COMP6237 Data Mining

Discovering Groups

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Introduction

- Modelling text documents as vectors 101
- Clustering
  - Hierarchical
  - K-Means
  - Mean-shift
- Visualisation in 2D
  - Principal Component Analysis
  - Self Organising Maps
  - Multidimensional Scaling

Problem statement

- Understanding large datasets is **hard**
  - especially if the data is represented by high dimensional features

- In order to explore a dataset we might:
  - want to be able to understand which *data items* are *similar* to each other
  - want to be able to understand which *features* are *similar* to each other

Aside: Representing text documents as vectors

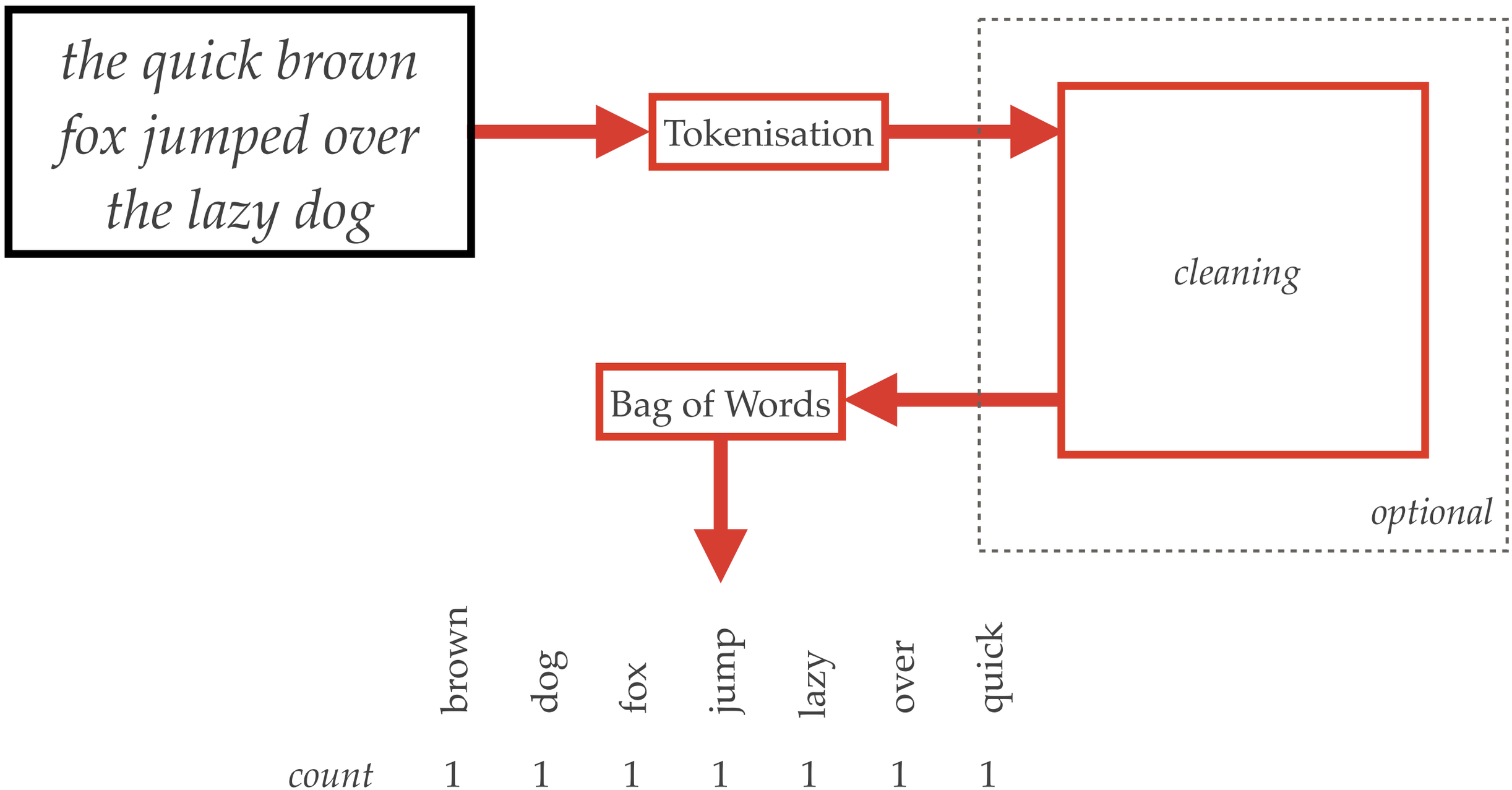
Bag of Words

A document

the quick brown fox jumped over the lazy dog

The bag of words describing the document

Text processing (feature extraction)

