Homework 2 Questions

1 Programming exercise

Using scikit-learn, train an SVM to do classification on the iris data set and evaluate the significance of the obtained classification accuracy. As a hint, consider the following steps:

1. Consider two possible models - one linear and one with an RBF kernel.
2. Determine which model is better for the classification task.
3. Using the better of the two models, obtain a test accuracy.
4. Evaluate whether the test classification accuracy is significant using a permutation test.
5. Report the p-value you obtained.

Question 1: In class, we considered one way of doing feature selection through quantifying the mutual information between features and class labels. Which regularization penalty can be used as another way to discard irrelevant features?

a. ℓ_1

b. ℓ_2

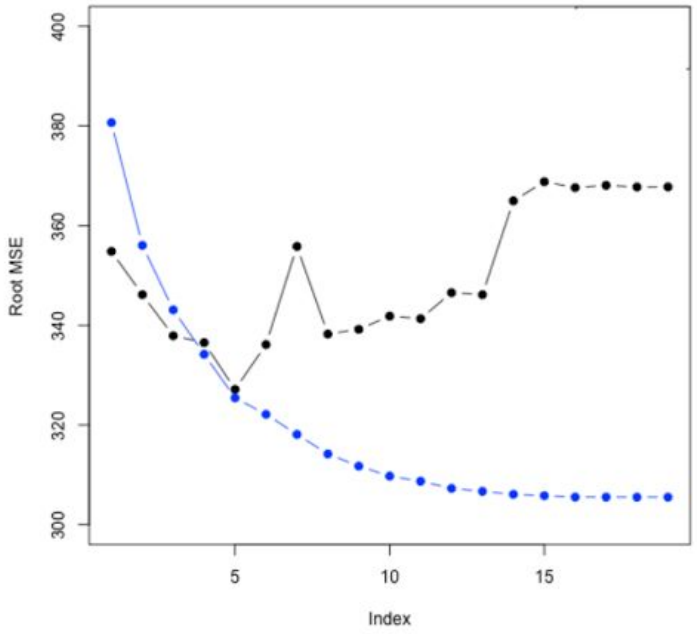
c. none of the above

Question 2: Consider a data set with 19 features per data instance. You decide to do feature selection in a brute force way by selecting subsets of features and performing cross validation to determine whether the selected subset of features is a good one for some task. You form 19 subsets of features with sizes 1, 2,...,19. Note that you decide not to investigate all possible subsets (that would be 2^{19} possible subsets). You have better things to do with your life.

You have performed 19 complete cross validations, and plot the training and validation errors in order of increasing subset size. Which of the following lines is the training error? (note that "root MSE" (mean squared error) is one way to quantify error, and "Index" is the subset index in the list, which is equivalent to the size of the subset)

a. blue

b. black



Question 3: Consider the setting of question 2. Based on the training and validation error plots, which size subset would you choose for the final evaluation of your model?

a. 5

b. 7

c. 14

d. 19

Question 4: Consider performing leave-2-out cross validation on a data set with 150 total data instances. If you decide to leave 10% of the data for testing, how many folds of cross validation will you need to run?

a. 2

b. 9045

c. 11175

d. none of the above

Question 5: Consider performing 2-fold cross validation on the same data set as in question 4. Now, if you decide to leave 20% of the data for testing, how many folds of cross validation will you need to run?

a. 2

b. 9045

c. 11175

d. none of the above

Question 6: Which of the following methods will be best to use to determine the best number of nearest neighbors k in kNN for a certain data set?

a. feature selection

b. cross validation

c. regularization

Dimensionality reduction and clustering

06/17/2016

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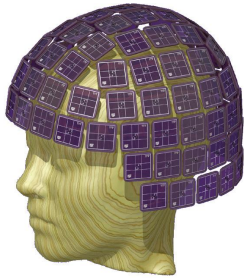
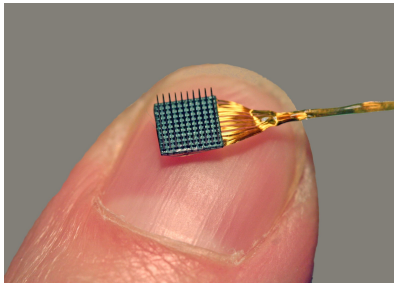
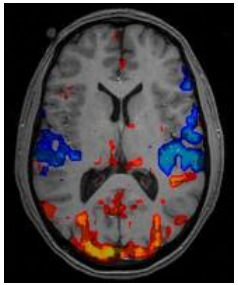
Some figures derived from slides by Alona Fyshe, Aarti Singh, Barnabás Póczos, Tom Mitchell

How can ML help neuroscientists?

