Week 8 - Dimensionality Reduction II

COM2004/3004

Jon Barker

Department of Computer Science
University of Sheffield

Autumn Semester

Lecture Objectives

In this lecture we will,

- introduce the idea of a dimensionality reducing transform.
- introduce three types of transform,
  - a fixed transform – e.g. the Discrete Cosine Transform
  - a data dependent transform – e.g. principal component transform
  - a data and class dependent transform – e.g. linear discriminant analysis

Week 8 - Dimensionality Reduction II
Jon Barker
Recap
Dimensionality reducing transforms
Discrete Cosine Transform
Principal Components Analysis
Linear Discriminant Analysis
Summary

How can we reduce dimensionality of $\mathbf{x}$

Consider our face data.

- Select some subset of elements, e.g. keep just a line of pixels down the center of the image
  - Will loose information.
  - How do we select which pixels to keep. . . ?
- Use feature selection techniques like those discussed last week
  - But are any individual pixels likely to discriminate between classes?
  - People can't be identified by looking at individual pixels.
  - Need to find features that are less 'local'.
- Note the high degree of correlation between the features
  - Note, adjacent pixels tend to have similar values – they are correlated
  - A pair of correlated features hold less information that a pair of independent features
  - Intuitively, the 'effective' dimensionality of the face images in less than 17×17

Dimensionality reducing transforms

- Consider some function, H that takes our feature vector x and returns a vector of lower dimensionality y
  - $y = H(x)$ where $\mathbf{x} = \{x_1, x_2, ..., x_N\}$ and $\mathbf{y} = \{y_1, y_2, ..., y_M\}$ and $M < N$.
- We will consider class of functions, H, known as linear transforms.
  - $y_1 = a_{11}x_1 + a_{12}x_2 + ... + a_{1N}x_N$;
  - $y_2 = a_{21}x_1 + a_{22}x_2 + ... + a_{2N}x_N$;
  - $y_M = a_{M1}x_1 + a_{M2}x_2 + ... + a_{MN}x_N$;
- These equations can be written more compactly as,
  - $\mathbf{y} = A\mathbf{x}$ where A is the M by N matrix of parameters a_{ij}

Week 8 - Dimensionality Reduction II

Jon Barker

Recap

Dimensionality reducing transforms

Discrete Cosine Transform

Principal Components Analysis

Linear Discriminant Analysis

Summary

Dimensionality reducing transforms

- Note, feature selection can be seen as a linear transform.
- Special case where for y_i one a_{ij} is 1 and all others are 0.
- For example, consider we are reducing our letter images down to a 3-d feature vector by choosing pixels 20, 145 and 179, then,
  - $y_1 = 0x_1 + 0x_2 + ... + 1x_{20} ... + 0x_{900}$;
  - $y_2 = 0x_1 + 0x_2 + ... + 1x_{145} ... + 0x_{900}$;
  - $y_3 = 0x_1 + 0x_2 + ... + 1x_{179} ... + 0x_{900}$;
- Or $\mathbf{y} = A\mathbf{x}$ with A having 3 rows and 900 column, all 0's except for 1's at $\{1, 20\}$ $\{2, 245\}$ and $\{3, 179\}$
- **Question**: Can we design *better* dimensionality reducing transforms by allowing the matrix A to have an arbitrary form?

What would make a good y?

Some questions that we might consider:

- Is the dimensionality of y much lower than that of the input vector x?
- Does y 'capture the information' that is in x?
- Are the features of y uncorrelated?
- Does y separate out the classes?

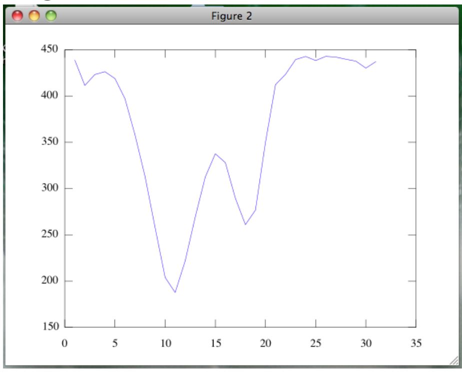
Week 8 - Dimensionality Reduction II
Jon Barker
Recap
Dimensionality reducing transforms
Discrete Cosine Transform
Principal Components Analysis
Linear Discriminant Analysis
Summary

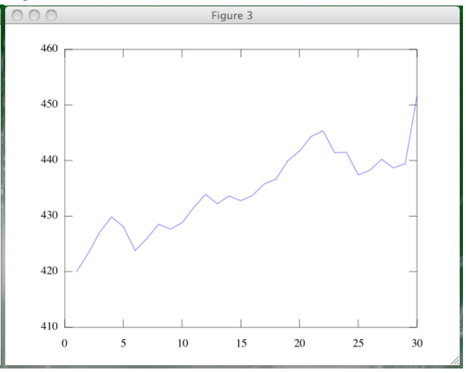
Three different approaches

- Discrete Cosine Transform
  - A fixed transform which does not depend on the data.
- Principal Component Analysis
  - A data dependent approach but which does not consider class labels.
- Linear Discriminant Analysis
  - A transform which considers both the data and the class labels.

