Inf2b - Learning

Lecture 3: Clustering and data visualisation

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http://www.inf.ed.ac.uk/teaching/courses/inf2b/
https://piazza.com/ed.ac.uk/spring2020/infr08028
Office hours: Wednesdays at 14:00-15:00 in IF-3.04

Jan-Mar 2020

Today's Schedule

1. What is clustering
2. K-means clustering
3. Hierarchical clustering
4. Example – unmanned ground vehicle navigation
5. Dimensionality reduction with PCA and data visualisation
6. Summary

Clustering

- Clustering: partition a data set into meaningful or useful groups, based on distances between data points
- Clustering is an unsupervised process — the data items do not have class labels
- Why cluster?

  Interpreting data Analyse and describe a situation by automatically dividing a data set into groupings

  Compressing data Represent data vectors by their cluster index — vector quantisation

Clustering

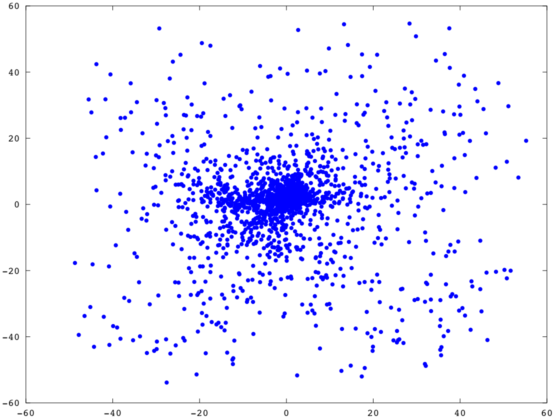
"Human brains are good at finding regularities in data. One way of expressing regularity is to put a set of objects into groups that are similar to each other. For example, biologists have found that most objects in the natural world fall into one of two categories: things that are brown and run away, and things that are green and don't run away. The first group they call animals, and the second, plants."

Recommended reading: David MacKay textbook, p284–

http://www.inference.phy.cam.ac.uk/mackay/itila/

Visualisation of film review users

MovieLens data set
(http://grouplens.org/datasets/movielens/)
$C \approx 1000$ users, $M \approx 1700$ movies

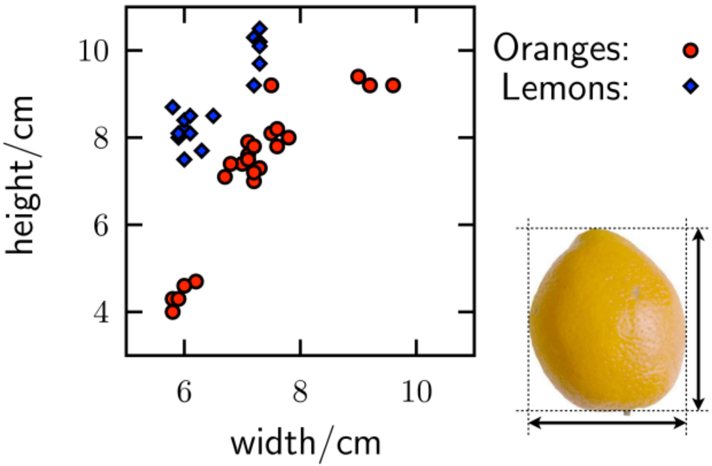


2D plot of users based on rating similarity

Application of clustering

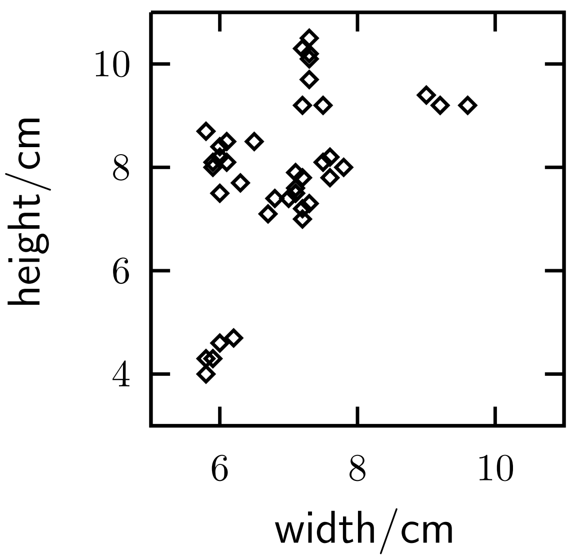
- Face clustering
  doi: 10.1109/CVPR.2013.450
  LHI-Animal-Face dataset
- Image segmentation
  http://dx.doi.org/10.1093/bioinformatics/btr246
- Document clustering
  Thesaurus generation
- Temporal Clustering of Human Behaviour
  http://www.f-zhou.com/tc.html

