THE UNIVERSITY *of* EDINBURGH
informatics

Applied Machine Learning (AML)

Exploratory Data Analysis

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Data Visualisation

Plotting Data

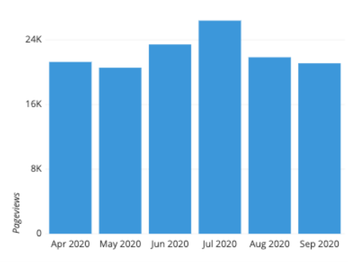
Figures: chartio.com

Plotting Data

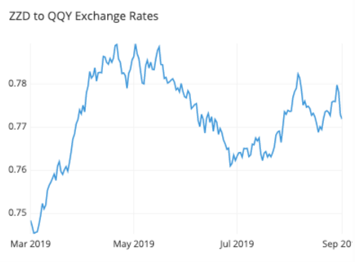
Plot Types

- temporal change

Bar chart



Line chart



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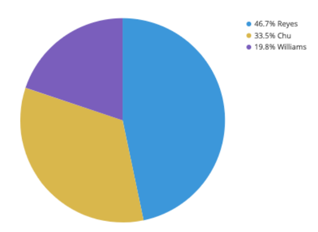
Plotting Data

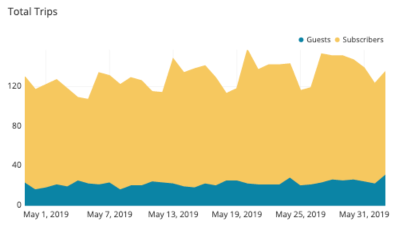
Plot Types

- temporal change
- part-to-whole composition

Pie chart



Stacked area chart



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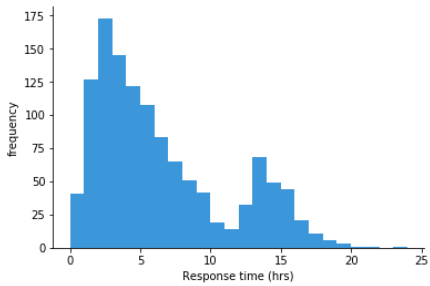
Plotting Data

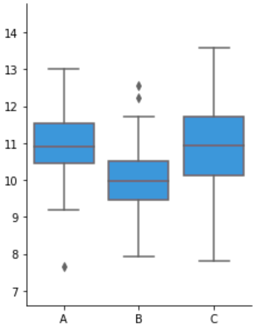
Plot Types

- temporal change
- part-to-whole composition
- distribution

Histogram



Box plot



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Plotting Data

Plot Types

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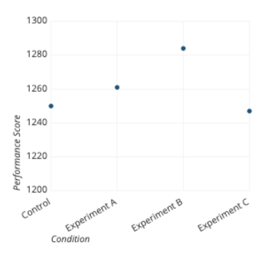
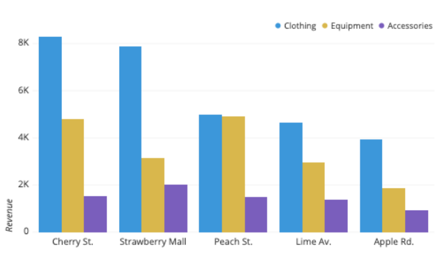
- distribution
- group comparison

Point plot



Grouped bar chart



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Plotting Data

Plot Types

- temporal change
- part-to-whole composition
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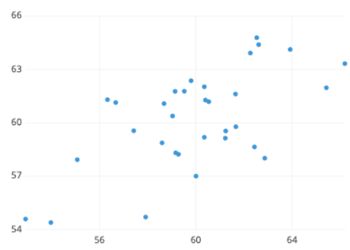
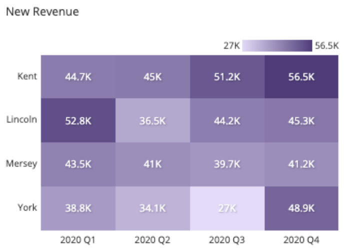
- inter-variable relations