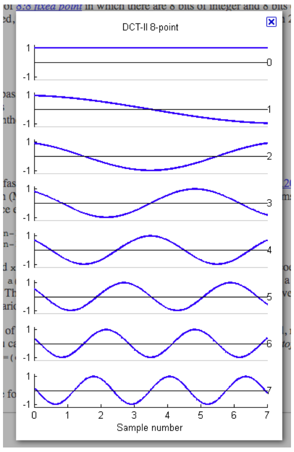
Discrete Cosine Transform

- Consider raw feature vectors made of sequence data
  - temporal sequence - e.g., sound samples, share price history
  - spatial sequence - e.g., pixels in an image
- There are two general observations,
  - adjacent samples in the sequence may be highly correlated
  - rapid fluctuations in the sequence are often uninteresting noise effect
- e.g., consider two rows of pixel data taken from letter 'A'



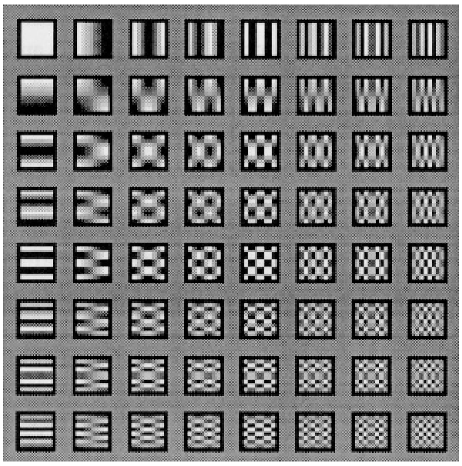


Discrete Cosine Transform

- The Discrete Cosine Transform is a linear transform $\mathbf{y} = A\mathbf{x}$, with
  - $a_{ij} = \cos\left(\frac{\pi}{N}(j + \frac{1}{2})i\right)$
- Can consider the transform as breaking the sequence $\mathbf{x}$ into a weighted sum of a set of basis functions.
  - 

- y_1 how much DC component, y_2 how much tilt, y_3 how much dip in middle etc
- Rapid variations represented by parameters at end of the vector y
- The elements of y tend to be fairly independent.

Discrete Cosine Transform

- There is a 2-D form of the DCT that can be used to transform 2-D images
- Equivalent to describing image as a weighted sum of 'basis images' of the form below.
  - 
- This is how JPEG image compression works.

Week 8 - Dimensionality Reduction II
Jon Barker
Recap
Dimensionality reducing transforms
Discrete Cosine Transform
Principal Components Analysis
Linear Discriminant Analysis
Summary

Principal Component Analysis (PCA)

- DCT is a fixed data-independent transform.
- Generally does a good just of decorrelating features and removing irrelevant fine detail.
- Can we do better by tailoring a transform to our particular training data?
- Principal Component Analysis is one approach.
- PCA aims to reduce the dimensionality of the data while preserving its spread.