A two-dimensional space

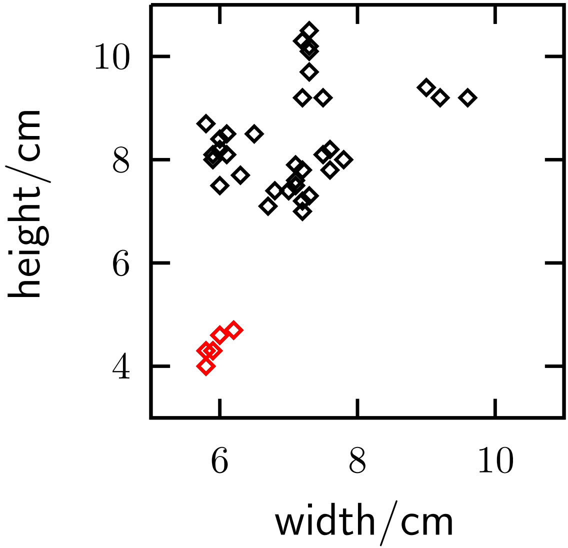


http://homepages.inf.ed.ac.uk/imurray2/teaching/oranges_and_lemons/

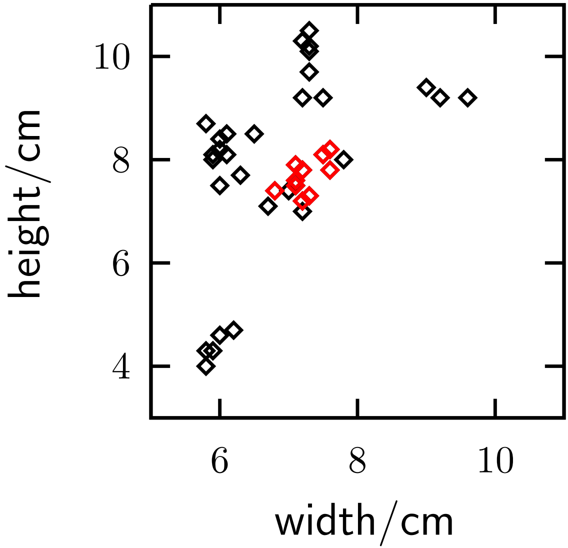
The Unsupervised data



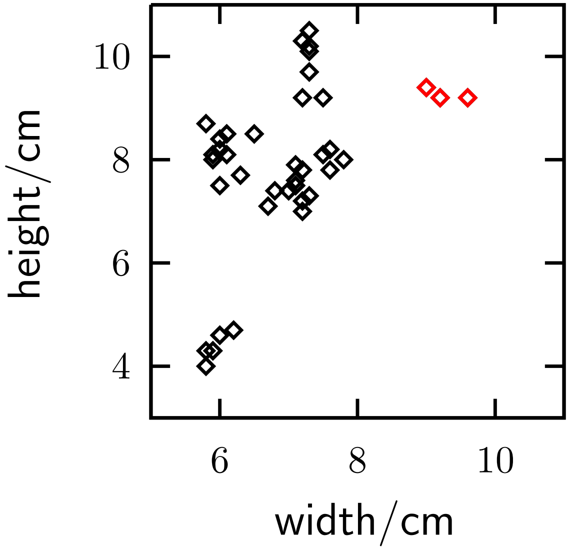
Manderins



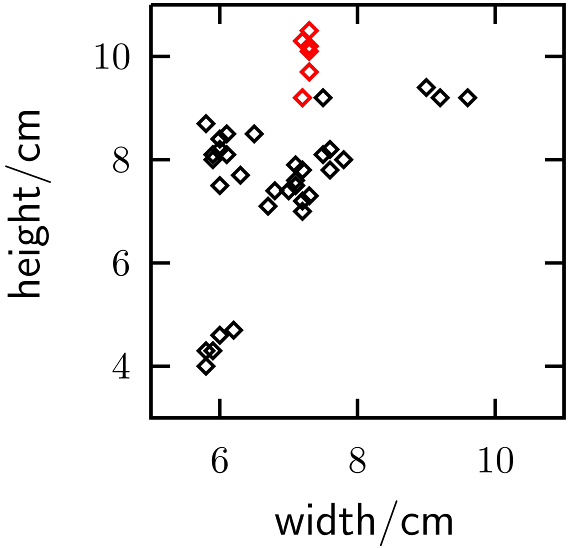
Navel oranges



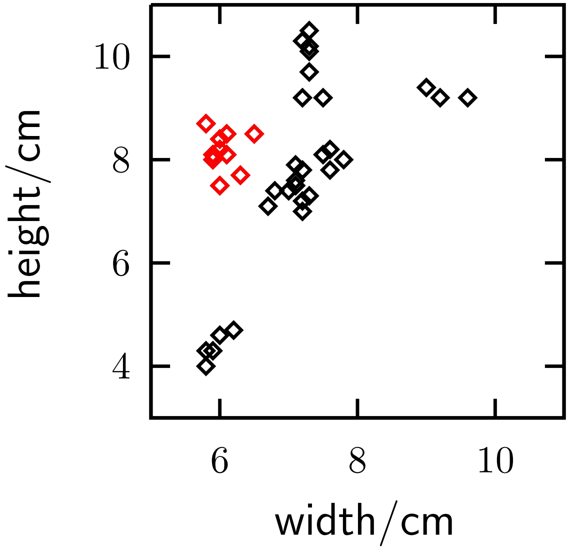
Spanish jumbo oranges



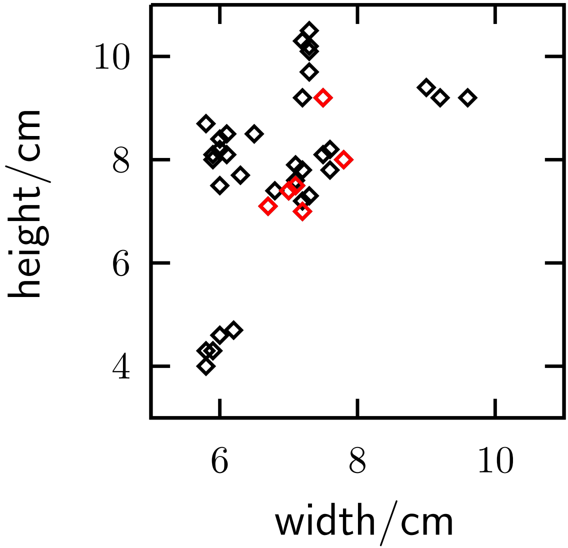
Belsan lemons



Some other lemons



"Selected seconds" oranges



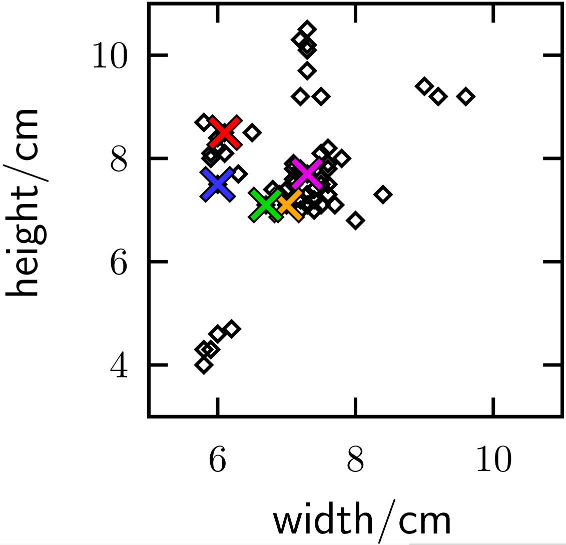
K-means clustering

A simple algorithm to find clusters:

1. Pick K random points as cluster centre positions
2. Assign each point to its nearest centre*
3. Move each centre to mean of its assigned points
4. If centres moved, `goto` 2.

* In the unlikely event of a tie, break tie in some way. For example, assign to the centre with smallest index in memory.

K-means clustering



Evaluation of clustering

- One way to measure the quality of a k-means clustering solution is by a *sum-squared error function*, i.e. the sum of squared distances of each point from its cluster centre.
- Let $z_{kn} = 1$ if the point $\mathbf{x}_n$ belongs to cluster k and $z_{kn} = 0$ otherwise. Then:

$$E = \sum_{k=1}^{K} \sum_{n=1}^{N} z_{kn} \| \mathbf{x}_n - \mathbf{m}_k \|^2$$

$\mathbf{x}_n = (x_{n1}, \ldots, x_{nD})^T$
$\mathbf{m}_k = (m_{k1}, \ldots, m_{kD})^T$
$\|\cdot\|$: Euclidean (L^2) norm

  where $\mathbf{m}_k$ is the centre of cluster k.
- Sum-squared error is related to the variance — thus performing k-means clustering to minimise E is sometimes called minimum variance clustering.
- This is a within-cluster error function — it does not include a between clusters term

