ where $\boldsymbol{\epsilon}$ is isotropic noise with variance 2

Illustrative Example

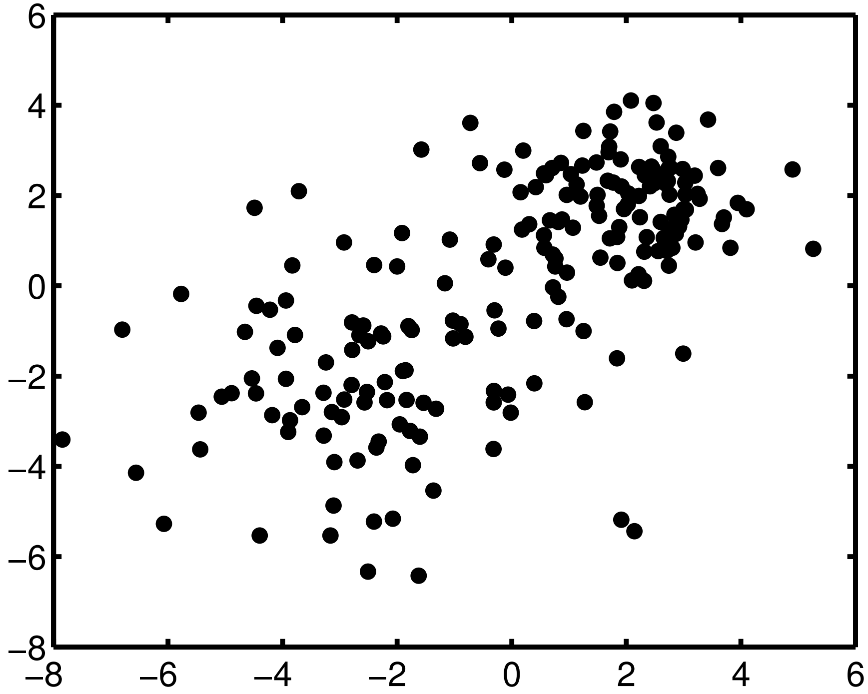

Figure 1: A scatter diagram of the 2-D data.

Illustrative Example

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- Given this 10-D data let us perform PCA on the data and study how the errors are distributed throughout the ten dimensions by plotting the 10 eigenvalues $\lambda_1 \cdots \lambda_{10}$.

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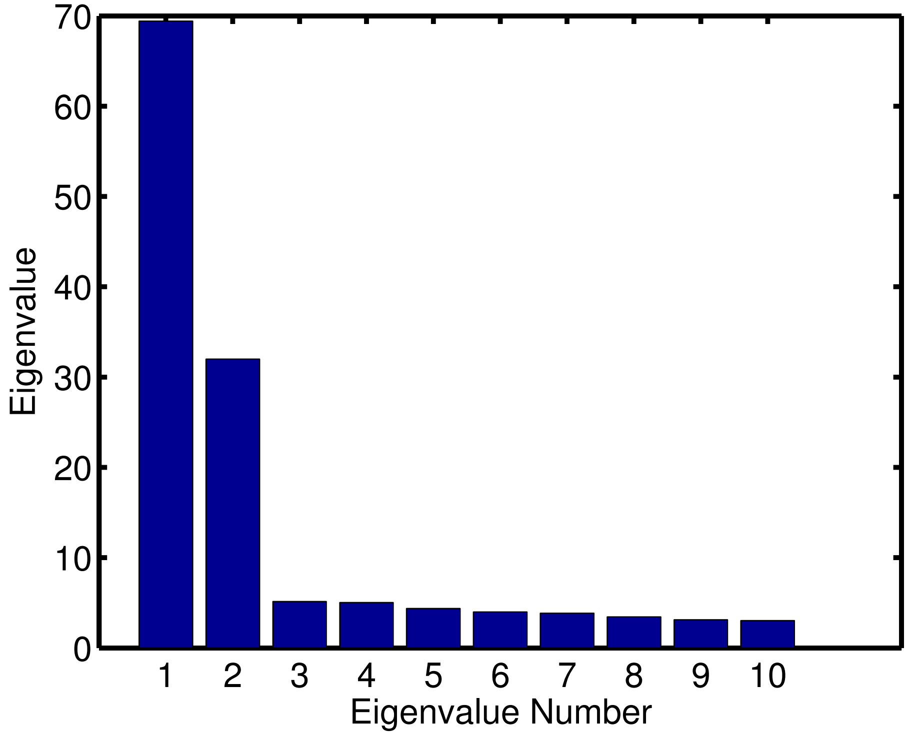

Illustrative Example

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- The face data matrix $\mathbf{X}$ has dimension 400×4096 and so the covariance matrix will have dimension 4096×4096 which is huge relative to the number of examples available.