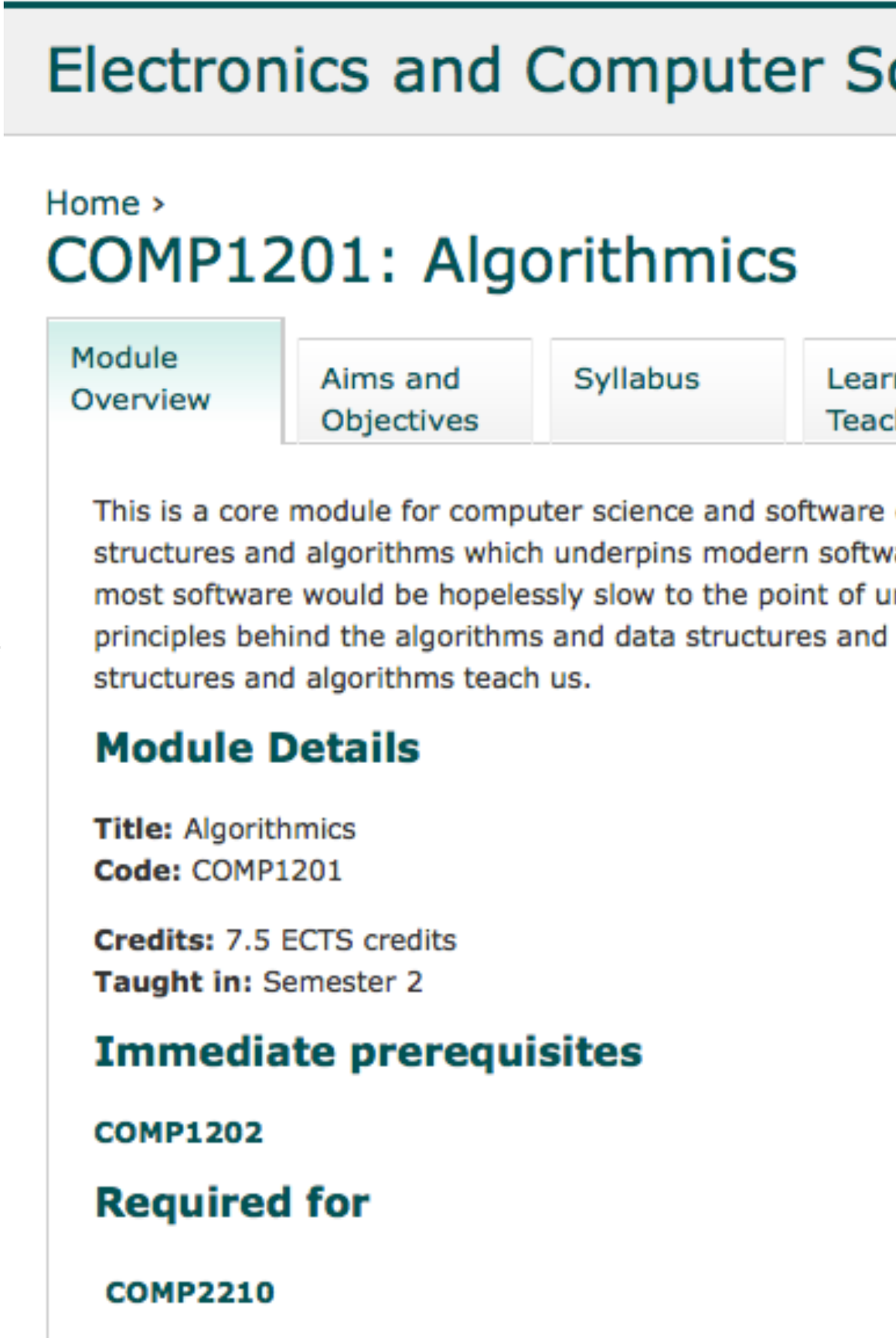


Sparsity

- The bag of words histogram representing an individual document is very sparse
    - i.e. not all words appear in all documents!
- This is subtly different to the sparse vectors we encountered when we were talking about recommender systems
    - there, vectors were sparse because we had unknown values; this time they are sparse because the value is zero
    - The tricks we applied to distance functions don’t apply here - we need to account for the zeros
    - **But** we can still modify our implementations of distance functions to be more efficient given sparse vectors

A sample data set

- The syllabus description pages from all ECS COMPXXXX modules
- Relevant sections from the overview, aims and syllabus parts
- Tokenised by splitting on
  [^A-Z^a-z]+
- Terms with a **document frequency** of <10% and >70% removed
- Words with 2 or less characters removed



Clustering

Clustering

- Clustering aims to group data without any prior knowledge of what the groups should look like or contain.

- In terms of featurevectors, items with similar vectors should be grouped together by a clustering operation.

- Some clustering operations create overlapping groups; others assign an item to a single group.

Hierarchical clustering

- Important set of techniques for understanding the structure of data
    - Creates a binary tree that recursively groups pairs of similar items or clusters
- Two approaches:
    - Agglomerative clustering (bottom up)
    - Divisive clustering (top-down)

Hierarchical Agglomerative Clustering

- Simple algorithm:
  - `Initially every item is in a cluster of its own`
  - `While there is more than one single cluster:`
    - `The closest pair of clusters according to a` **`linkage criterion`** `are merged into a bigger cluster`
- By recording the merges at each step a binary tree structure linking the clusters can be formed
  - Often a useful way of utilising this is by drawing a diagram known as a **dendrogram** that shows the structure of the tree

Linkage criterion

- A measure of dissimilarity between clusters
  - **Centroid-based**
    - Dissimilarity between clusters is equal to the distance between their centroids (for an arbitrary distance measure)
    - Requires items being clustered are represented by numeric feature vectors
  - **Distance-based**
    - Dissimilarity between clusters is a function of the distances between the items in those clusters (for an arbitrary distance measure)
    - Don’t need a feature vector for each item; only need a precomputed measure of similarity between items

Centroid-based linkage

- **Weighted Centroid Clustering** (**WPGMC** - *Weighted Pair Group Method with Centroids*)
  - When two clusters *s* and *t* are combined into a new cluster *u*, the average of centroids *s* and *t* give the new centroid *u*
- **Unweighted Centroid Clustering** (**UPGMC** - *Unweighted Pair Group Method with Centroids*)
  - When two clusters *s* and *t* are combined into a new cluster *u*, the average of the positions of all the items within *s* and *t* give the new centroid *u*

Distance-based linkage

- Common linkage criteria between two sets of items *A* and *B*:
  - **Minimum** or **single-linkage clustering**: min{ *d*(*a*,*b*) : $a \in A$, $b \in B$ }
    - tends to produce long, thin, clusters
  - **Maximum** or **complete-linkage clustering**: max{ *d*(*a*,*b*) : $a \in A$, $b \in B$ }
    - Avoids problems of single-linkage clustering; tends to find compact clusters of approximately equal diameter
- **Mean** or **average linkage clustering** (**UPGMA** - *Unweighted Pairwise Group Method with Arithmetic Mean*):

$$\frac{1}{|A||B|}\sum_{a\in A}\sum_{b\in B} d(a,b)$$

Demo showing 2d hierarchical agglomerative clustering

Demo showing hierarchical agglomerative clustering on real data

Aside: Hierarchical Divisive Clustering

- Divisive clustering algorithms do exist
  - e.g. DIANA (DIvisive ANAlysis)
- Not widely used in practice
- Computationally much harder problem to compute divisive clustering compared to agglomerative