- **Deal with large number of sensors/recording sites**







  - investigate high-dimensional representations
    - classification (what does this high-dimensional data represent?)
    - regression (how does it represent it? can we predict a different representation?)
    - model selection (what model would best describe this high dimensional data?)
    - **clustering (which high-dimensional representations are similar to each other?)**
  - **uncover few underlying processes that interact in complex ways**
    - **dimensionality reduction techniques**

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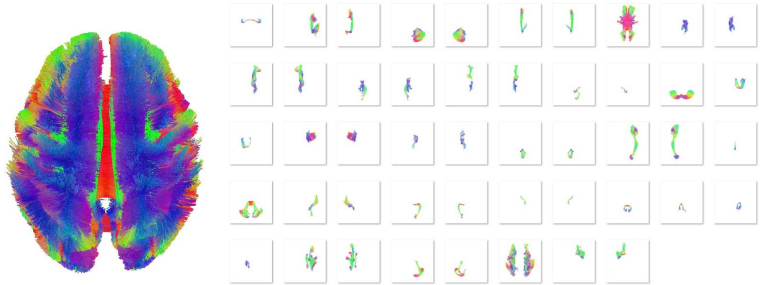

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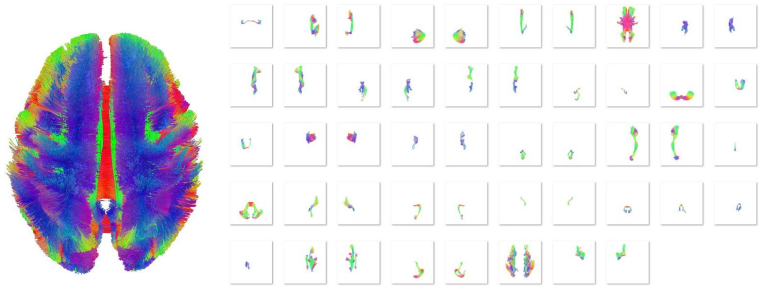

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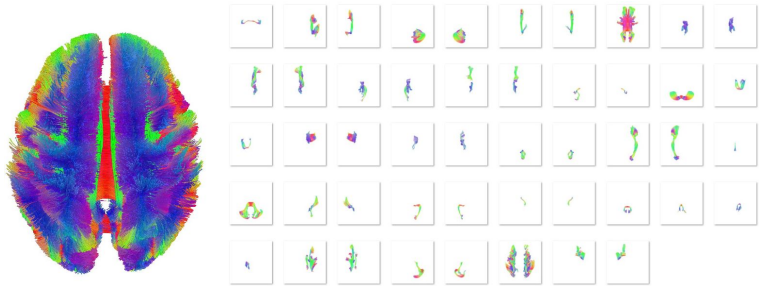

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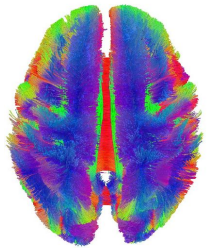

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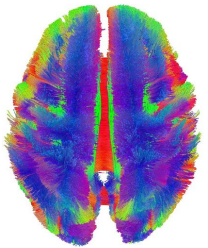

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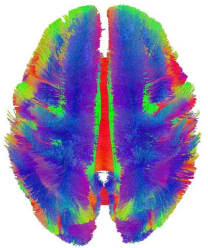

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    - For unsupervised methods, want to learn P(data)

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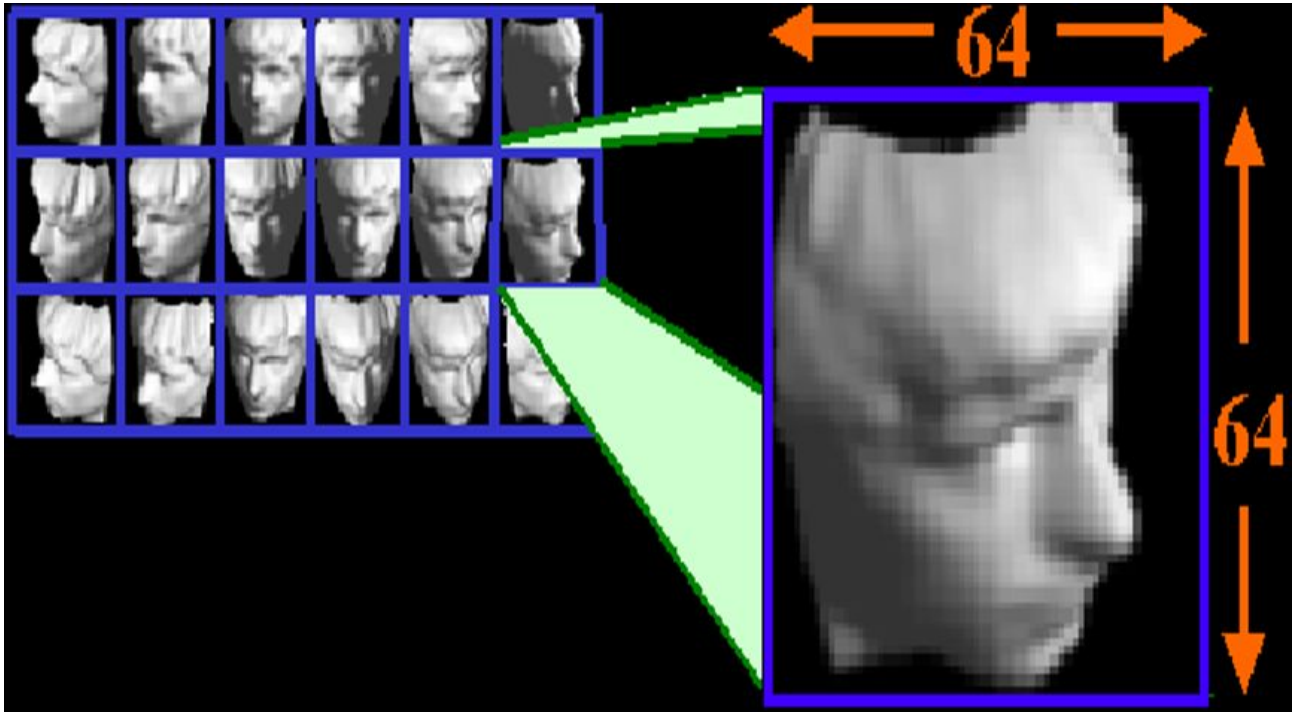
    - Some linear or nonlinear combination of observed features provides more efficient representation for the data than observed features