Illustrative Example

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$$
\begin{aligned}
\widehat{\mathbf{C}} &= \mathbf{B}\mathbf{D}\mathbf{B}^{\mathsf{T}} \\
&\Rightarrow \frac{1}{N}\mathbf{X}^{\mathsf{T}}\mathbf{X} = \mathbf{B}\mathbf{D}\mathbf{B}^{\mathsf{T}} \\
&\Rightarrow \frac{1}{N}\mathbf{X}^{\mathsf{T}}\mathbf{X}\mathbf{B} = \mathbf{B}\mathbf{D} \\
&\Rightarrow \frac{1}{N}\mathbf{X}\mathbf{X}^{\mathsf{T}}\mathbf{X}\mathbf{B} = \mathbf{X}\mathbf{B}\mathbf{D} \\
&\Rightarrow \frac{1}{N}\mathbf{X}\mathbf{X}^{\mathsf{T}}\mathbf{U} = \mathbf{U}\mathbf{D}
\end{aligned}
$$

where we have defined $\mathbf{U} = \mathbf{X}\mathbf{B}$. Now as there are only N non-zero eigenvalues then we can see that

$$\frac{1}{N}\mathbf{X}\mathbf{X}^{\mathsf{T}}\mathbf{U} = \mathbf{U}\mathbf{D}$$

Face Images

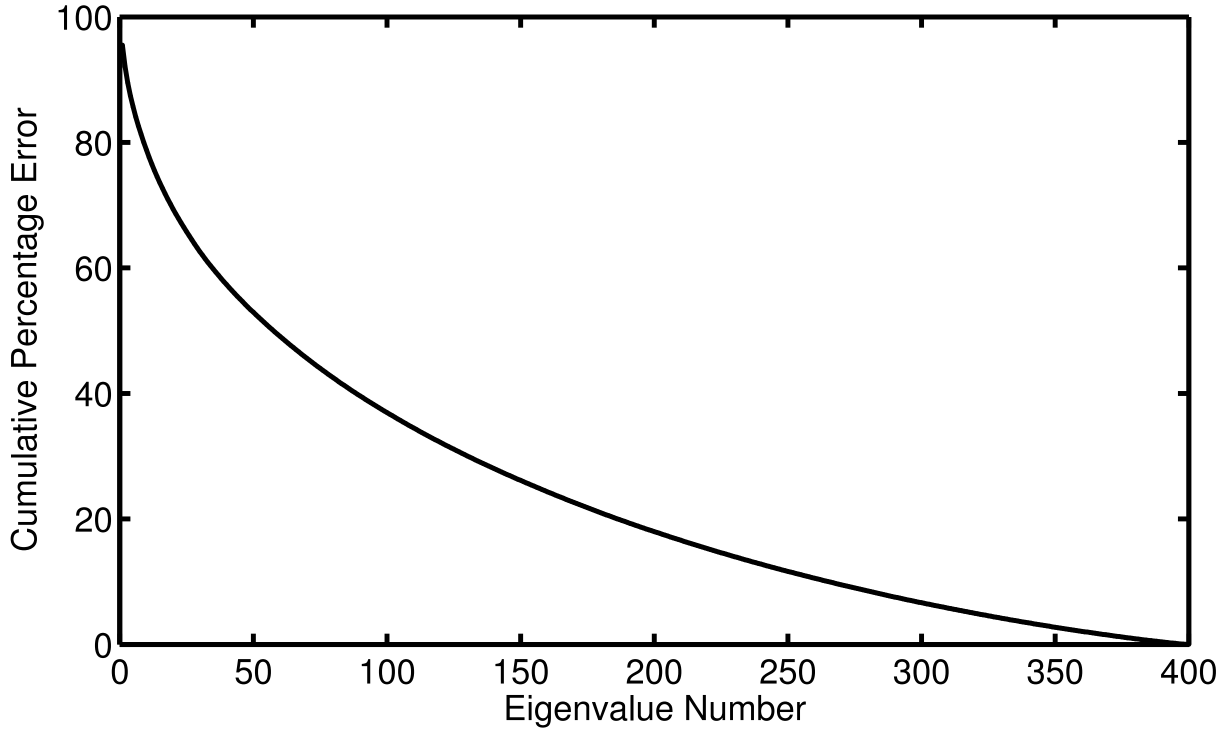

Figure 2: The percentage reconstruction error as principal components are included within the image representation.