K-Means Clustering

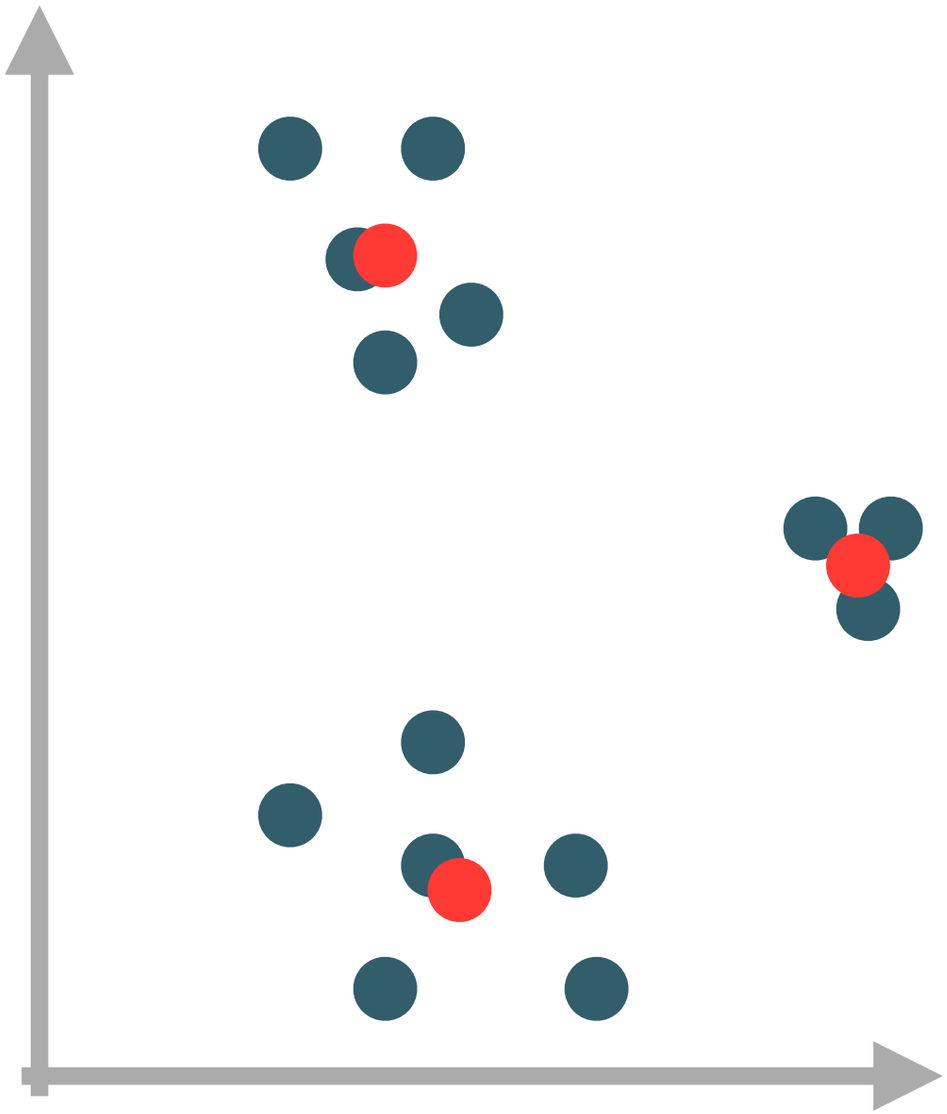
- K-Means is a classic featurespace clustering algorithm for grouping data into K groups with each group represented by a *centroid*:
  - The value of K is chosen
  - K initial cluster centres are chosen
  - Then the following process is performed iteratively until the centroids don’t move between iterations:
    - Each point is assigned to its closest centroid
    - The centroid is recomputed as the mean of all the points assigned to it. If the centroid has no points assigned it is randomly re-initialised to a new point.
  - The final clusters are created by assigning all points to their nearest centroid.

2D K-Means Demo

Demo showing K-Means of Real Data

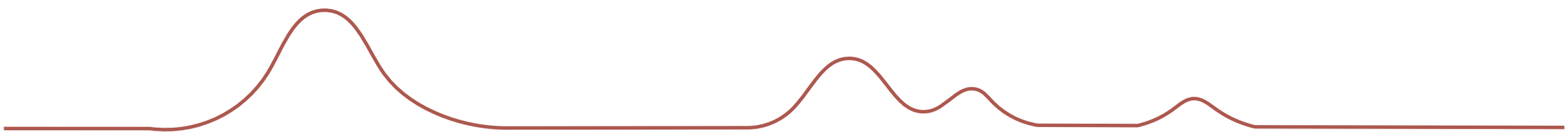
Mean shift clustering

- Mean shift is an algorithm that finds the modes of a probability density function
    - Quite literally this means it finds the points in a feature space with the highest feature density
        - Points in the feature space that are most likely given the dataset
- Doesn't need to know the number of clusters *a priori*
    - But does need a *kernel* and a *kernel bandwidth*



Probability Density Functions

PDF of the features



unbiased sample of 1D features from a dataset

PDF Estimation

- How can we estimate the PDF?
  - Histogram?

  - Crude/coarse/discrete
  - How to choose bin size?