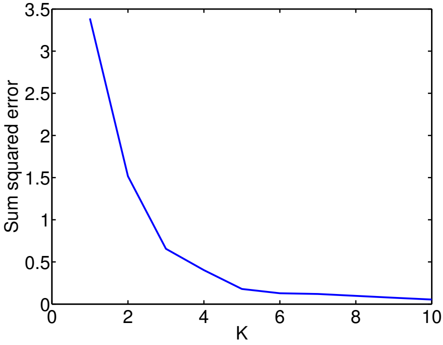
Theory of K-means clustering

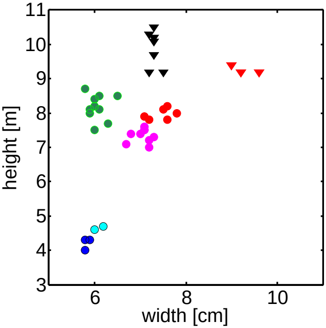
- If assignments don't change, algorithm terminates.
- **Can assignments cycle, never terminating?**
- **Convergence proof technique:** find a *Lyapunov function* $\mathcal{L}$, that is bounded below and cannot increase.
  $\mathcal{L}$ = sum of square distances between points and centres

  NB: $E^{(t+1)} \leq E^{(t)}$
- K**-means is an optimisation algorithm** for $\mathcal{L}$.
  Local optima are found, i.e. there is no guarantee of finding global optimum. Running multiple times and using the solution with best $\mathcal{L}$ is common.

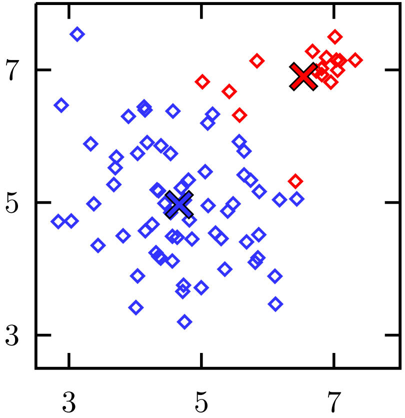
How to decide K?

- The sum-squared error decreases as K increases ($E \rightarrow 0$ as $K \rightarrow N$)
- We need another measure?!



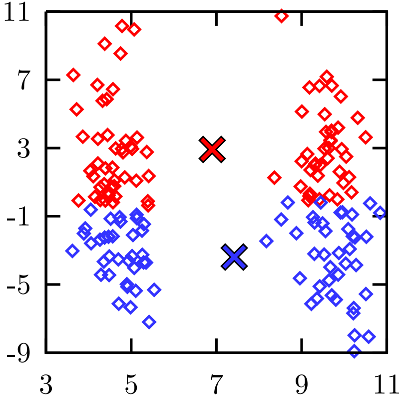


Failures of K-means (e.g. 1)



Large clouds pull small clusters off-centre

Failures of K-means (e.g. 2)



Distance needs to be measured sensibly.

Clustering clustering methods *(NE)*

- K-means clustering is not the only method for clustering data
- See: http://en.wikipedia.org/wiki/Cluster_analysis

Hierarchical clustering *(NE)*

Form a 'dendrogram' / binary tree with data at leaves

Bottom-up / Agglomerative:

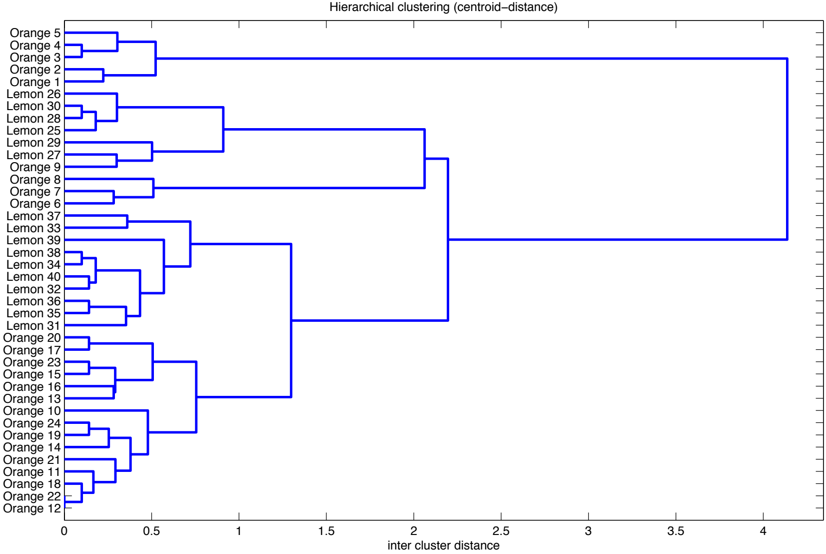
- Repeatedly merge closest groups of points
- Often works well. Expensive: $O(N^3)$