Face Images

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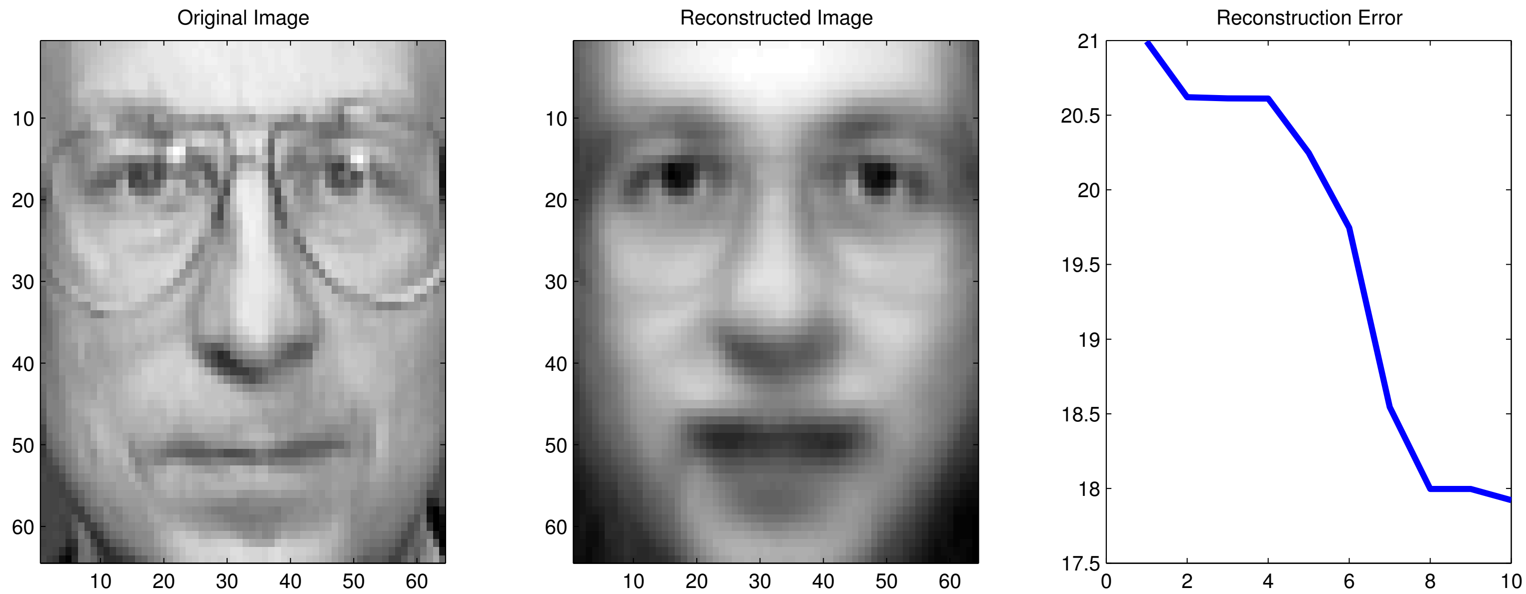

Figure 3: The original image (left) and the reconstructed image (middle) after ten principal components have been employed. The right hand plot shows how the error has decreased for this particular face over the ten PC's employed.