Kernel Density Estimation (aka Parzen Window)

- Really want a technique that will give us a smooth, continuous estimate

  - use a “kernel density estimator” that can compute the value of the PDF at an arbitrary position **x**:

$$f(\mathbf{x}) = \frac{1}{nh^d} \sum_{i=1}^{n} K(\frac{\mathbf{x} - \mathbf{x}_i}{h})$$

featurevector of the *i*-th item

number of items

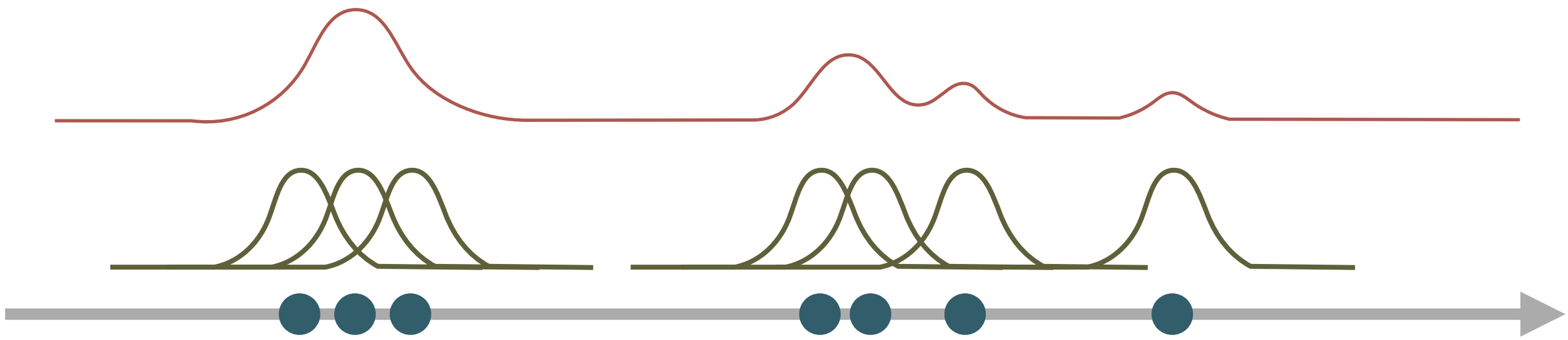
dimensionality of feature space

kernel function

kernel bandwidth

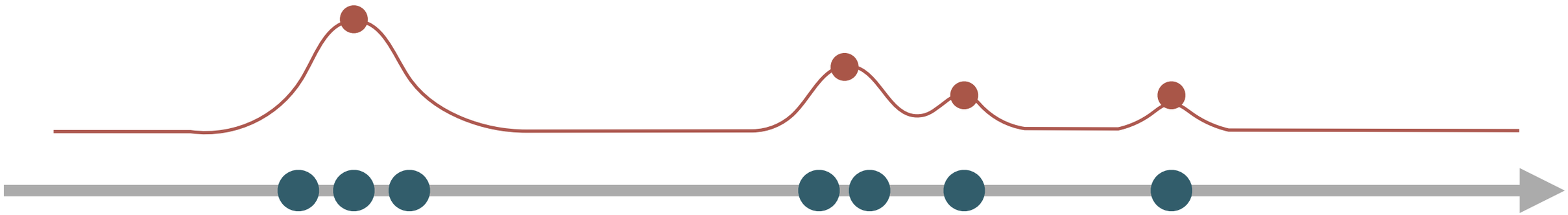
Kernel Density Estimation (aka Parzen Window)

- Commonly we'll use a Gaussian kernel with unit s.d.
  - If the kernel is radially symmetric, then only need to consider the profile of the kernel, $k(\mathbf{x})$ that satisfies $K(\mathbf{x})=c_{k,d}k(||\mathbf{x}||^2)$



The Mean Shift Procedure

- Mean shift finds the modes of the PDF
  - points where gradient is zero: $\nabla f(\mathbf{x})=0$



Assume radially symmetric kernel:

$g(\bullet) = -f'(\bullet)$

$$\nabla f(\mathbf{x}) = \frac{2c_{k,d}}{nh^{d+2}} \sum_{i=1}^{n} (\mathbf{x} - \mathbf{x}_i) g\left(\left\| \frac{\mathbf{x} - \mathbf{x}_i}{h} \right\|^2 \right)$$

$$= \boxed{\frac{2c_{k,d}}{nh^{d+2}} \left[\sum_{i=1}^{n} g\left(\left\| \frac{\mathbf{x} - \mathbf{x}_i}{h} \right\|^2 \right) \right]} \boxed{\left[\frac{\sum_{i=1}^{n} \mathbf{x}_i g\left(\left\| \frac{\mathbf{x} - \mathbf{x}_i}{h} \right\|^2 \right)}{\sum_{i=1}^{n} g\left(\left\| \frac{\mathbf{x} - \mathbf{x}_i}{h} \right\|^2 \right)} - \mathbf{x} \right]}$$

This is proportional to a density estimate with kernel $G(\mathbf{x}) = c_{g,d} g(\|\mathbf{x}\|^2)$

This is the **mean shift** …it's a vector that always points in the direction of maximum density

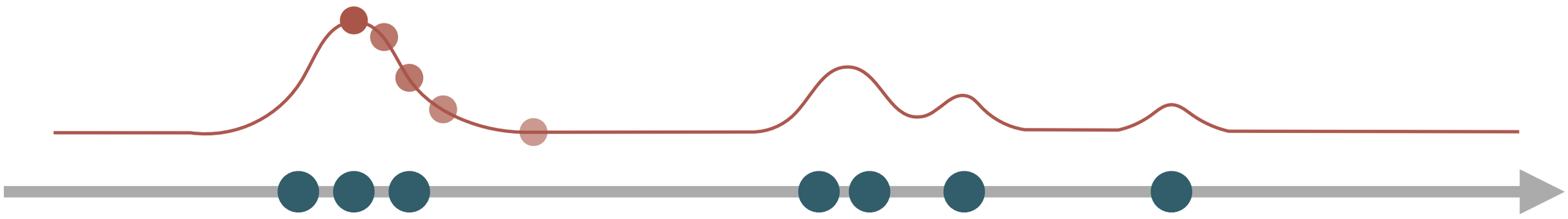
Mean shift procedure:

1. Start at a point $\mathbf{x}_t$

2. Compute the mean shift vector $\mathbf{m}_h(\mathbf{x}_t)$

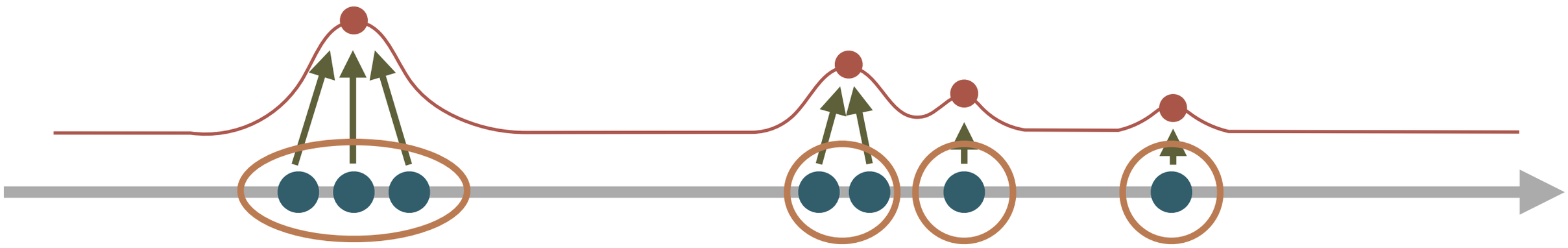
3. Move x towards the mode: $\mathbf{x}_{t+1} = \mathbf{m}_h(\mathbf{x}_t)$

4. Stop if $\mathbf{x}_{t+1} = \mathbf{x}_t$; otherwise goto step 2



Mean Shift Clustering

- Simple extension of the mean shift procedure:
- for each feature vector
  - apply the mean shift procedure until convergence and store the resultant mode
- the set of featurevectors that converge to the same mode define the *basin of attraction* of that mode; all features that converged to the same mode belong to the same cluster



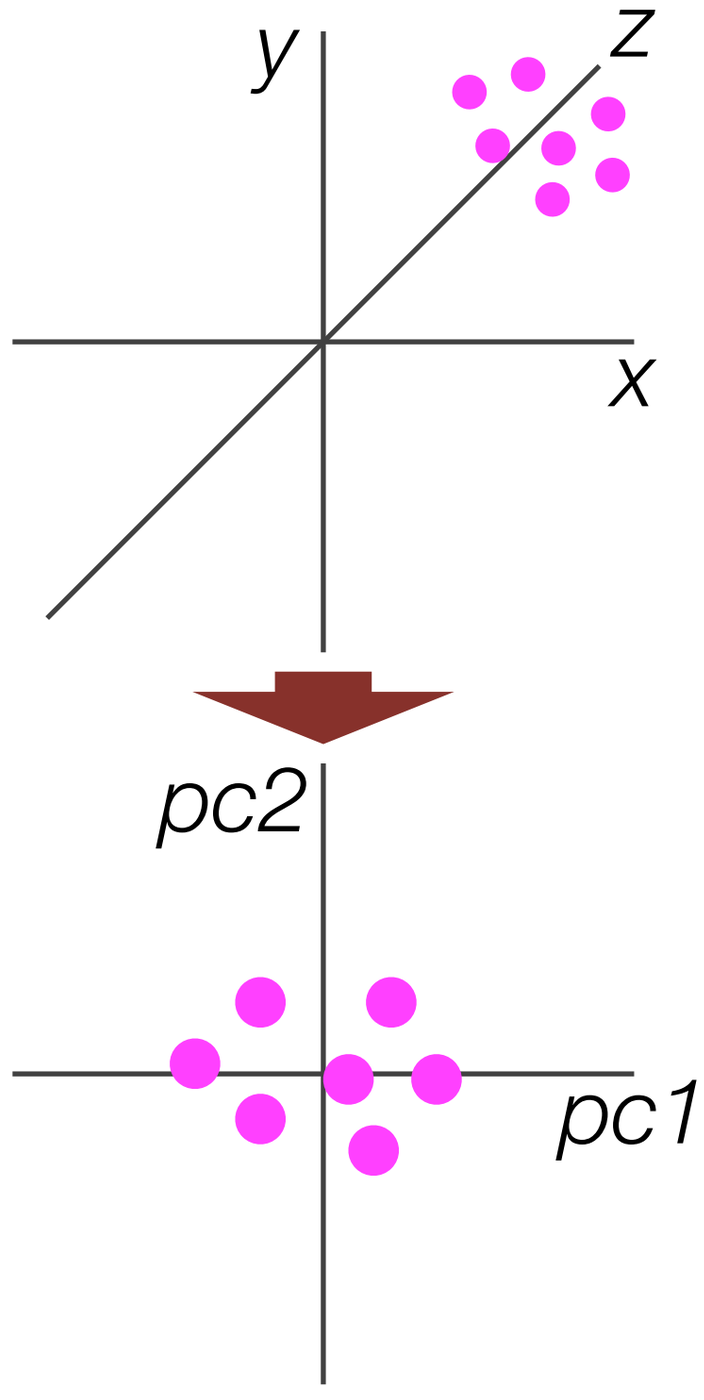
Demo showing Mean-Shift in 2D

Visualising data in two dimensions

- Sometimes we just want to visualise how items of data relate to each other
    - i.e. want to plot them on a 2D surface in such a way that things that are similar are close together (specifically have a small Euclidean distance)

PCA

- We've already looked at how PCA works
  - Can use PCA to project features to a 2D space based on the first and second principle axes