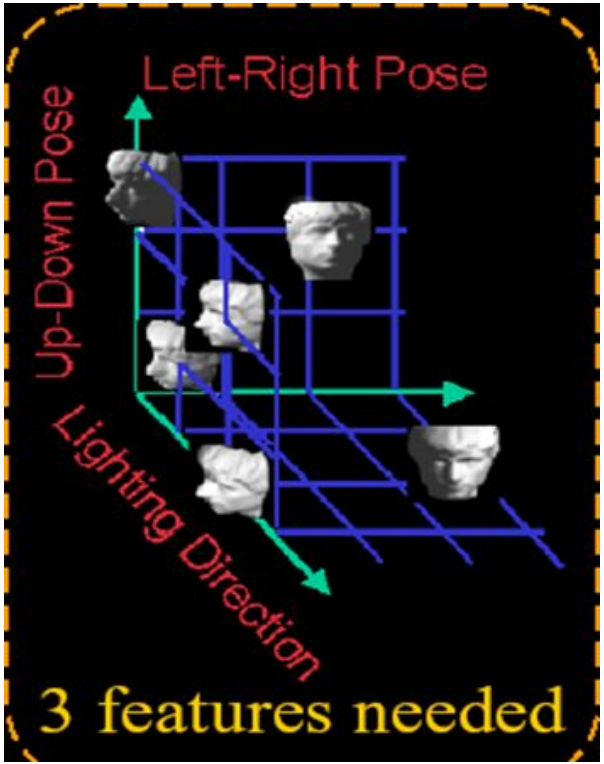
Example: how does the brain store these pictures?

Data: 64x64 dimensions, but are there fewer underlying relevant dimensions?



We can condense data to 3 underlying informative dimensions

- Don’t need every pixel (64x64)



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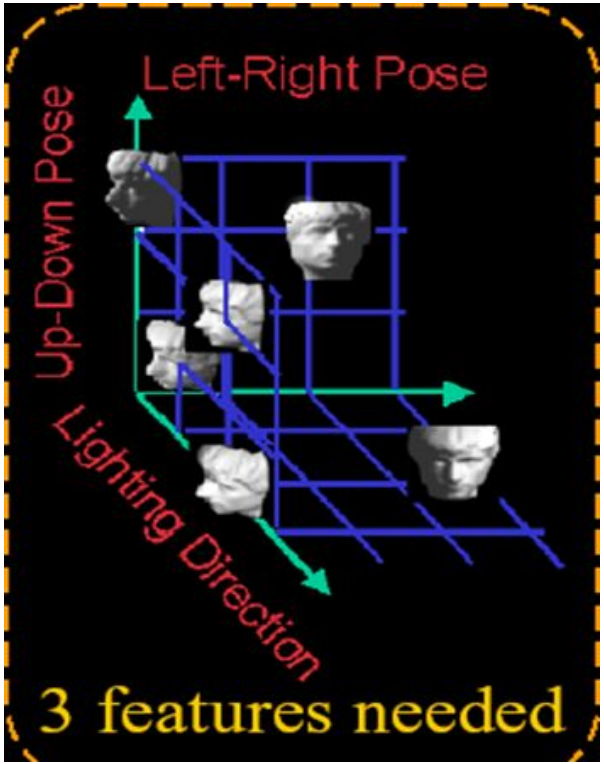