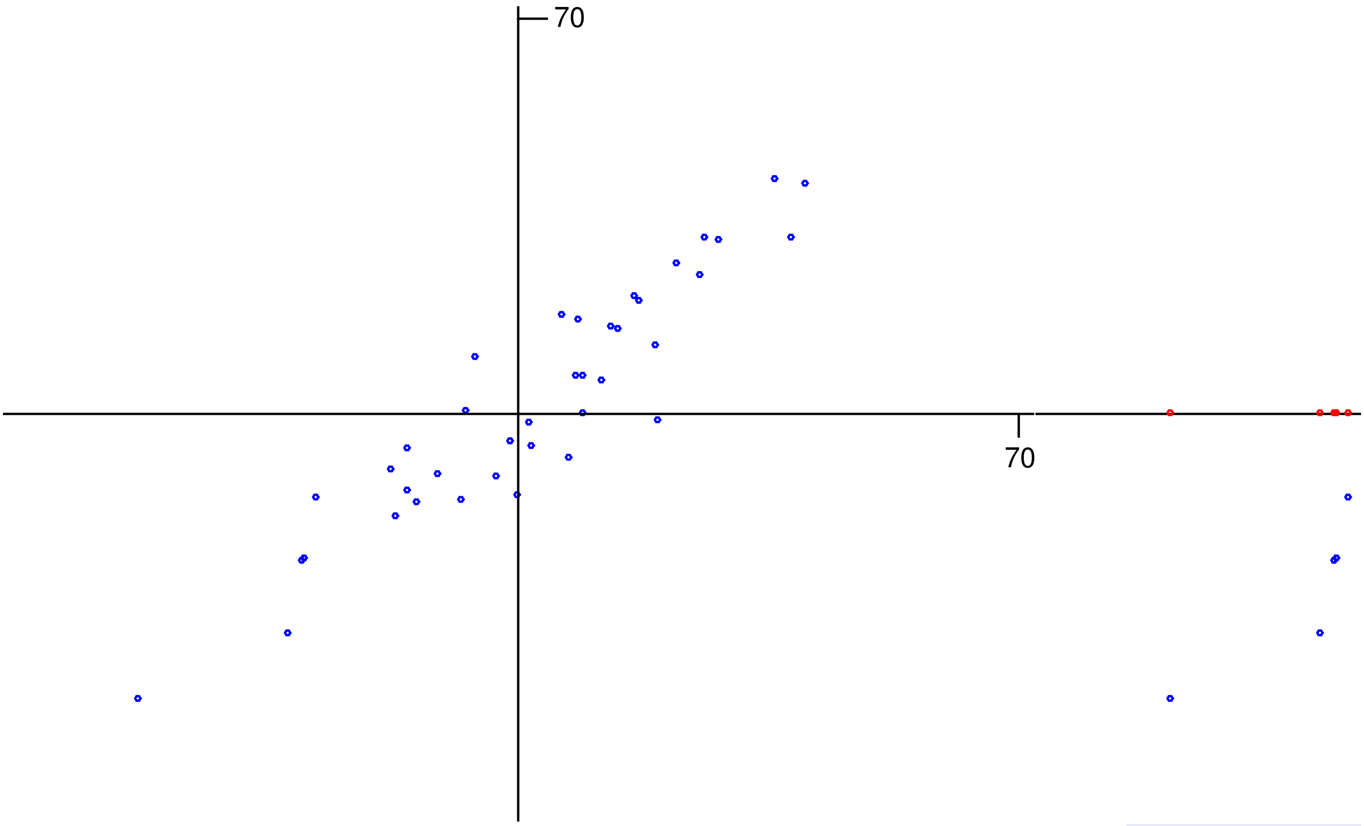
PCA – the basic idea

- Consider the act of photographing a 3D object.
- You are reducing a set of 3D points in the real world to a set of 2D points in the image.
- Dimensionality has been reduced and some information has been lost.
- What angle would you choose to photograph the object from in order to preserve as much information as possible?
- Example: photographing a teapot

Teapot example

Principal Component Analysis (PCA)

- Consider the following highly correlated data.!!