Scatter plot



Heat map



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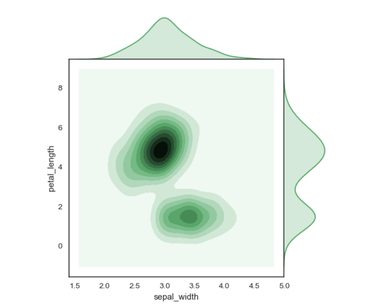
Plotting Data

Plot Types

- temporal change
- part-to-whole composition
- distribution
- group comparison
- inter-variable relations
- and more …

Wordcloud

Joint plot



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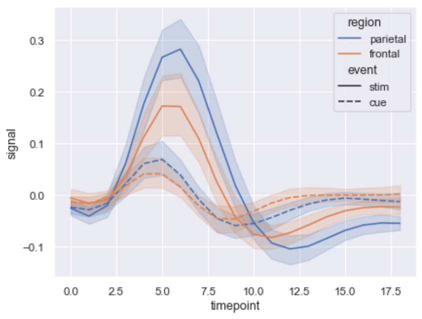
Features of a good plot

Figures: Matplotlib—anatomy of a figure

Features of a good plot

- title
- labelled axes
- axes ranges and ticks
- clarity (colour/thickness)
- legend

Neural response (BOLD)



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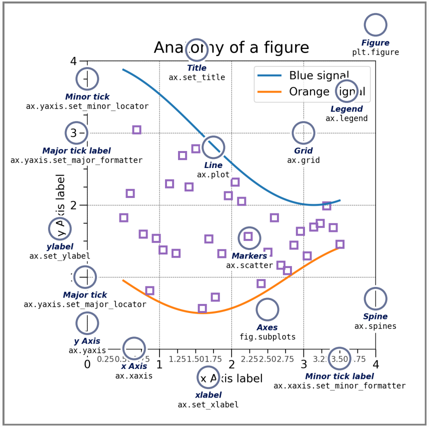
informative:
convey as much as necessary

clean:
avoid overfilling & redundancy



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Relatively easy to think about when data is low dimensional

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Relatively easy to think about when data is low dimensional

What do we do when data is high dimensional?

Figures: Matplotlib—anatomy of a figure

Dimensionality Reduction

Curse of Dimensionality

Manifold Hypothesis

High-dimensional data in the real world really lies on low-dimensional manifolds within that high-dimensional space.

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  vision: 10^4 pixels, text: 10^6 words

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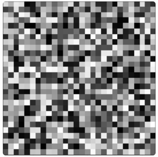
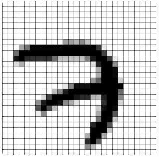
- Example: handwritten digits (MNIST)
  - 28×28 pixels $\rightarrow \{0,1\}^{784}$ possible “images”
  - only a very small number of these images are actually real
  - true dimensionality: actual variation of pen strokes!





Dealing with high dimensionality

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Statistics

- ML involves some form of “counting” observations and features
  - count within some regions
    e.g. constructing histograms
  - use counts to construct predictors
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- domain knowledge / feature engineering
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- reduce data dimensionality
  construct a new set of dimensions / variables

Dimensionality Reduction

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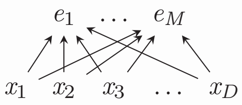
- construct a new set of dimensions



$$M \ll D$$

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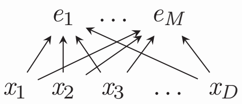

$$M \ll D$$

- transformation of original

  e.g. linear $F \implies \boldsymbol{e} = F\boldsymbol{x}$

Dimensionality Reduction

PCA

Principal Components Analysis (PCA)

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Define principal components (PCs)

- 1st PC: direction of *greatest* variation in the data
- 2st PC: ⊥ 1st PC; greatest *remaining* variation

…and so on until D, for $\boldsymbol{x} \in \mathbb{R}^D$.