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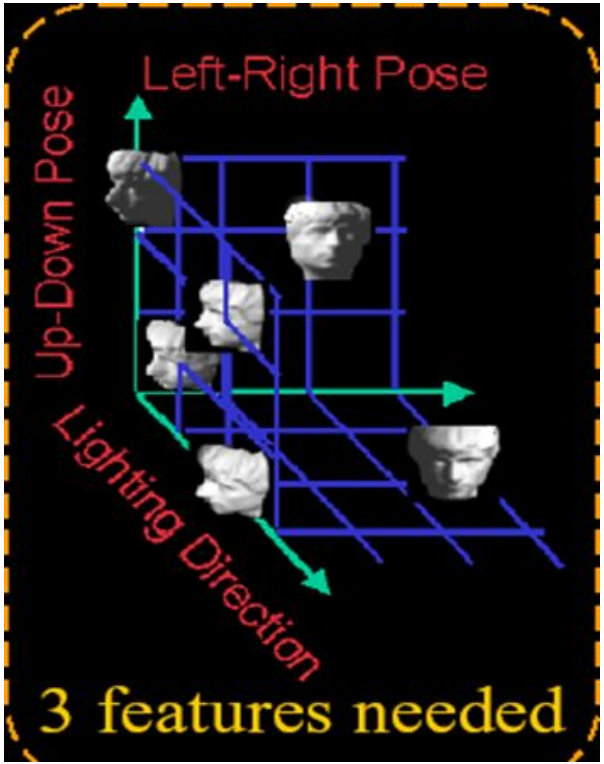

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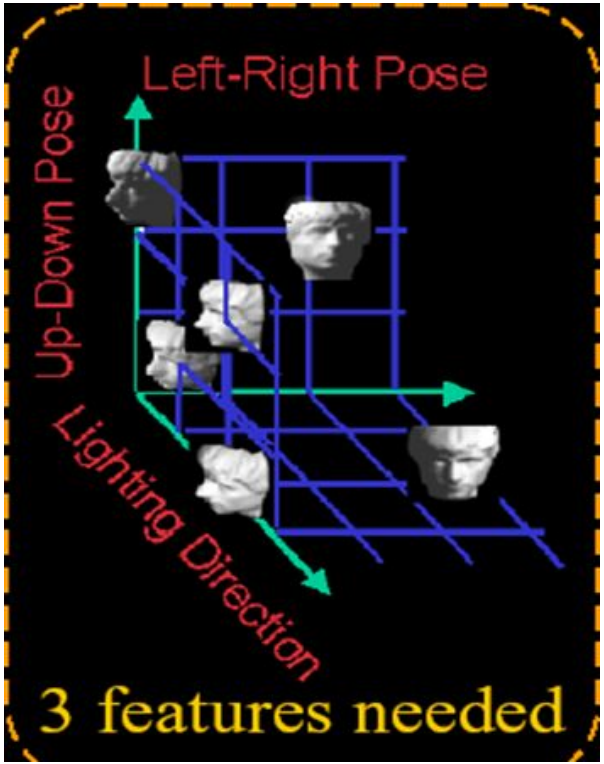
- Reduction of high-dimensional inputs to 3-dimensional intrinsic manifold



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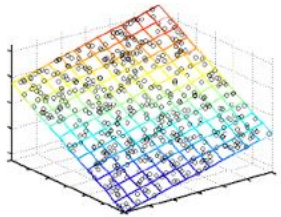

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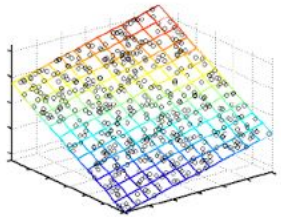

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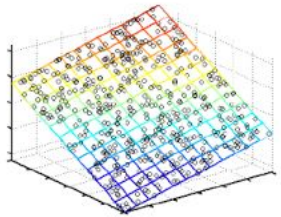

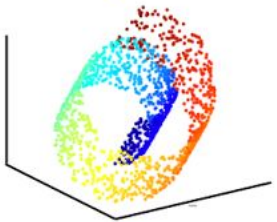

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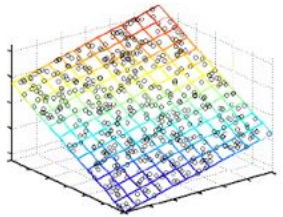

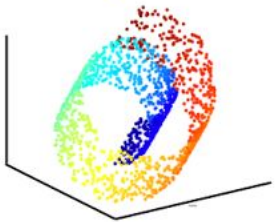

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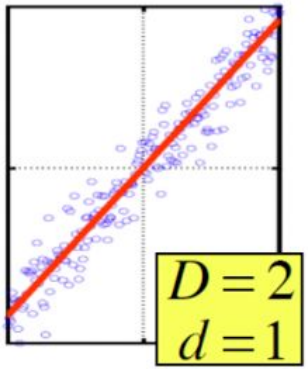