Top-down / Divisive:

- Recursively split groups into two (e.g. with k-means)
- Early choices might be bad.
- Much cheaper! $\sim O(N^2)$ or $O(N^2 \log N)$

More detail:
Pattern Classification (2nd ed.), Duda, Hart, Stork. §10.9

Bottom-up clustering of the lemon/orange data

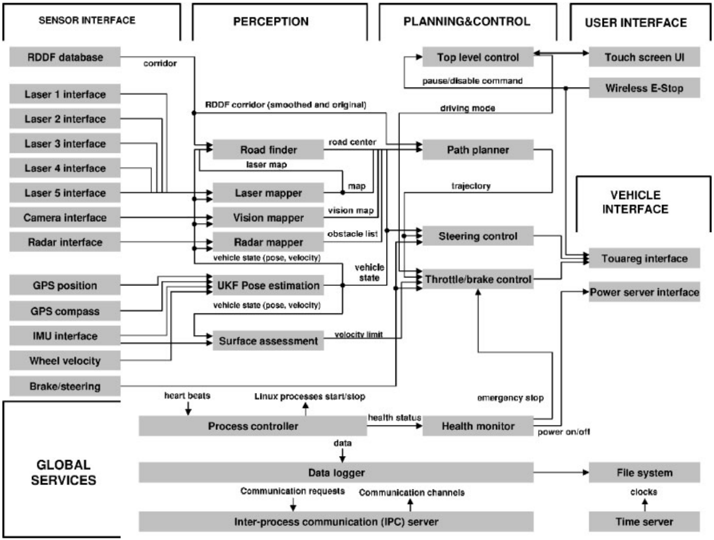


Stanley

Stanford Racing Team; DARPA 2005 challenge

http://robots.stanford.edu/talks/stanley/

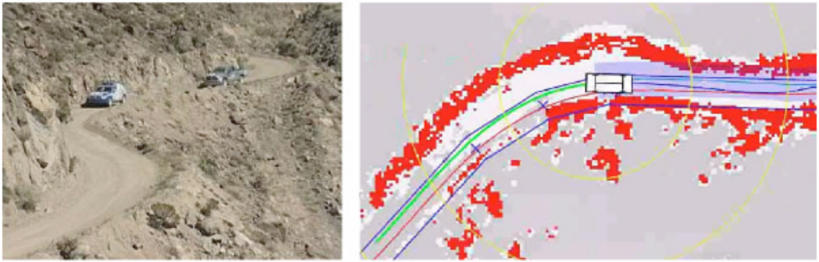
Inside Stanley



Stanley figures from Thrun et al., J. Field Robotics 23(9):661, 2006.

Perception and intelligence

(a) Beer Bottle Pass (b) Map and GPS corridor

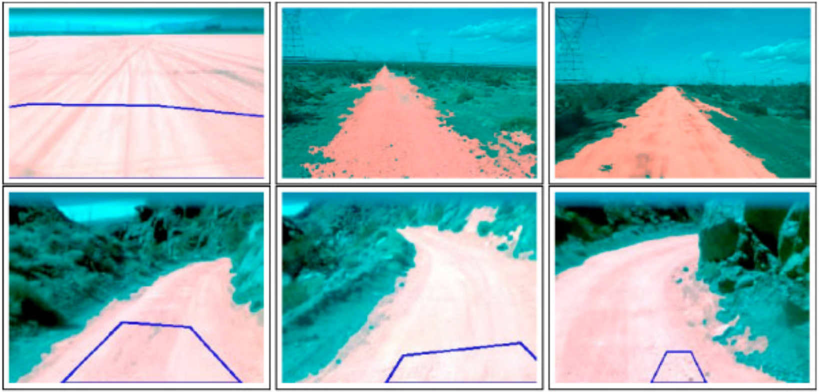


It would look pretty stupid to run off the road,
just because the trip planner said so.

How to stay on the road?

Classifying road seems hard. Colours and textures change: road appearance in one place may match ditches elsewhere.