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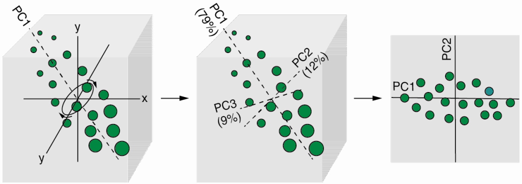
- First $M \ll D$ components $\rightarrow$ new basis dimensions
- …transform coordinates of each data point to new basis



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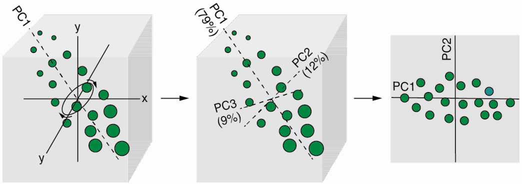


Rationale

- variation along direction
= *information*
- transform basis →
fit maximum information
into M dimensions

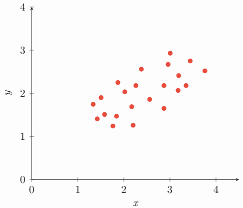
PCA: Basics

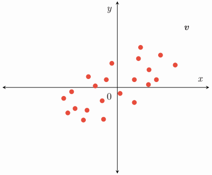
$$X = \begin{bmatrix} \boldsymbol{x}_1^\top \\ \vdots \\ \boldsymbol{x}_N^\top \end{bmatrix} \qquad X \in \mathbb{R}^{N \times D}, \ \boldsymbol{x}_i \in \mathbb{R}^D$$

(data)

$$S = \frac{1}{N} X^\top X \qquad S \in \mathbb{R}^{D \times D}$$

(covariance, assuming 0-mean)





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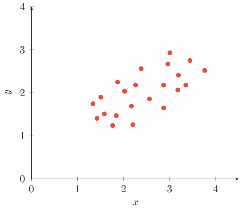

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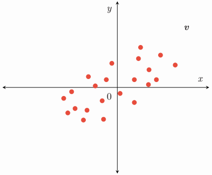
Intuition

Repeated transformation using the covariance (S) turns towards direction of maximum variance

(example)



$$S\boldsymbol{v} = \begin{bmatrix} 2.0 & 0.8 \\ 0.8 & 0.6 \end{bmatrix} \begin{bmatrix} -1 \\ 1 \end{bmatrix} = \begin{bmatrix} -1.2 \\ 0.2 \end{bmatrix} \stackrel{S}{=} \ldots \stackrel{S}{=} \begin{bmatrix} -14.1 \\ -6.4 \end{bmatrix} \stackrel{S}{=} \begin{bmatrix} -33.3 \\ -15.1 \end{bmatrix}$$

where the *slope* converges to 0.454

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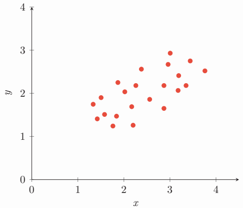

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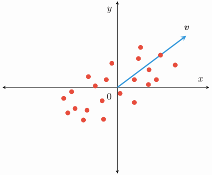

Goal: Find $\boldsymbol{v}$ such that

$$S\boldsymbol{v} = \lambda \boldsymbol{v}$$

PCA: Maximising Variance

Recall $X\boldsymbol{v}$ projects X onto $\boldsymbol{v}$

PCA: Maximising Variance

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$$\begin{aligned}
\mathrm{Var}[X\boldsymbol{v}] &= \frac{1}{N}(X\boldsymbol{v})^\top(X\boldsymbol{v}) \\
&= \frac{1}{N}\boldsymbol{v}^\top X^\top X\boldsymbol{v} \\
&= \boldsymbol{v}^\top \frac{X^\top X}{N}\boldsymbol{v} \\
&= \boldsymbol{v}^\top S\boldsymbol{v}
\end{aligned}$$