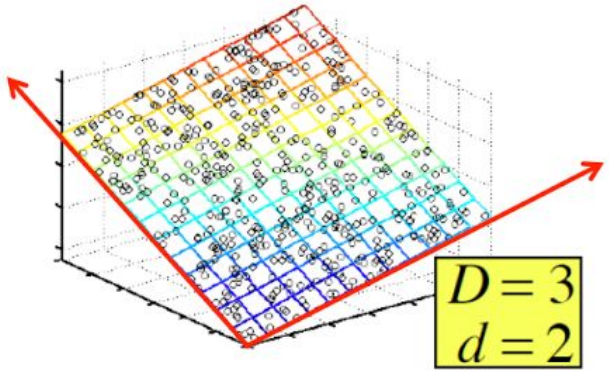

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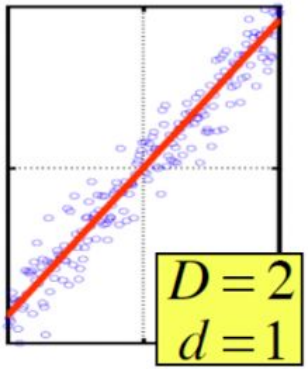

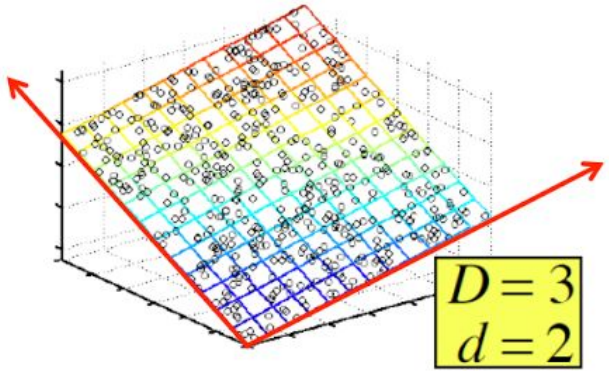

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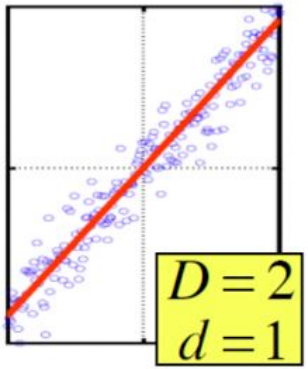

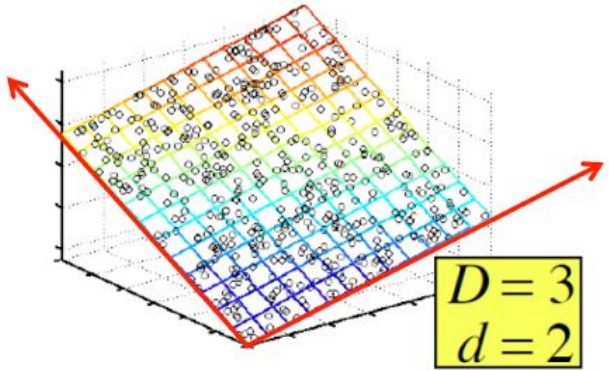

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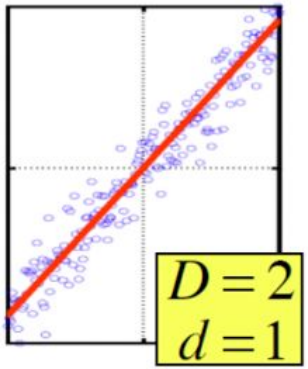

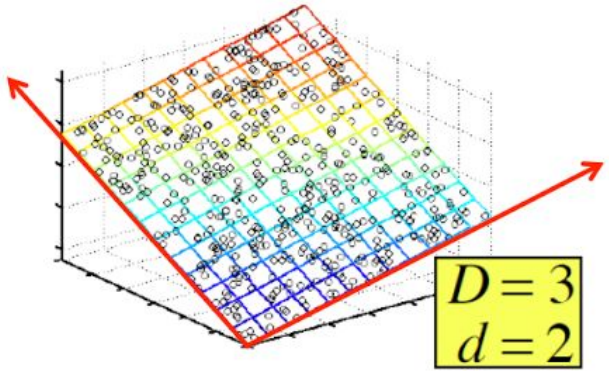

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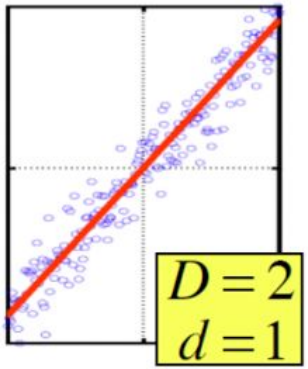