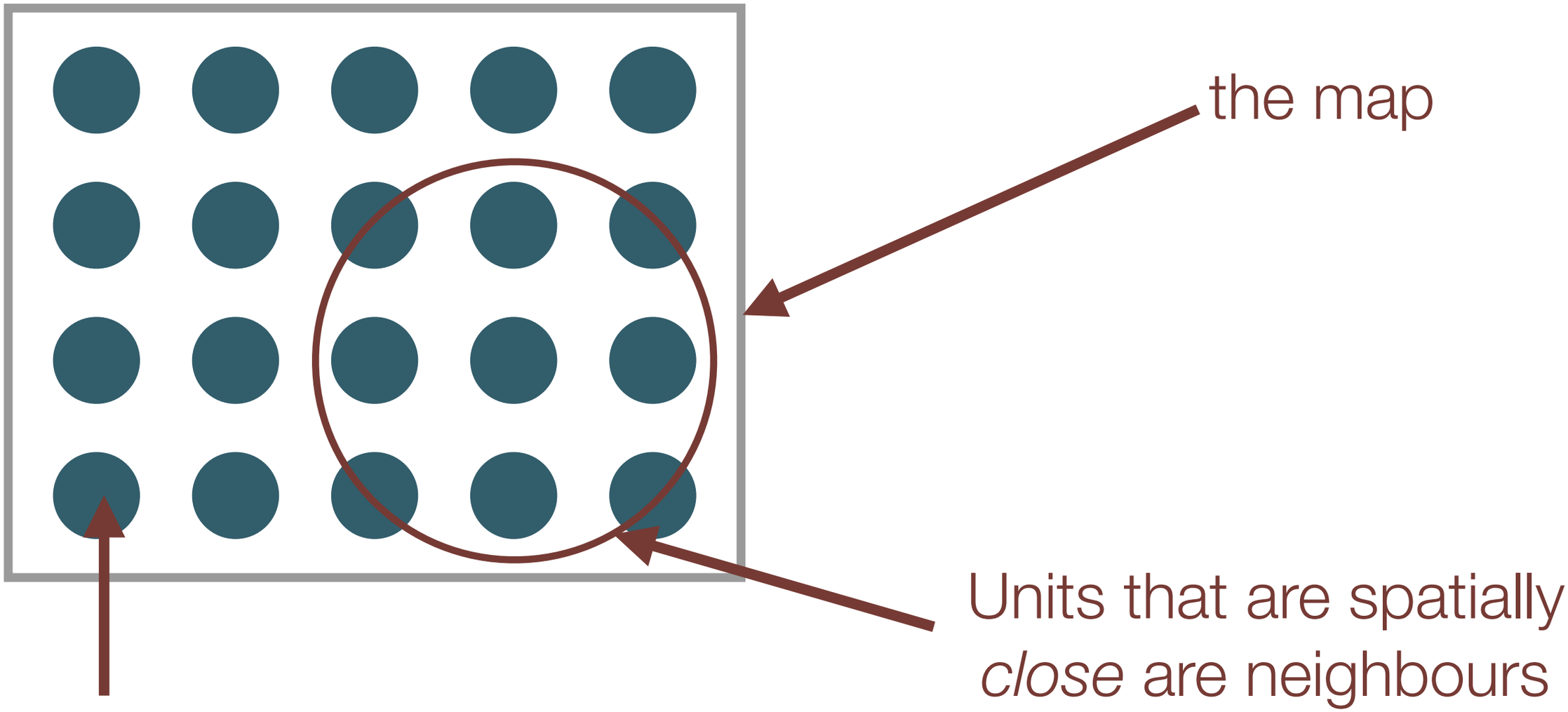
Demo showing PCA on real data

PCA Problems

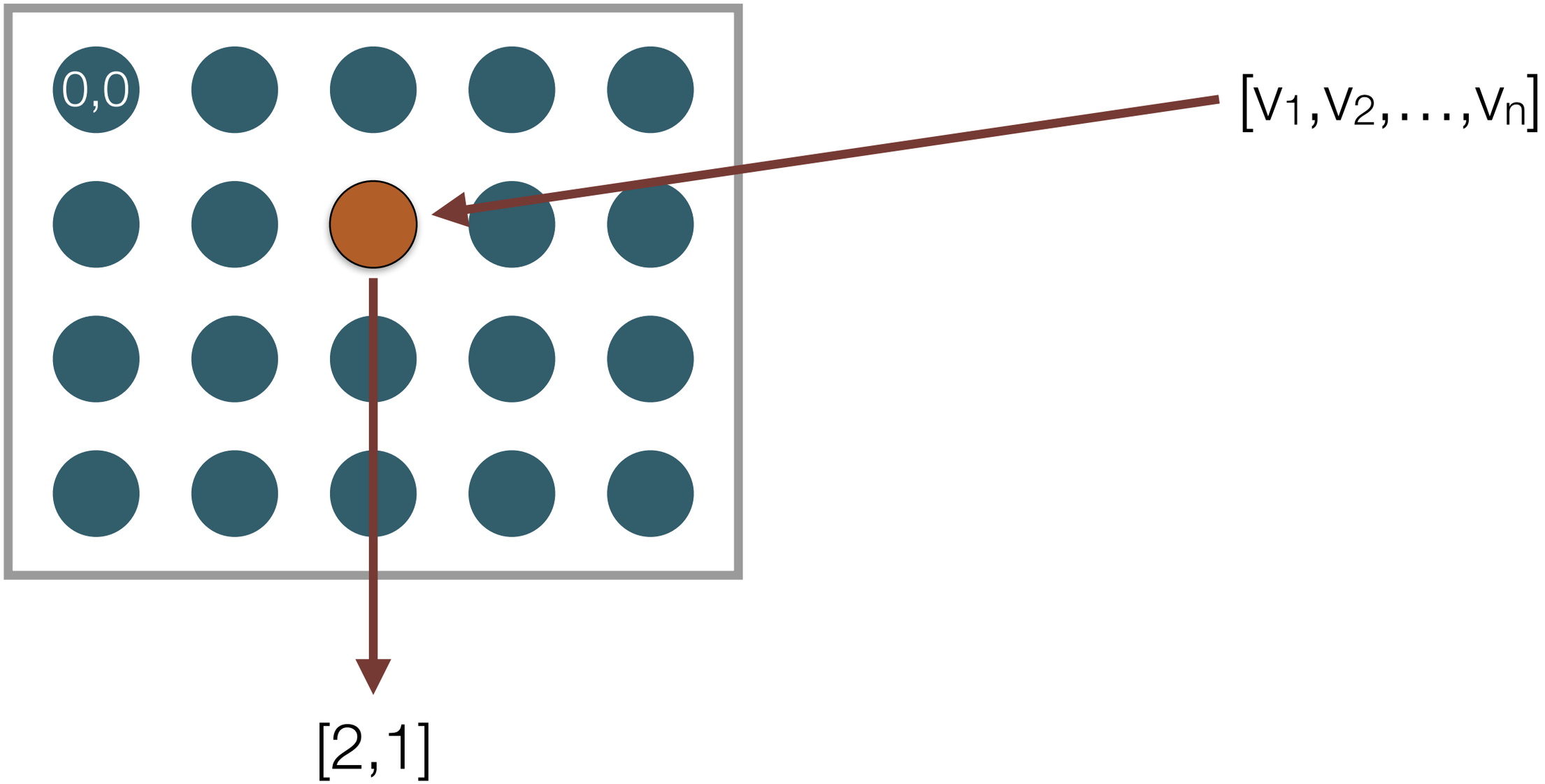
- No control over the distance measure
- Just because axes are oriented along greatest variance, doesn't mean similar things will appear close together
- bear in mind PCA is only a rotation of the original space followed by truncation of less significant dimensions