Face Images

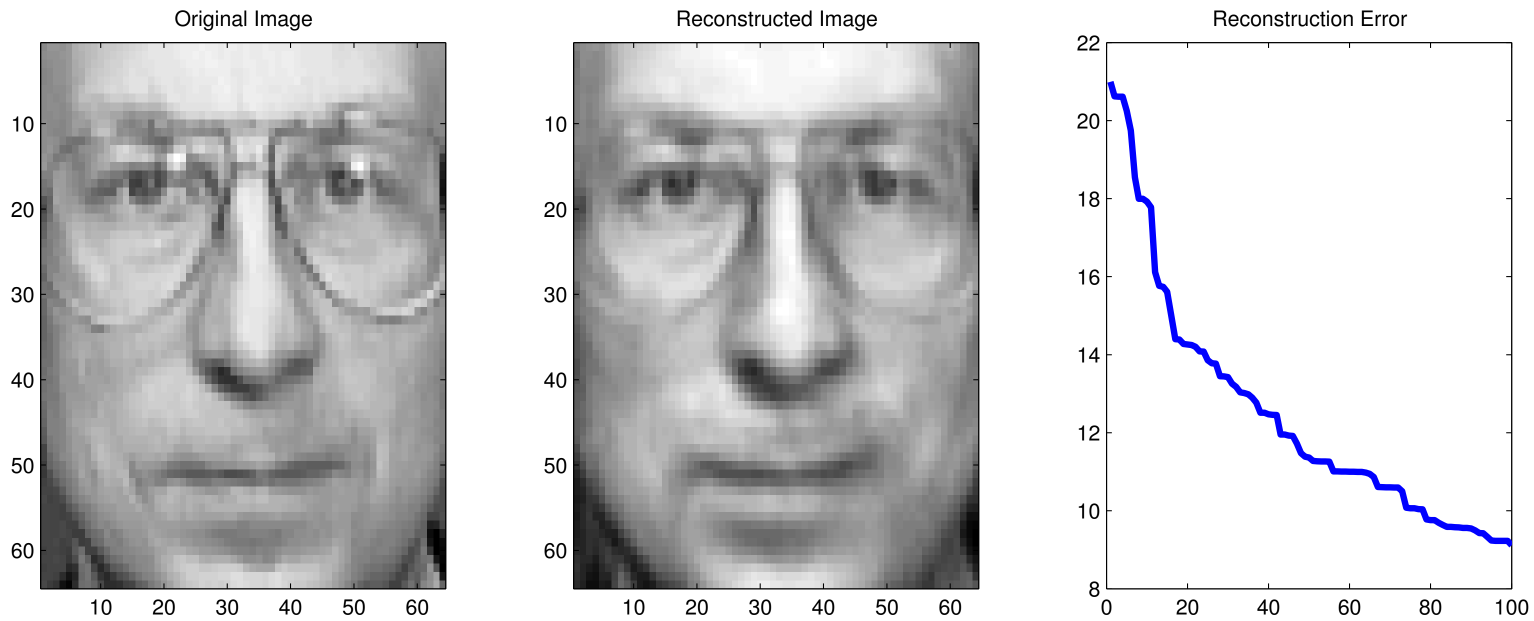

Figure 4: The original image (left) and the reconstructed image (middle) after one hundred principal components have been employed. The right hand plot shows how the error has decreased for this particular face over the one hundred PC's employed.

Generalisation

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- Recall that the variance of predictions made by linear regression models on data points $\mathbf{x}_*$ can be given as

$$\sigma^2 \mathbf{x}_*^{\mathsf{T}} (\mathbf{X}^{\mathsf{T}} \mathbf{X})^{-1} \mathbf{x}_*$$

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Generalisation

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- and as

$$\mathbf{X}^\top \mathbf{X} = N\mathbf{B}\mathbf{D}\mathbf{B}^\top$$

- then given that $\mathbf{B}$ is an orthonormal matrix such that $\mathbf{B}^\top \mathbf{B} = \mathbf{I}$ then $\mathbf{B}^{-1} = \mathbf{B}^\top$ we can write
-

$$(\mathbf{X}^\top \mathbf{X})^{-1} = \frac{1}{N}\mathbf{B}\mathbf{D}^{-1}\mathbf{B}^\top = \frac{1}{N}\sum_{p=1}^{D} \frac{1}{\lambda_p} \boldsymbol{\beta}_p \boldsymbol{\beta}_p^\top$$

Visualistion

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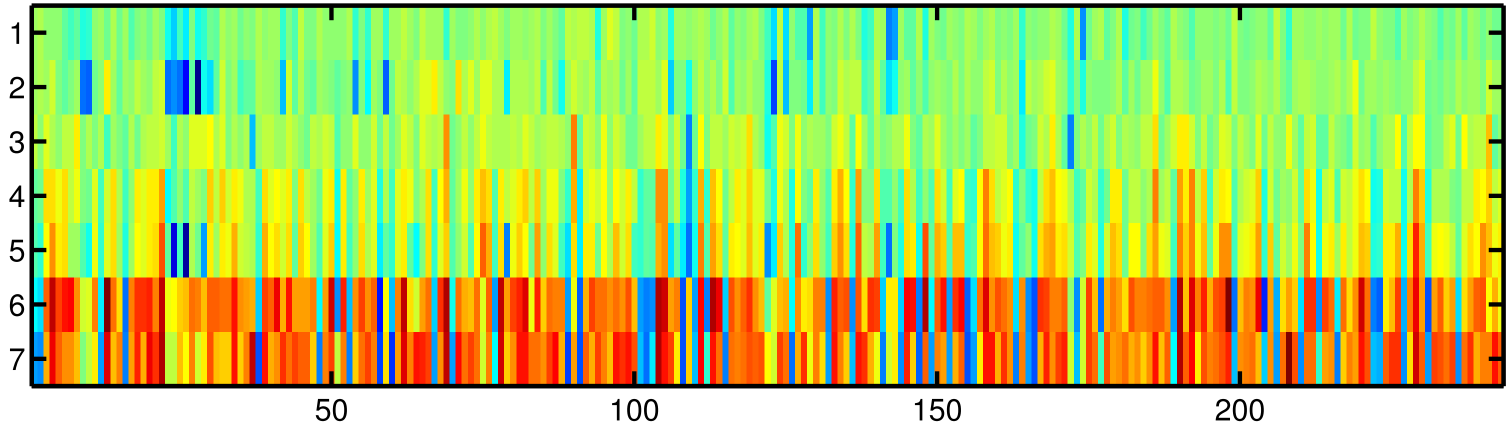