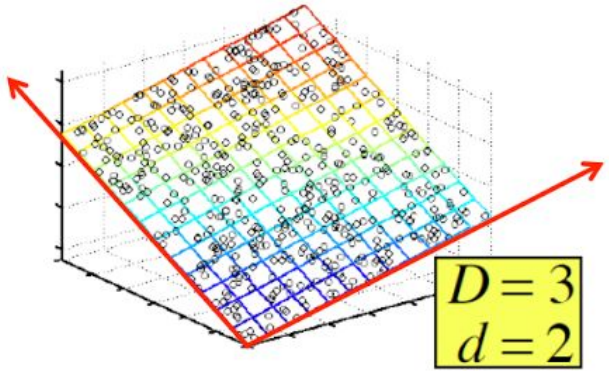

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- Goal: identify these axes = also known as the principal components (PCs)

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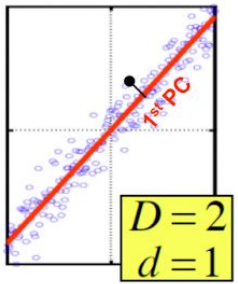
- Intuitively, PCs are the orthogonal directions that capture most of the variance in the data



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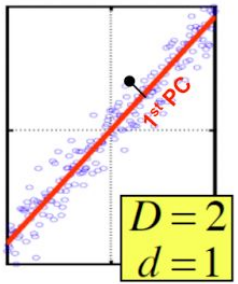

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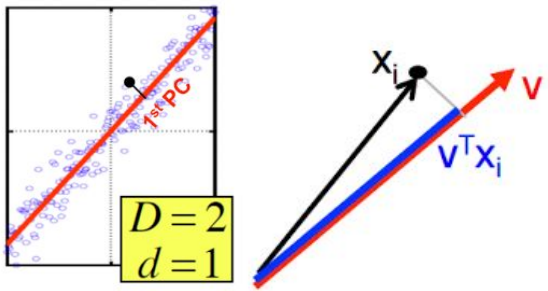

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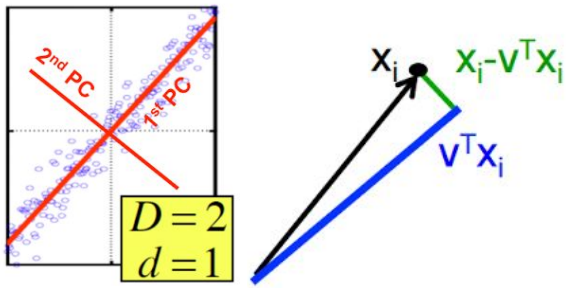

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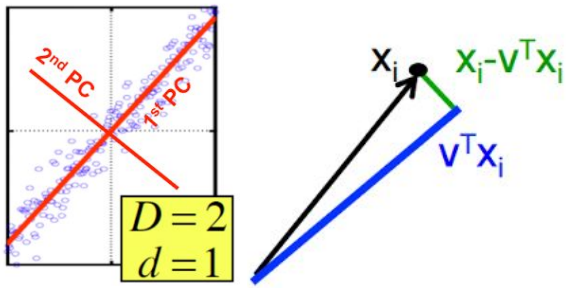

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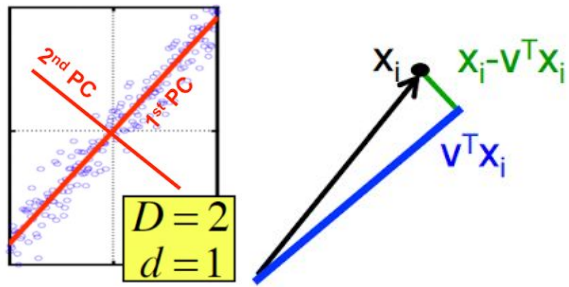

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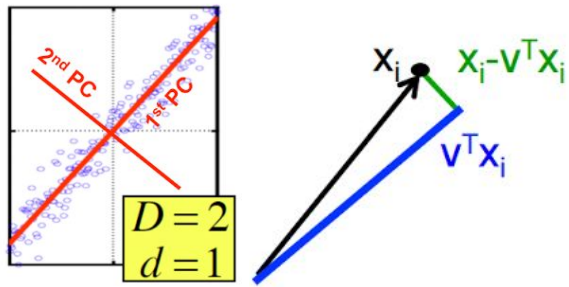

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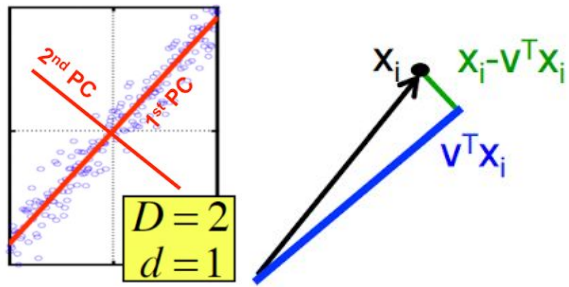