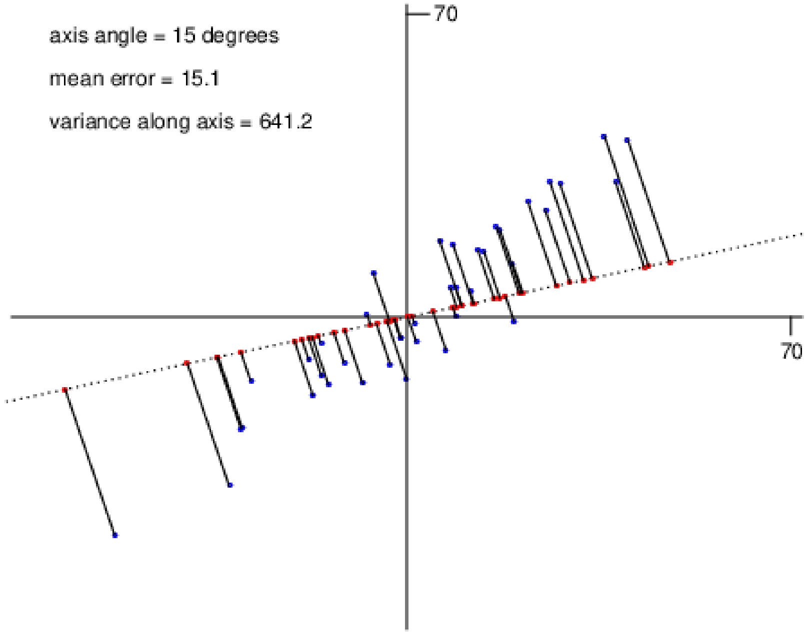


Week 8 - Dimensionality Reduction II
Jon Barker

Recap
Dimensionality

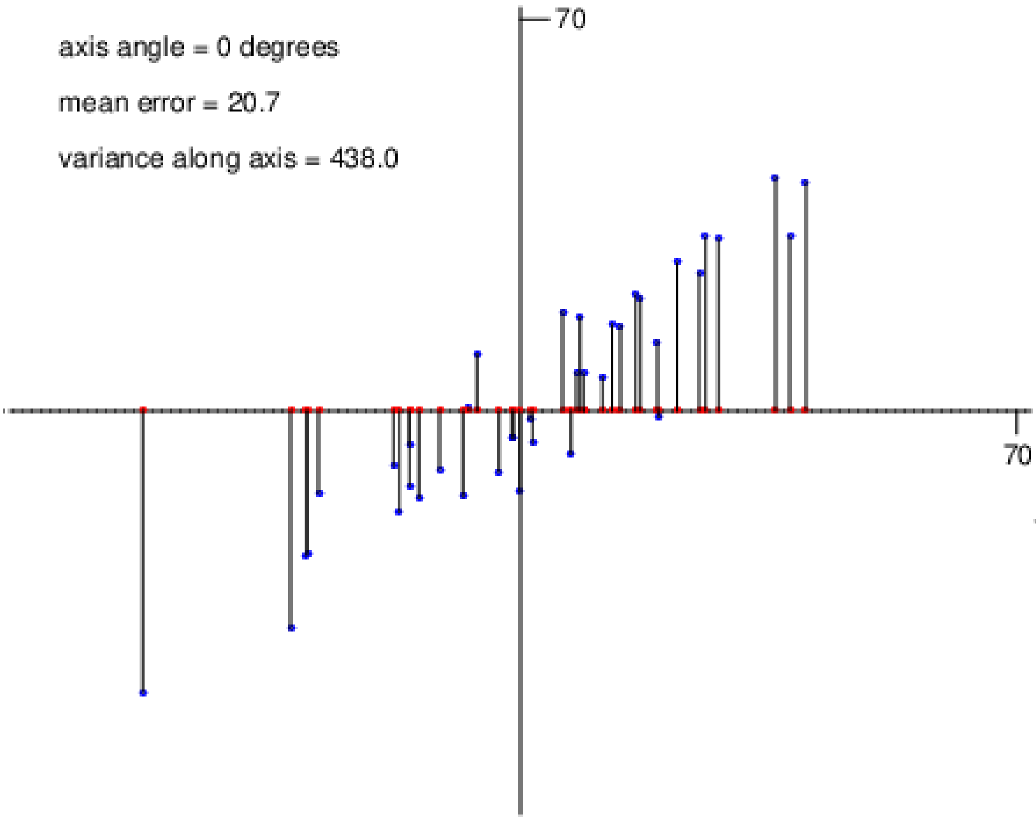
Projecting points onto a new axis

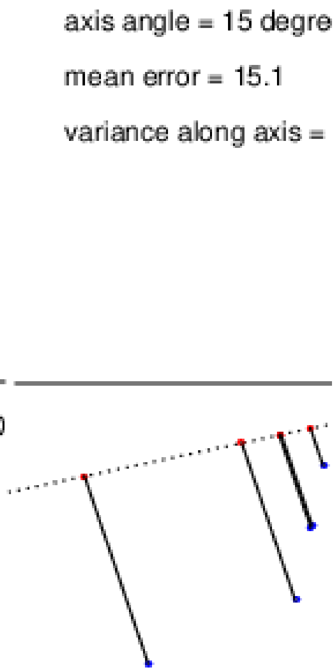
- Points can be ‘projected’ onto any axis.
- The projection of a point is the point on the axis which lies closest to it.
- Note how the line from a point to its projection meets the axis at right angles.



Finding the principal axis

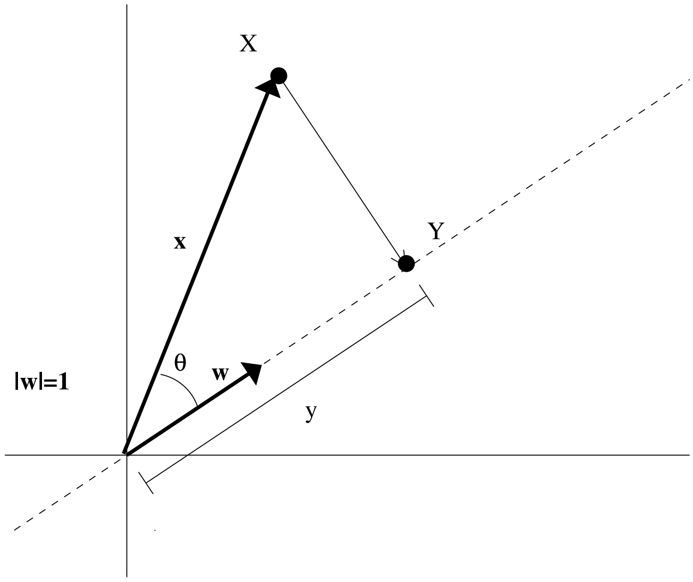
- The principal axis is the one that best represents the data, i.e. projected points lie close to original points.





Position of projected point

- Given a point X and an axis direction $\mathbf{w}$ we wish to know the distance, y, of the point's projection along the axis.