Self Organising Maps

- SOMs invented by Kohonen in the ‘80s
  - A type of neural net
    - Use competitive learning rather than back-prop against an known objective
    - Use a neighbourhood function to preserve the topology of the input features
- Best not to think to hard about the neural network analogy though!

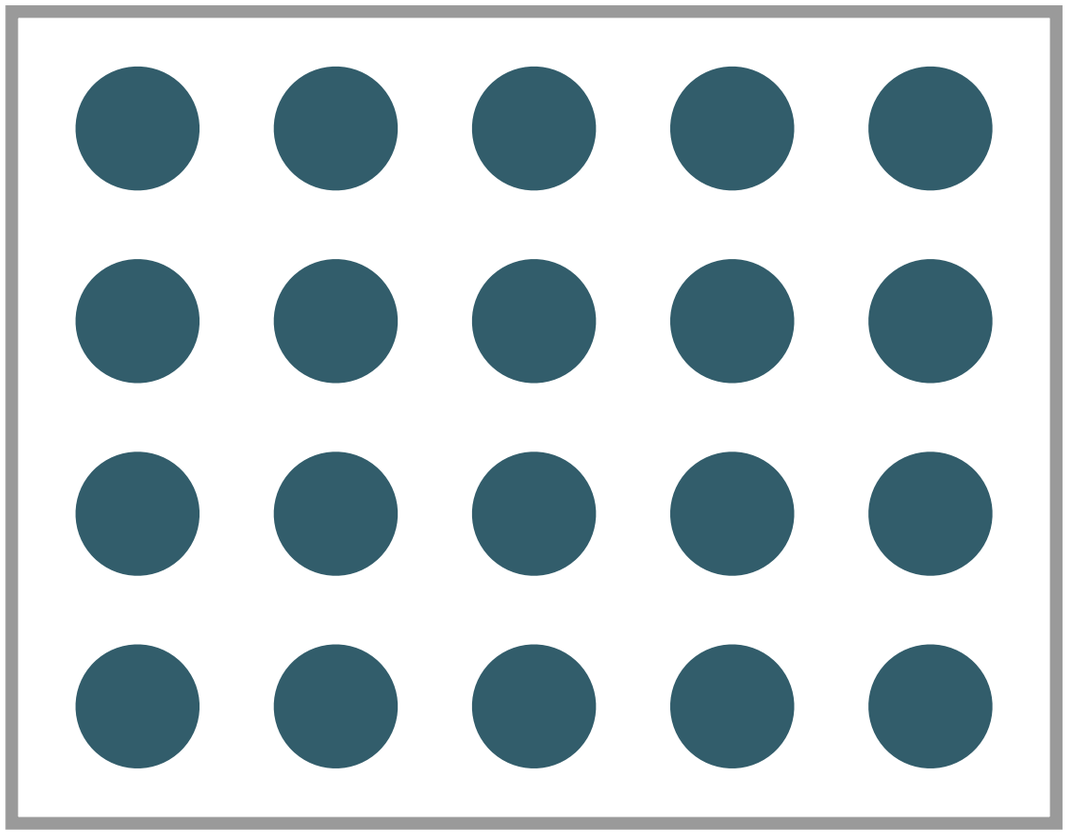


- Each unit has an associated *weight vector*
  - The dimensionality of this vector is equal to the dimensionality of the input feature space
- The location of a unit in the map can be considered to be its (2D) coordinate



In the **projection** phase, the SOM maps high dimensional vectors to a 2D coordinate through the unit that has the closest weight vector (in terms of Euclidean distance)

This is the **Best Matching Unit** (**BMU**)



Before a SOM can be used to project data, it must first be trained - the weights of each unit need to be learned

1. Randomly assign weights to each unit

2. Traverse each input vector in the input data set

    1. Find the BMU by computing the Euclidean distance of the input vector to each unit and picking the unit with the smallest distance

    2. Update the units in the **neighbourhood** of the BMU (including the BMU itself) by pulling them closer to the input vector:
    $\mathbf{W}_v(s+1) = \mathbf{W}_v(s)+\Theta(u,v,s)\alpha(s)(\mathbf{D}(t)-\mathbf{W}_v(s))$