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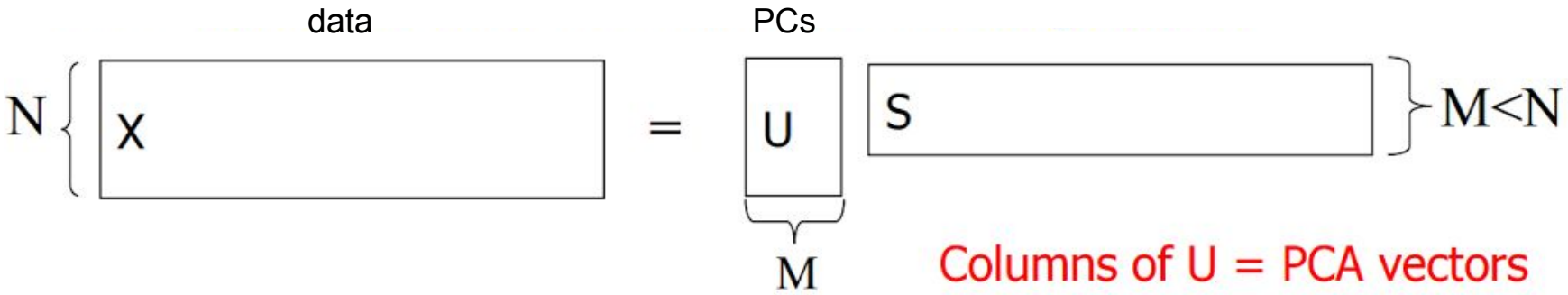
PCA: low rank matrix factorization for compression



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  - Cut off when certain % of variance explained is reached or when you see a sharp decrease in % variance explained

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Do we need the latent dimensions to be orthogonal?

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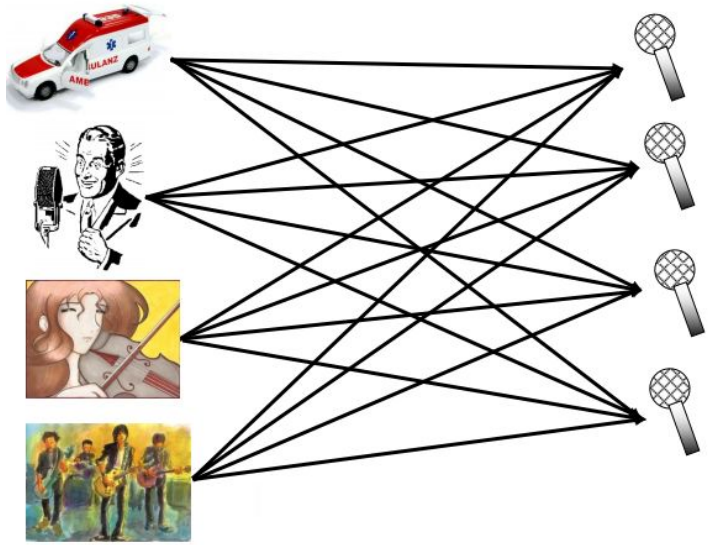
- What if instead, they're statistically independent? => Independent component analysis (ICA)

ICA aims to separate the observed data into some underlying signals that have been mixed



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mixed observations

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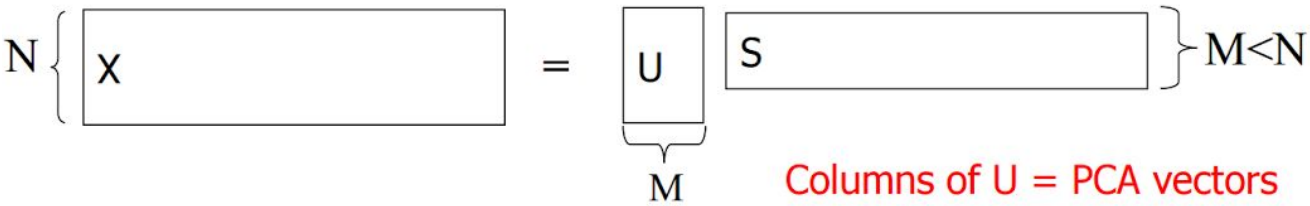