- From the figure we can see that $y = |\mathbf{x}| \cos \theta$
- Remember, $\mathbf{x}.\mathbf{w} = |\mathbf{x}||\mathbf{w}| \cos \theta$ where θ is the angle between the vectors.
- $\mathbf{w}$ has unit length, so $\mathbf{x}.\mathbf{w} = |\mathbf{x}| \cos \theta = y$
- i.e., $y = \mathbf{x}.\mathbf{w}$, distance y is the dot product of the data point $\mathbf{x}$ and the axis direction vector $\mathbf{w}$

Week 8 - Dimensionality Reduction II
Jon Barker
Recap
Dimensionality reducing transforms
Discrete Cosine Transform
Principal Components Analysis
Linear Discriminant Analysis
Summary

Principal Component Analysis

- Consider n d-dimensional samples, $\mathbf{x}_1, \ldots, \mathbf{x}_n$,
- Consider, y_i, the coordinate of the projection of these points onto a new axis $\mathbf{w}$

$$y_i = \mathbf{w}^t \mathbf{x}_i$$

- The first principal axis, $\mathbf{w}_1$ is defined as the linear combination $y_i = \mathbf{w}_1^t \mathbf{x}_i$ for which the y_i have the largest possible variance given $\mathbf{w}_1^t \mathbf{w}_1 = 1$.
- i.e. the axis $\mathbf{w}_1$ along which the projected points are most spread out.

Principal Component Analysis

- The first principal axis, $\mathbf{w}_1$ is defined as the linear combination $y_i = \mathbf{w}_1^t \mathbf{x}_i$ for which the y_i have the largest possible variance given $\mathbf{w}^t\mathbf{w} = 1$.
- The second principal axis, $\mathbf{w}_2$ is the linear combination $y_i = \mathbf{w}_2^t \mathbf{x}_i$ for which the y_i have the largest possible variance given $\mathbf{w}_2^t\mathbf{w}_2 = 1$ **and** such that $\mathbf{w}_2^t\mathbf{w}_1 = 0$ (orthogonal)
- The third principal axis, $\mathbf{w}_3$ is the linear combination $y_i = \mathbf{w}_3^t \mathbf{x}_i$ for which the y_i have the largest possible variance given $\mathbf{w}_3^t\mathbf{w}_3 = 1$ **and** such that $\mathbf{w}_3^t\mathbf{w}_1 = 0$ **and** $\mathbf{w}_3^t\mathbf{w}_2 = 0$
- etc
- Once we have found all the first M axes we can project an x onto the new set of axes by simply computing $\mathbf{y} = A\mathbf{x}$ where the matrix $\mathbf{A}$ is $\{\mathbf{w}_1^T, \mathbf{w}_2^T, ..., \mathbf{w}_M^T\}$
- But how do we find the axes $\mathbf{w}$?

Principal Component Analysis

Let $S(y)$ be the variance of the values y.

By definition

$$S(y) = \frac{1}{n-1}\sum_{i=1}^{n}(y_i - \tilde{y})^2$$

Substituting $y_i = \mathbf{w}^t\mathbf{x}_i$ and performing a little algebra,

$$\begin{aligned} S(y) &= \frac{1}{n-1}\sum_{i=1}^{n}(y_i - \tilde{y})^2 \\ &= \frac{1}{n-1}\sum_{i=1}^{n}\mathbf{w}^t(\mathbf{x}_i - \tilde{\mathbf{x}})(\mathbf{x}_i - \tilde{\mathbf{x}})^t\mathbf{w} \\ &= \mathbf{w}^t[\frac{1}{n-1}\sum_{i=1}^{n}(\mathbf{x}_i - \tilde{\mathbf{x}})(\mathbf{x}_i - \tilde{\mathbf{x}})^t]\mathbf{w} \end{aligned}$$

Principal Component Analysis

So, we have,

$$S_y = \mathbf{w}^t \left[\frac{1}{n-1} \sum_{i=1}^{n} (\mathbf{x}_i - \tilde{\mathbf{x}})(\mathbf{x}_i - \tilde{\mathbf{x}})^t \right] \mathbf{w}$$

but the bit inside [] is just the definition of the covariance matrix $\mathbf{S}_x$ computed from the original data points x.

So we can compute, $\mathbf{S}_x$ from our data, and then find the $\mathbf{w}$ that maximises, S_y

$$S_y = \mathbf{w}^t \mathbf{S}_x \mathbf{w}$$

The $\mathbf{w}$ is constrained to be of unit length, i.e.,

$$\mathbf{w}^t \mathbf{w} = 1$$

Principal Component Analysis

Week 8 - Dimensionality Reduction II

Jon Barker

Recap

Dimensionality reducing transforms

Discrete Cosine Transform

Principal Components Analysis

Linear Discriminant Analysis

Summary

Now it turns out that the $\mathbf{w}$ that maximises $S_y = \mathbf{w} S_x \mathbf{w}$ must also satisfy,

$$S_x \mathbf{w} = \lambda \mathbf{w}$$

i.e. $\mathbf{w}$ is an eigenvector of the covariance matrix S_x.