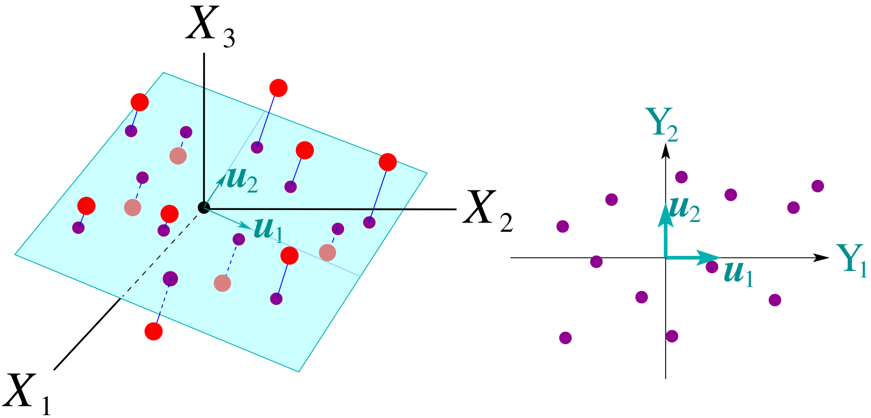
Clustering to stay on the road



Stanley used a Gaussian mixture model. “Souped up *k*-means.”
The cluster just in front is road (unless we already failed).

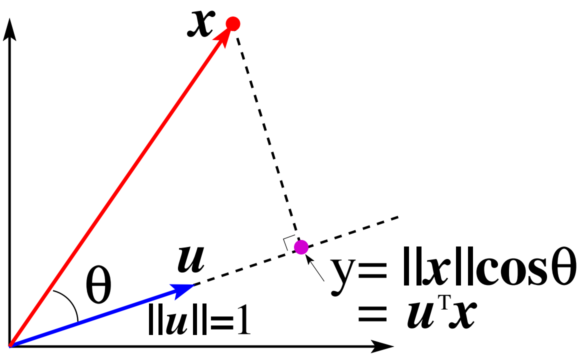
Dimensionality reduction and data visualisation

- High-dimensional data are difficult to understand and visualise.
- Consider dimensionality reduction of data for visualisation

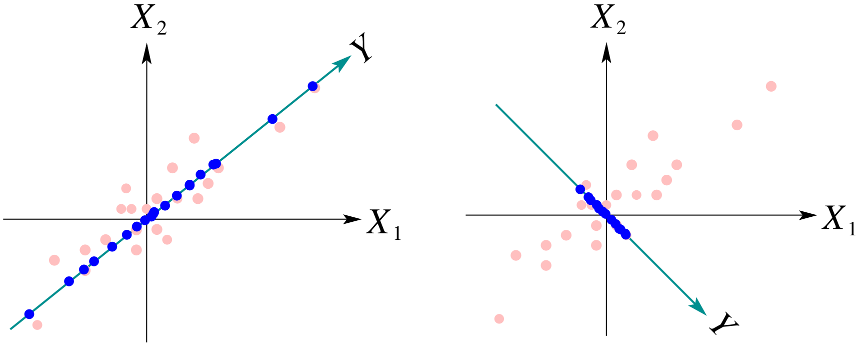


Project each sample in 3D onto a 2D plane

Orthogonal projection of data onto an axis



Optimal projection of 2D data onto 1D



- Mapping 2D to 1D: $y_n = \mathbf{u}^T \mathbf{x}_n = u_1 x_{n1} + u_2 x_{n2}$
- Optimal mapping: $\max\limits_{\mathbf{u}} \mathrm{Var}\,(y)$

$$\mathrm{Var}\,(y) = \frac{1}{N-1} \sum_{n=1}^{N} (y_n - \bar{y})^2$$

- cf. least squares fitting (linear regression)

Principal Component Analysis (PCA)

- Mapping D-dimensional data to a *principal component axis* $\mathbf{u} = (u_1, \ldots, u_D)^T$ that maximises $\mathrm{Var}(y)$:

  $$y_n = \mathbf{u}^T \mathbf{x}_n = u_1 x_{n1} + \cdots + u_D x_{nD} \qquad \text{NB: } \|\mathbf{u}\| = 1$$

- $\mathbf{u}$ is given as the eigenvector with the largest eigenvalue of the covariance matrix, S:

  $$S = \frac{1}{N-1} \sum_{n=1}^{N} (\mathbf{x}_n - \bar{\mathbf{x}})(\mathbf{x}_n - \bar{\mathbf{x}})^T, \quad \bar{\mathbf{x}} = \frac{1}{N} \sum_{n=1}^{N} \mathbf{x}_n$$

- Eigen values λ_i and eigenvectors $\mathbf{p}_i$ of S:

  $$S\,\mathbf{p}_i = \lambda_i\,\mathbf{p}_i, \quad i = 1, \ldots, D$$

  If $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_D$, then $\mathbf{u} = \mathbf{p}_1$, and $\mathrm{Var}(y) = \lambda_1$

NB: $\mathbf{p}_i^T \mathbf{p}_j = 0$, i.e. $\mathbf{p}_i \perp \mathbf{p}_j$ for $i \neq j$

$\mathbf{p}_i$ is normally normalised so that $\|\mathbf{p}_i\| = 1$.