PCA: Maximising Variance

Recall $X\boldsymbol{v}$ projects X onto $\boldsymbol{v}$ $max\ \boldsymbol{v}^\top S\boldsymbol{v},$ s.t. $\boldsymbol{v}^\top\boldsymbol{v} = 1$

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solved using *Lagrange multipliers* as

$$max\ \underbrace{\boldsymbol{v}^\top S\boldsymbol{v} - \lambda\left(\boldsymbol{v}^\top\boldsymbol{v} - 1\right)}_{\mathcal{L}}$$

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computing derivative w.r.t $\boldsymbol{v}$ and setting $= 0$

$$\frac{d\mathcal{L}}{d\boldsymbol{v}} = 2S\boldsymbol{v} - 2\lambda\boldsymbol{v} = 0$$

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$$S\boldsymbol{v} = \lambda\boldsymbol{v}$$

left multiply by $\boldsymbol{v}^\top$

$$\begin{aligned}\boldsymbol{v}^\top S\boldsymbol{v} &= \boldsymbol{v}^\top\lambda\boldsymbol{v} \\ &= \lambda\boldsymbol{v}^\top\boldsymbol{v} \\ &= \lambda \quad \square\end{aligned}$$

PCA: Maximising Variance

Recall Xv projects X onto v

$$\mathrm{Var}[Xv] = \frac{1}{N}(Xv)^\top(Xv)$$
$$= \frac{1}{N}v^\top X^\top Xv$$
$$= v^\top \frac{X^\top X}{N} v$$
$$= v^\top S v$$

$max\ v^\top Sv$, s.t. $v^\top v = 1$

solved using *Lagrange multipliers* as

$$max\ \underbrace{v^\top Sv - \lambda\left(v^\top v - 1\right)}_{\mathcal{L}}$$

computing derivative w.r.t v and setting $= 0$

$$\frac{d\mathcal{L}}{dv} = 2Sv - 2\lambda v = 0$$
$$Sv = \lambda v \quad \square$$

$v \longrightarrow$ direction of max variance

$$Sv = \lambda v$$

left multiply by $v^\top$

$$v^\top Sv = v^\top \lambda v$$
$$= \lambda v^\top v$$
$$= \lambda \quad \square$$

$\lambda \longrightarrow$ max variance

PCA: Finding Principal Components

More generally, solve for $SV = \Lambda V$ using Eigen decomposition

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Eigenvalues

Solve $|S - \lambda I| = 0$

$$\begin{vmatrix} 2.0 - \lambda & 0.8 \\ 0.8 & 0.6 - \lambda \end{vmatrix} = 0$$

$$\lambda^2 - 2.6\lambda + 0.56 = 0$$

$$\implies \{\lambda_1, \lambda_2\} = \{2.36, 0.23\}$$

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Eigenvectors

Find i^{th} eigenvector by solving $S\boldsymbol{v}_i = \lambda_i \boldsymbol{v}_i$

$$\begin{bmatrix} 2.0 & 0.8 \\ 0.8 & 0.6 \end{bmatrix} \begin{bmatrix} v_{1,1} \\ v_{1,2} \end{bmatrix} = 2.36 \begin{bmatrix} v_{1,1} \\ v_{1,2} \end{bmatrix} \quad \Longrightarrow \quad \boldsymbol{v}_1 = \begin{bmatrix} 2.2 \\ 1 \end{bmatrix}$$

$$\begin{bmatrix} 2.0 & 0.8 \\ 0.8 & 0.6 \end{bmatrix} \begin{bmatrix} v_{2,1} \\ v_{2,2} \end{bmatrix} = 0.23 \begin{bmatrix} v_{2,1} \\ v_{2,2} \end{bmatrix} \quad \Longrightarrow \quad \boldsymbol{v}_2 = \begin{bmatrix} -0.41 \\ 0.91 \end{bmatrix}$$