But S_x will have more than one eigenvector. Which one do we pick?

Note, premultiplying both sides of the equation above by $\mathbf{w}^t$,

$$\mathbf{w}^t S_x \mathbf{w} = \lambda \mathbf{w}^t \mathbf{w} = \lambda$$

We want to maximise $\mathbf{w}^t S_x \mathbf{w}$, so we choose the eigenvector $\mathbf{w}$ corresponding to the eigenvalue, λ, which has the largest value.

Principal Component Analysis

For the second axis, p_1, we again want to maximise $S_y^t = \mathbf{p}_2 S_x \mathbf{p}_2$ but now subject:to the two constraints:

- $\mathbf{p}_2^t \mathbf{p}_2 = 1$ and
- $\mathbf{p}_2^t \mathbf{p}_1 = 0$ (i.e. 2nd axis is orthogonal to 1st).

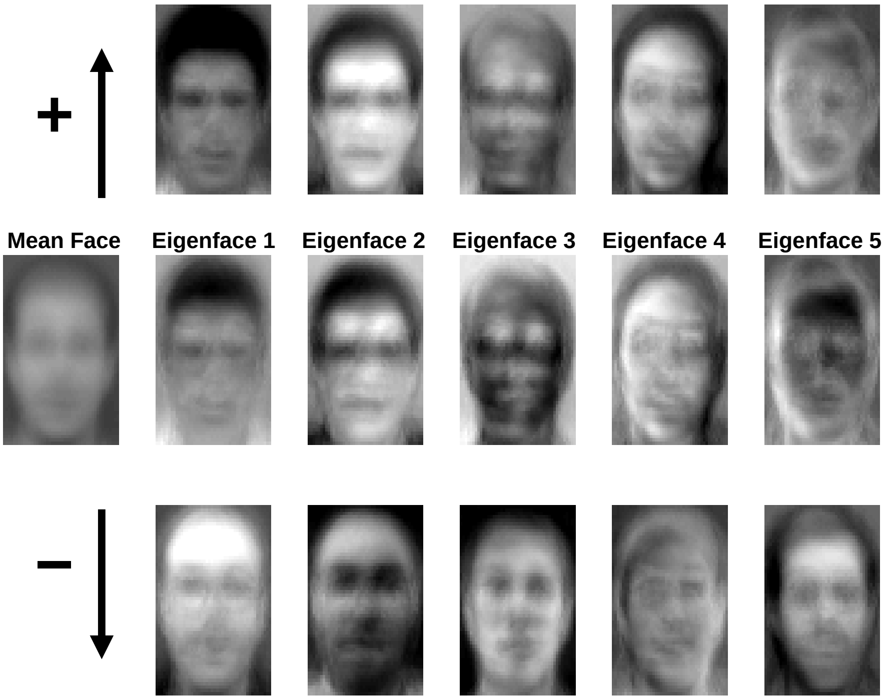
With these constraints it can be shown that $\mathbf{p}_2$ is in fact the eigenvector of S_x associated with the 2nd largest eigenvalue. We continue the process, so that each new axis maximised S_y^t while being constrained to be orthogonal to all the others found so far. It turns out, the new axes are simply the eigenvectors of S_x, ordered by their respective eigenvalues.

Principal Components as ‘Basis’ Vectors

- The principle components, $\mathbf{w}_1$, $\mathbf{w}_2$ ... $\mathbf{w}_M$ can also be seen as a set of ‘basis’ vectors.
- $\mathbf{y} = \mathbf{A}\mathbf{x}$ can be written as $\mathbf{A}^T\mathbf{y} = \mathbf{x}$
  - this is because $\mathbf{A}$ is orthogonal, i.e. $\mathbf{A}\mathbf{A}^T = I$
- Remember, $\mathbf{A} = \{\mathbf{w}_1^T, \mathbf{w}_2^T, ..., \mathbf{w}_M^T\}$ so $\mathbf{A}^T\mathbf{y} = \mathbf{x}$ is just saying,
  - $\mathbf{x} = y_1 * \mathbf{w}_1 + y_2 * \mathbf{w}_2 + ... + y_N * \mathbf{w}_N$
  - i.e., $\mathbf{x}$ is made up of a weighted sum of the principle component where the y vector is storing the weights.
- If we truncate the sum and use just the first few dimensions of $\mathbf{y}$ then,
  - $\mathbf{x} \approx y_1 * \mathbf{w}_1 + y_2 * \mathbf{w}_2 + ... + y_M * \mathbf{w}_M$ with $M < N$

Faces – variability represented by first 5 principal components

After applying PCA to image data we can reshape the principle component vectors into matrices and display them as images.