Figure 5: The differential gene expression levels of 243 genes measured at seven time points.

Visualistion

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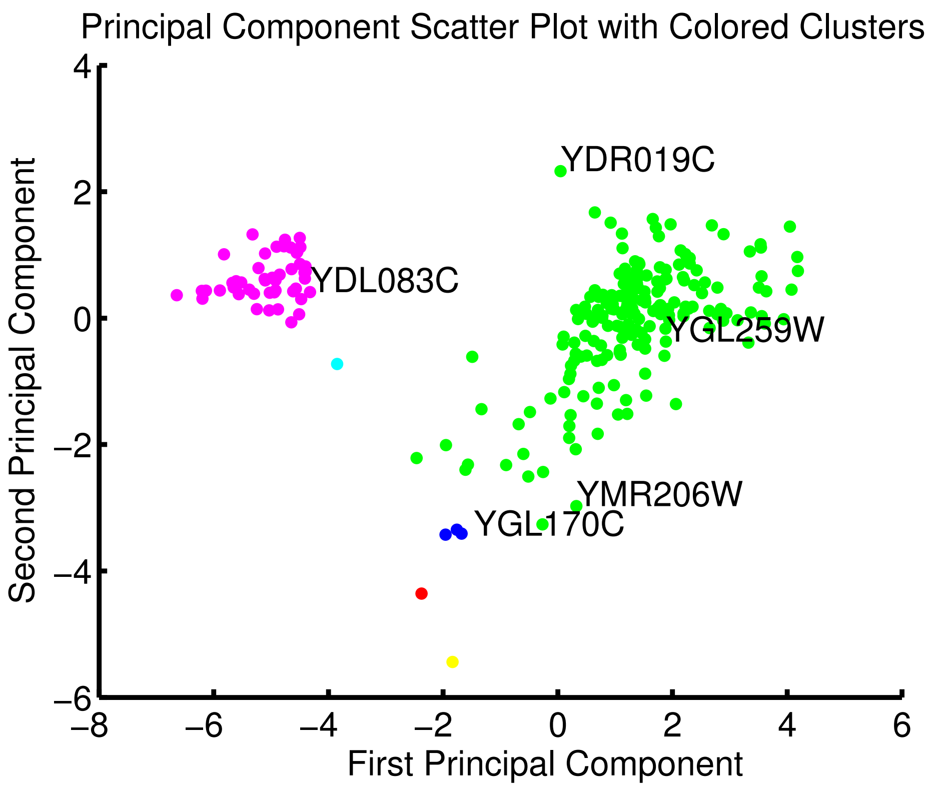

Figure 6: The projection of the differential gene expression levels of 243 genes onto the first two principal directions.

Computing a PCA

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- The following iteration will converge to the principal eigenvector of the covariance matrix $\mathbf{C}$.

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- The following iteration will converge to the principal eigenvector of the covariance matrix $\mathbf{C}$.

$$\begin{aligned} \mathbf{x}_t &= \mathbf{C}\mathbf{y}_{t-1} \\ \mathbf{y}_t &= \frac{\mathbf{x}_t}{\sqrt{\mathbf{x}_t^\top \mathbf{x}_t}} \end{aligned}$$

as $t \to \infty$ then $\mathbf{y}_t \to \boldsymbol{\beta}_1$ and $\sqrt{\mathbf{x}_t^\top \mathbf{x}_t} \to \lambda_1$. Covariance matrix is deflated as detailed previously $\mathbf{C} \leftarrow \mathbf{C} - \lambda_1 \boldsymbol{\beta}_1 \boldsymbol{\beta}_1^\top$ and the above iteration is applied to the deflated matrix to obtain the second eigenvector and associated eigenvalue. This is repeated until all the eigenvector/value pairs are obtained.