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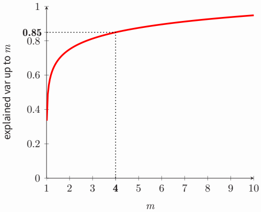

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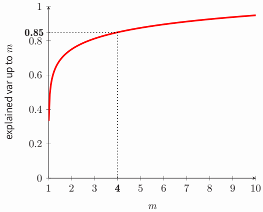
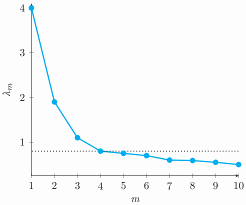


Elbow plot

- plot eigenvalues in descending order $\lambda_1 \geq \ldots \geq \lambda_D$
- choose point at which curve "bends" most (i.e. elbow)



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Let $V_M = [\boldsymbol{v}_1, \ldots, \boldsymbol{v}_M] \in \mathbb{R}^{D \times M}$ denote the *truncated* eigenvector matrix for $M \ll D$

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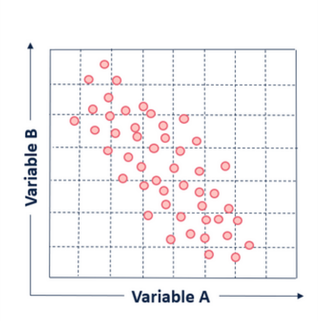
$V_M V_M^\top \in \mathbb{R}^{D \times D}$ is the data *projection* matrix

Dimensionality Reduction

PCA: Examples

PCA: Overview and Use

Characteristics



Figures: Sydney Firmin @ towardsdatascience.com

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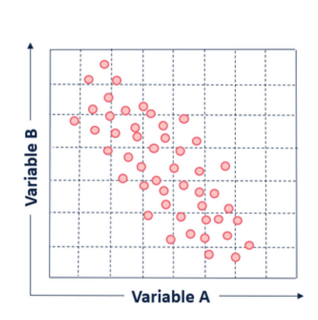

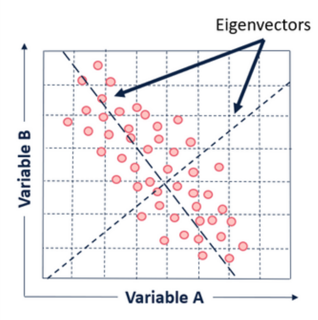

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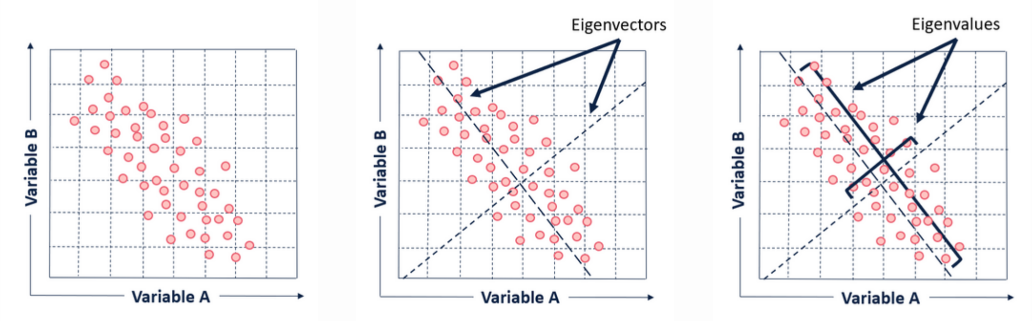

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PCA: Overview and Use

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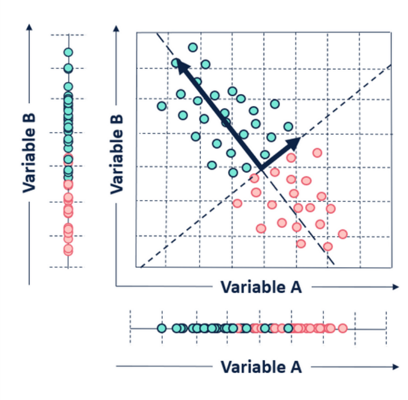