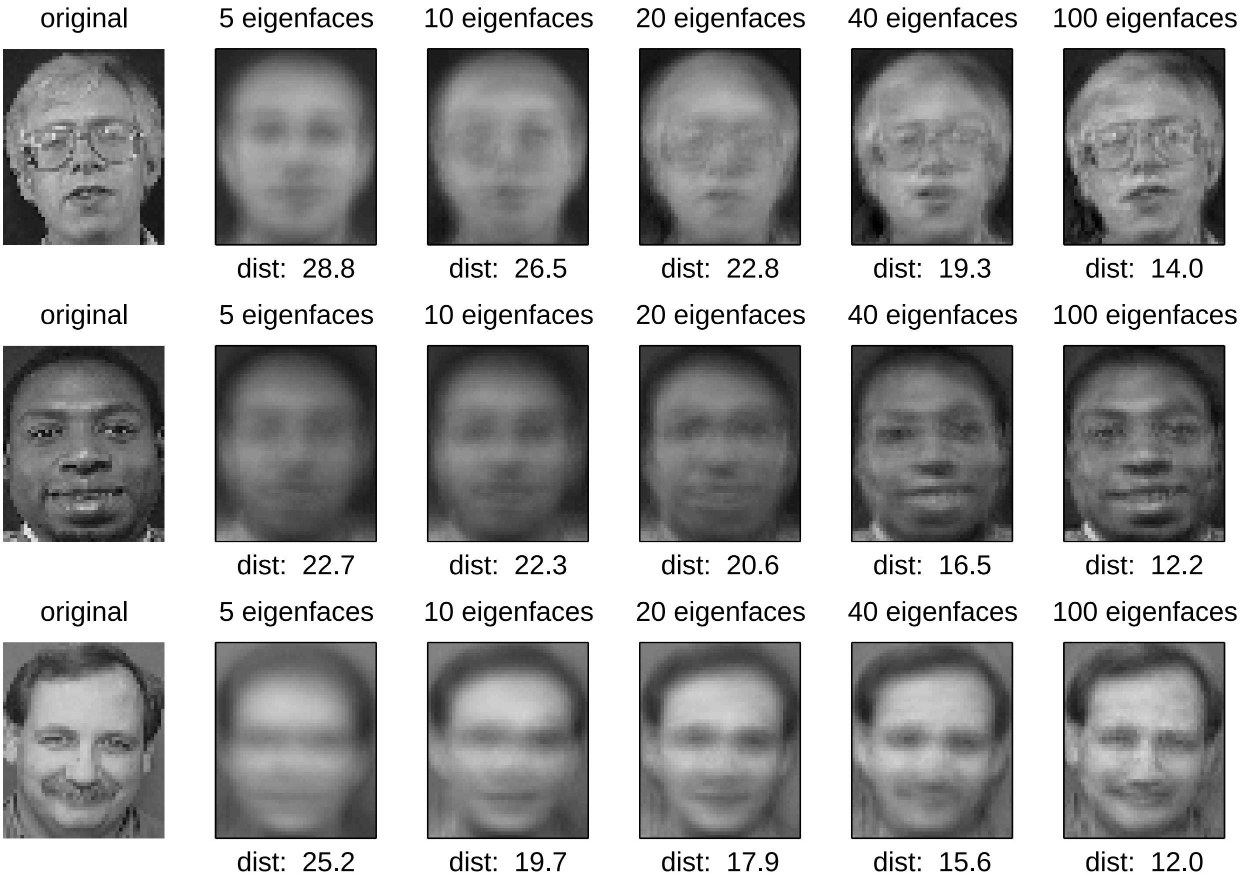


Week 8 - Dimensionality Reduction II

Jon Barker

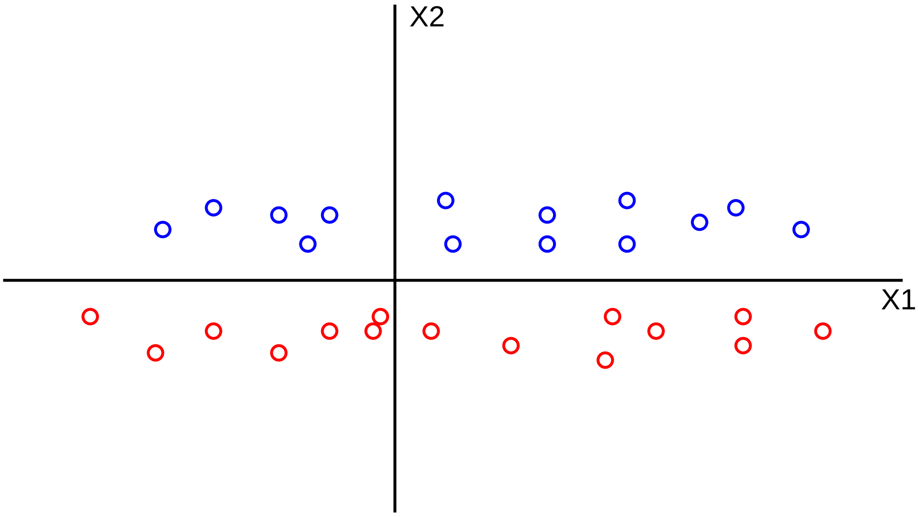
Recap
Dimensionality reducing transforms
Discrete Cosine Transform
Principal Components Analysis
Linear Discriminant Analysis
Summary