Covariance matrix

$$S = \begin{pmatrix} s_{11} & \cdots & s_{1D} \\ \vdots & \ddots & \vdots \\ s_{D1} & \cdots & s_{DD} \end{pmatrix} \quad \cdots \ D\text{-by-}D \text{ symmetric matrix}$$

- In scalar representation:

$$s_{ij} = \frac{1}{N-1}\sum_{n=1}^{N}(x_{ni} - \bar{x}_i)(x_{nj} - \bar{x}_j), \qquad \bar{x}_i = \frac{1}{N}\sum_{n=1}^{N} x_{ni}$$

- Relation with Pearson's correlation coefficient:

$$\begin{aligned} r_{ij} &= \frac{1}{N-1}\sum_{n=1}^{N}\left(\frac{x_{ni} - \bar{x}_i}{s_i}\right)\left(\frac{x_{nj} - \bar{x}_j}{s_j}\right) \\ &= \frac{1}{s_i s_j}\frac{1}{N-1}\sum_{n=1}^{N}(x_{ni} - \bar{x}_i)(x_{nj} - \bar{x}_j) \\ &= \frac{s_{ij}}{\sqrt{s_{ii}s_{jj}}} \qquad \text{cf: } s_i = \sqrt{s_{ii}} = \sqrt{\frac{1}{N-1}\sum_{n=1}^{N}(x_{ni} - \bar{x}_i)^2} \end{aligned}$$

Principal Component Analysis (PCA) *(cont.)*

- Let $\mathbf{v} = \mathbf{p}_2$, i.e. the eigenvector for the second largest eiven values, λ_2
- Map $\mathbf{x}_n$ on to the axis by $\mathbf{v}$:
$$z_n = \mathbf{v}^T \mathbf{x}_n = v_1 x_{n1} + \cdots + v_D x_{nD}$$
- Point $(y_n, z_n)^T$ in $\mathcal{R}^2$ is the projection of $\mathbf{x}_n \in \mathcal{R}^D$ on the 2D plane spanned by $\mathbf{u}$ and $\mathbf{v}$.
$$\mathrm{Var}\,(y) = \lambda_1, \quad \mathrm{Var}\,(z) = \lambda_2$$
- Can be generalised to a mapping from $\mathcal{R}^D$ to $\mathcal{R}^\ell$ using $\{\mathbf{p}_1, \ldots, \mathbf{p}_\ell\}$, where $\ell < D$.
- NB: Dimensionality reduction may involve loss of information. Some informaation will be lost if
$$\frac{\sum_{i=1}^{\ell} \lambda_i}{\sum_{i=1}^{D} \lambda_i} < 1$$

PCA on the film review toy data

	Australia	*Body of Lies*	*Burn After*	*Hancock*	*Milk*	*Rev Road*
Denby	3	7	4	9	9	7
McCarthy	7	5	5	3	8	8
M'stern	7	5	5	0	8	4
Puig	5	6	8	5	9	8
Travers	5	8	8	8	10	9
Turan	7	7	8	4	7	8

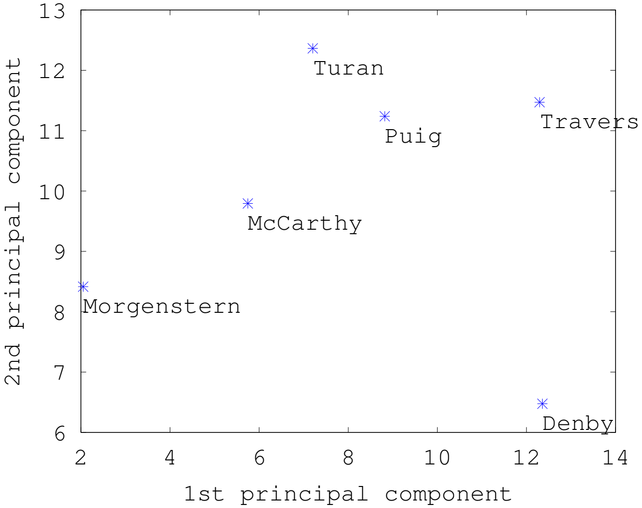
$$S = \begin{pmatrix} 2.66 & -1.07 & 0.53 & -4.67 & -1.20 & -0.67 \\ -1.07 & 1.47 & 1.07 & 3.27 & 0.60 & 1.27 \\ 0.53 & 1.07 & 3.47 & 0.67 & 0.20 & 1.87 \\ -4.67 & 3.27 & 0.67 & 10.97 & 2.30 & 3.67 \\ -1.20 & 0.60 & 0.20 & 2.30 & 1.10 & 0.60 \\ -0.67 & 1.27 & 1.87 & 3.67 & 0.60 & 3.07 \end{pmatrix}$$