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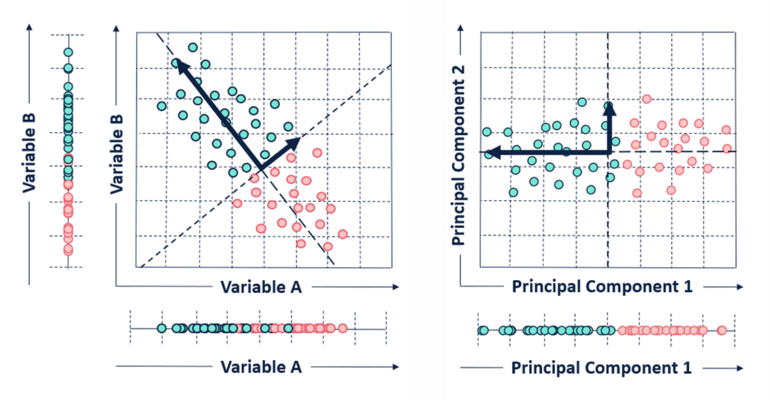

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PCA Example 1: UK Food Consumption

$X \in \mathbb{R}^{4\times 17}$

	England	N Ireland	Scotland	Wales
Alcoholic drinks	375	135	458	475
Beverages	57	47	53	73
Carcase meat	245	267	242	227
Cereals	1472	1494	1462	1582
Cheese	105	66	103	103
Confectionery	54	41	62	64
Fats and oils	193	209	184	235
Fish	147	93	122	160
Fresh fruit	1102	674	957	1137
Fresh potatoes	720	1033	566	874
Fresh Veg	253	143	171	265
Other meat	685	586	750	803
Other Veg	488	355	418	570
Processed potatoes	198	187	220	203
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Soft drinks	1374	1506	1572	1256
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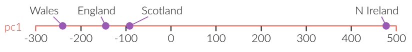

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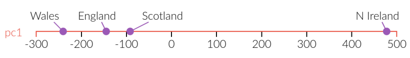
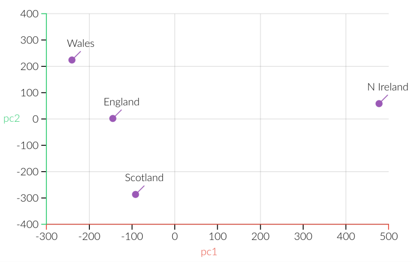


Projecting to 2 components (V_2)



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PCA Example 2: Eigenfaces

Data $X \in \mathbb{R}^{300\times4096}$

Image $\boldsymbol{x} \in \mathbb{R}^{64\times64}$ is flattened to $\mathbb{R}^{4096}$

...

PCA Example 2: Eigenfaces

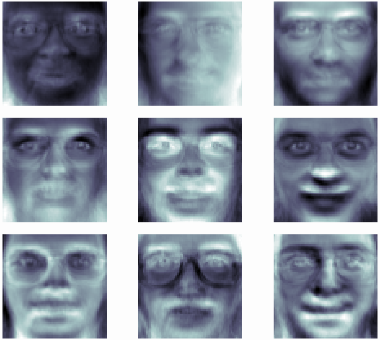
Data $X \in \mathbb{R}^{300\times 4096}$

Image $\boldsymbol{x} \in \mathbb{R}^{64\times 64}$ is flattened to $\mathbb{R}^{4096}$

...