Faces – using increasing number of PCA dimensions



Linear Discriminant Analysis

- PCA ensures that the data
  - has independent features – easy to model statistically
  - is well spread out – so classes are less likely to overlap
- But ‘spreadoutness’ has been maximised by looking at the data as a whole, i.e.,
  - the algorithm doesn’t make use of the class labels,
  - and spreading out the data doesn’t necessarily separate the classes,
  - e.g., in example below, X1 spreads the data but X2 separates the classes,

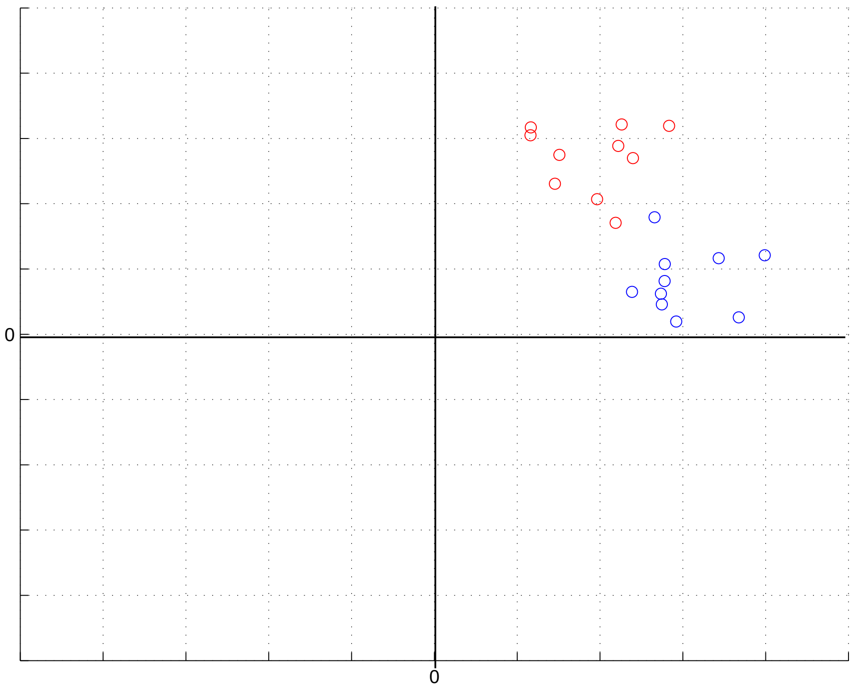


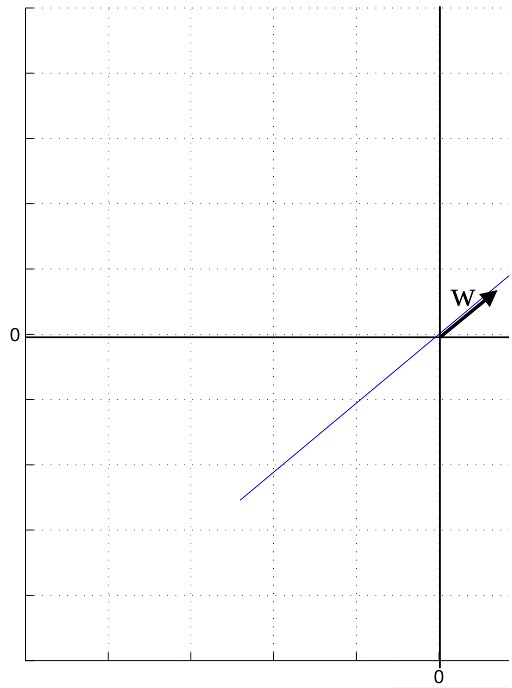
  -

Linear Discriminant Analysis

Week 8 - Dimensionality Reduction II
Jon Barker

Recap





Summary

- Dimensionality reduction is a generalisation of the feature selection idea
- A popular approach is to perform a linear transform of the data.
- DCT - a fixed transform that works well for sequence data.
- PCA - a data-driven transform that aims to reduce dimensionality while retaining the spread of the data.
- LDA - a data and label driven transform that reduces dimensionality while retaining the separability of the classes.
- PCA and LDA also result in decorrelated features that mean simple statistical models can be used for classification.