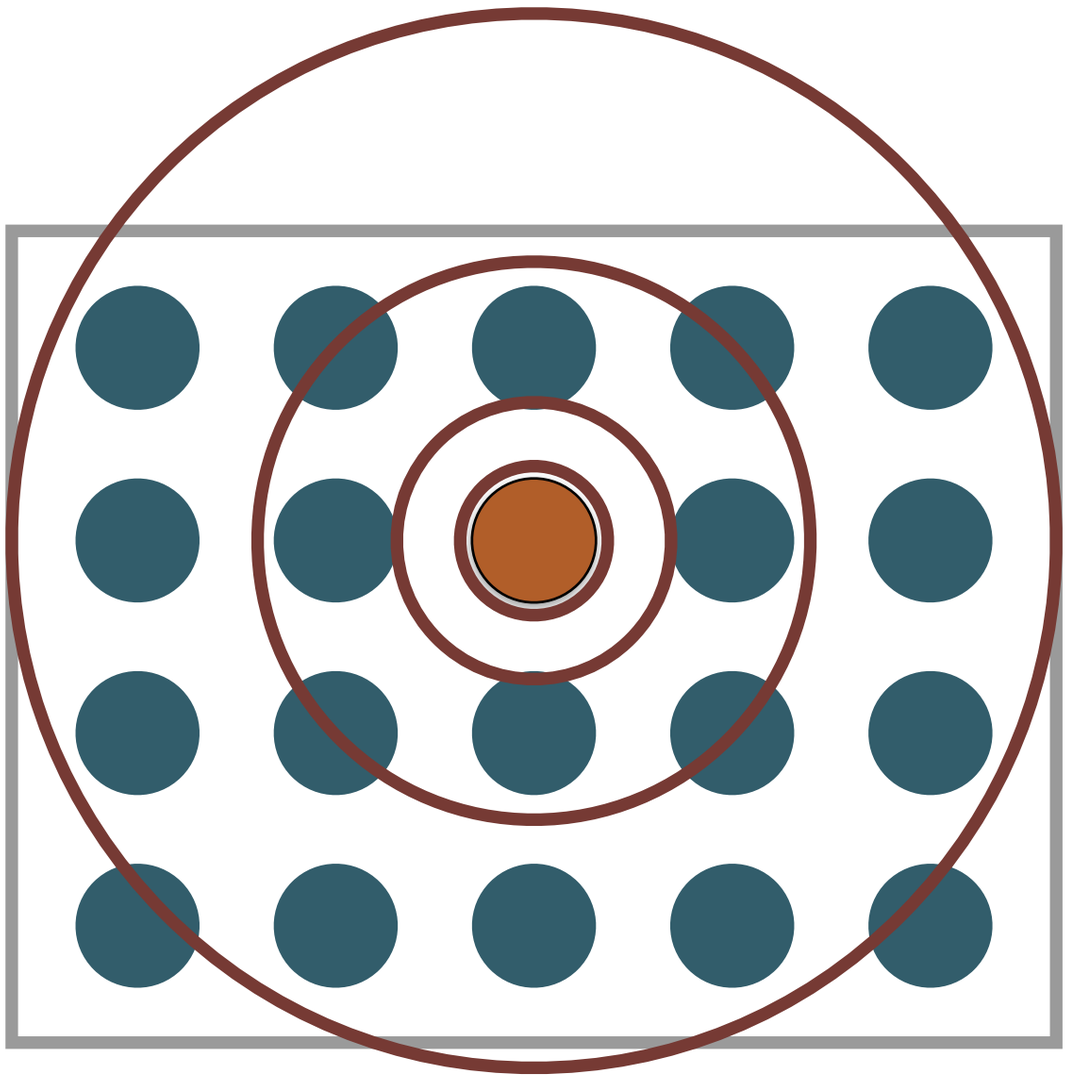
3. Increase s and repeat from step 2 while $s < \lambda$

current iteration

max iterations

$$W_v(s+1) = W_v(s) + \Theta(u,v,s)\alpha(s)(D(t) - W_v(s))$$

Learning rate decay
[gets smaller over time (*s*)]



Neighbourhood weighting function
(often Gaussian)
[gets smaller over time (*s*)]

Demo showing SOM on RGB Colours

Multidimensional Scaling

- Start with data in a high dimensional space and a set of corresponding points in a lower dimensional space

  - attempt to optimise the position of points in lower dimensional space so their Euclidean distances *are like* the distances between the high dimensional points

  - Can use any arbitrary distance measure in the high dimensional space

- Two main categories:
  - **Metric MDS**: tries to match distances
  - **Non-metric MDS**: tries to preserve rankings
- Only requires distances between items as input
  - Unlike PCA and SOM there is no explicit mapping
- Both categories work in the same way - try to minimise a **stress** function
  - Measures goodness of fit between two spaces
  - Can be linear or nonlinear

Stress Functions

- Lots of stress functions:
  - **Least-squares scaling/Kruskal-Shepard scaling**
  - **Shepard-Kruskal non-metric scaling** *Low-dimensional*
- **Sammon Mapping:**

$$S(\mathbf{z}_1, \mathbf{z}_2, \ldots, \mathbf{z}_n) = \sum_{i \neq j} \frac{(\delta_{ij} - \|\mathbf{z}_i - \mathbf{z}_j\|)^2}{\delta_{ij}}$$

Euclidean distance

All combinations of points with the exception of points to themselves

High-dimensional distance

Minimising the Sammon Mapping

- Non-linear… need to use *gradient descent*
  - Starting at an arbitrary point take steps in the direction of the gradient, with size equal to the *gradient* multiplied by a *learning rate,* until convergence:

$$\mathbf{z}_j(k+1) = \mathbf{z}_j(k) - \gamma_k \nabla_{\mathbf{z}_j} S(\mathbf{z}_1(k), \mathbf{z}_2(k), ..., \mathbf{z}_n(k))$$

where the derivative of the Sammon stress is :

$$\nabla_{\mathbf{z}_j} S(\cdot) = 2 \sum_{i \neq j} \left(\frac{\|\mathbf{z}_i(k) - \mathbf{z}_j(k)\| - \delta_{ij}}{\delta_{ij}} \right) \left(\frac{\mathbf{z}_j(k) - \mathbf{z}_i(k)}{\|\mathbf{z}_i(k) - \mathbf{z}_j(k)\|} \right)$$

Demo showing MDS

Other dimensionality reduction techniques

- We've only scratched the surface
  - Lots of other techniques and variants
    - ISOMAP
    - Locally Linear Embedding (LLE)
    - Principal curves
    - Autoencoders
    - …

Summary

- Clustering and dimensionality reduction of key importance to understanding data

- Lots of different approaches - we've barely scratched the surface

- We have however looked at the techniques you're most likely to start exploring a dataset with

    - …which leads on to the individual coursework…