Mean face: 

Principal Component Faces:



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PCA Example 2: Eigenfaces

Projection

Projecting face $\boldsymbol{x}_i$ onto $\boldsymbol{e}_i = [e_{i1}, \ldots, e_{iM}]$

 $=$  $+ \, e_1$  $+ \, e_2$  $+ \, e_3$  $+ \cdots$

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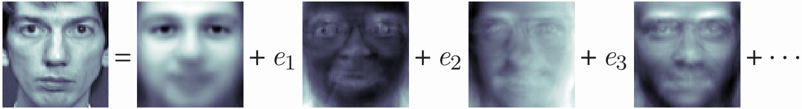


Reconstruction

Reconstructing face $\hat{\boldsymbol{x}}_i$ using M components

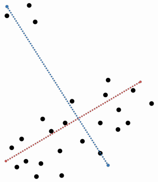
$M = 10$ $M = 30$ $M = 50$ $M = 70$ $M = 90$

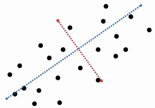
$(90 \ll 4096!)$

PCA: Limitations

Sensitivity

- outliers or scaling dimensions
  - changes variance along dimension
  - changes principal components





Removing outliers

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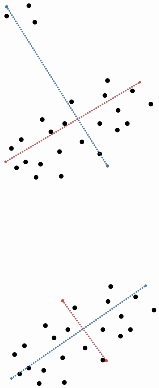
$$x' = \frac{x-\mu}{\sigma}$$



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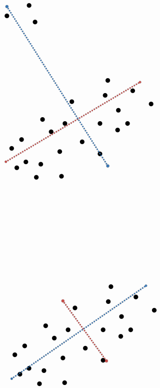

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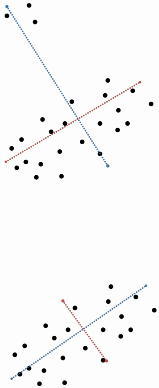

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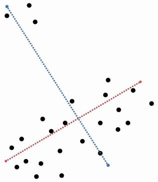

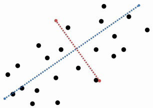

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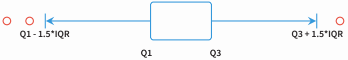
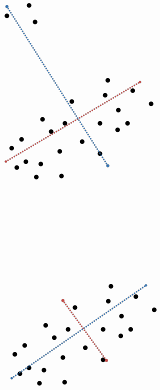


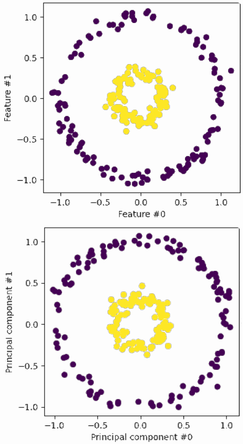


Removing outliers

PCA: Limitations

Linearity

- 1D: line; 2D: plane
- transform to handle non-linearity



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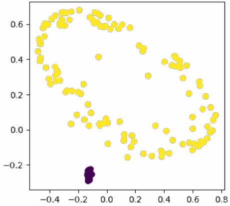
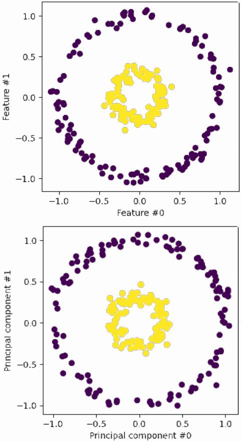


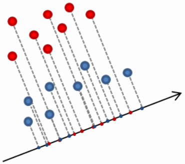


PCA: Limitations

Unsupervised

- maximises data variance along few directions
- ignorant of class labels
- could be hard to separate classes

Data



Projection on PC1

EDA: Summary

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  - for smaller number of components M, pack information

EDA: Summary

- Broad range of visualisation types
- Need to think about what information goes into a visualisation
- Actual data dimensionality $\ll$ observed dimensionality
- For high-dimensional data
  - domain knowledge / feature engineering
  - modelling assumption: independence / smoothness / symmetry etc.
  - dimensionality reduction: selection / transformation
- Principal Components Analysis (PCA)
  - choose directions that maximise variation (eigenvectors)
  - for smaller number of components M, pack information
  - examples: UK food consumption, Eigenfaces