$$P = \begin{pmatrix} -0.341 & 0.345 & 0.326 & -0.180 & 0.603 & -0.512 \\ 0.255 & 0.151 & -0.240 & -0.548 & 0.496 & 0.554 \\ 0.101 & 0.786 & -0.503 & 0.028 & -0.280 & -0.198 \\ 0.827 & -0.154 & 0.096 & -0.182 & 0.025 & -0.450 \\ 0.181 & -0.065 & -0.341 & 0.733 & 0.556 & 0.015 \\ 0.304 & 0.461 & 0.676 & 0.309 & -0.047 & 0.375 \end{pmatrix}$$

$$Q = \begin{pmatrix} 15.8 & 0 & 0 & 0 & 0 & 0 \\ 0 & 4.85 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1.13 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0.634 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0.288 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

where $P = (\mathbf{p}_1, \ldots, \mathbf{p}_6)$ and $(Q)_{ii} = \lambda_i$ for $i = 1, \ldots, 6$

PCA on the film review toy data (*cont.*)



Dimensionality reduction $D \rightarrow \ell$ by PCA

$$\begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_\ell \end{pmatrix} = \begin{pmatrix} \mathbf{p}_1^T \mathbf{x} \\ \mathbf{p}_2^T \mathbf{x} \\ \vdots \\ \mathbf{p}_\ell^T \mathbf{x} \end{pmatrix} = \begin{pmatrix} \mathbf{p}_1^T \\ \mathbf{p}_2^T \\ \vdots \\ \mathbf{p}_\ell^T \end{pmatrix} \mathbf{x}$$

where $\{\mathbf{p}_i\}_{i=1}^{\ell}$ are the eigenvectors for the ℓ largest eigenvalues of S. The above can be rewritten as

$\mathbf{y} = A^T \mathbf{x}$ $\cdots$ linear transformation from R^D to R^ℓ

$$\begin{aligned} \mathbf{y} &= (y_1, \ldots, y_\ell)^T : \quad \ell\text{-dimensional vector} \\ A &= (\mathbf{p}_1, \ldots, \mathbf{p}_\ell) : \quad D \times \ell \text{ matrix} \end{aligned}$$

In many applications, we normalise data before PCA, e.g. $\mathbf{y} = A^T(\mathbf{x} - \bar{\mathbf{x}})$.

Summary

- **Clustering**
  K-means for minimising 'cluster variance'
  Review notes, *not just slides*
  [other methods exist: hierarchical, top-down and bottom-up]
- **Unsupervised learning**
  Spot structure in unlabelled data
  Combine with knowledge of task
- **Principal Component Analysis (PCA)**
  Find principal component axes for dimensionality reduction and visualisation
- Try implementing the algorithms! (Lab 3 in Week 4)

Further reading *(NE)*

- Rui Xu, D. Wunsch, "Survey of clustering algorithsm," in IEEE Transactions on Neural Networks, vol. 16, no. 3, pp. 645-678, May 2005.
  https://doi.org/10.1109/TNN.2005.845141
- Dongkuan Xu, Yingjie Tian, "A Comprehensive Survey of Clustering Algorithms," Annals of Data Science, 2015, Volume 2, Number 2, Page 165.
  https://doi.org/10.1007/s40745-015-0040-1
- C. Bishop, "Pattern Recognition and Machine Learning," Chapter 12.1 (PCA).
  https://www.microsoft.com/en-us/research/people/cmbishop/prml-book/
- C.O.S. Sorzano, J. Vargas, A. Pascual Montano, "A survey of dimensionality reduction techniques," 2014.
  https://arxiv.org/abs/1403.2877

Quizes

Q1: Find computational complexity of k-means algorithm

Q2: For k-means clustering, discuss possible methods for mitigating the local minimum problem.

Q3: Discuss possible problems with k-means clustering and solutions when the variances of data (i.e. s_i, $i=1,\ldots,D$) are much different from each other.

Q4: For k-means clustering, show $E^{(t+1)} \leq E^{(t)}$. *(NE)*

Q5: At page 37, show $\mathbf{y} = \mathbf{u}^T\mathbf{x}$.

Q6: At page 39, show $\mathrm{Var}\,(y) = \lambda_1$, where λ_1 is the largest eigenvalue of S. *(NE)*

Q7: The first principal component axis is sometimes confused with the line of least squares fitting (or regression line). Explain the difference.