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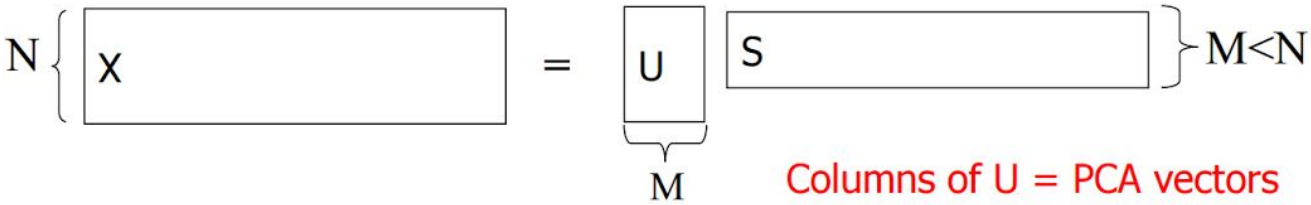
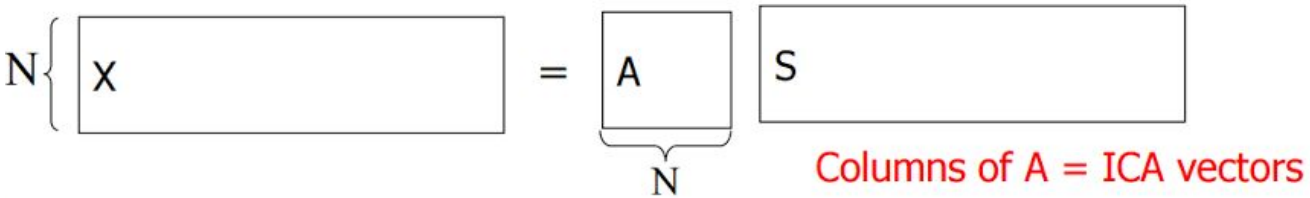


ICA: **full rank** matrix factorization to **remove dependencies** among rows



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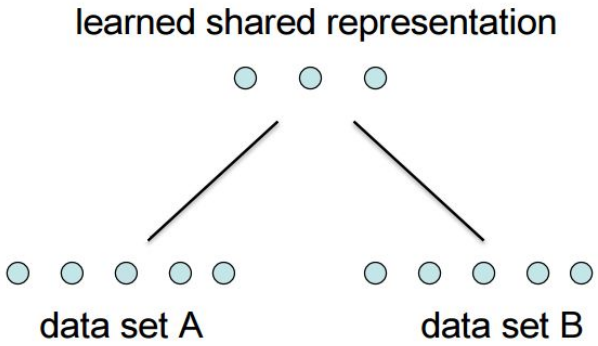
- Unlike PCA, which finds orthogonal latent components, ICA finds components that are statistically independent
- Used for denoising and source localization in neuroimaging

What if we're interested in explaining variance in multiple data sets at the same time?



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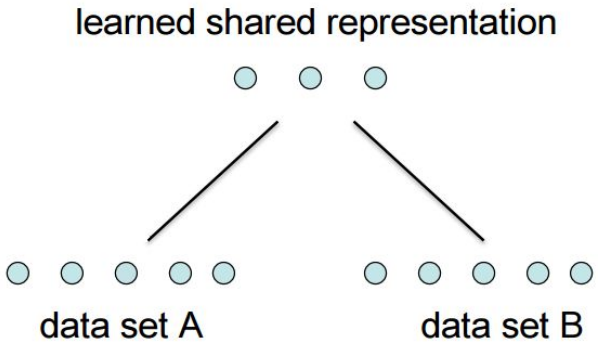

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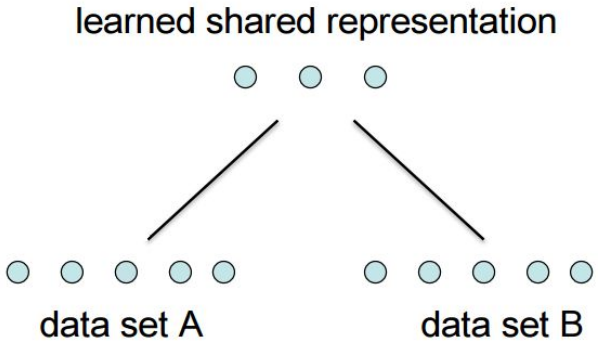
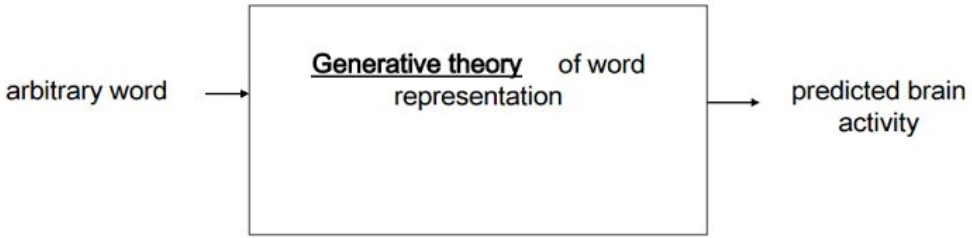


- Example: simultaneous recordings of NIRS (data set A) and fMRI (data set B), can we find the common brain processes?
- Canonical correlation analysis (CCA) maximizes the correlation of the projected data A and data B in the common latent lower-dimensional space

CCA: example use in neuroscience = discovering shared semantic basis between people



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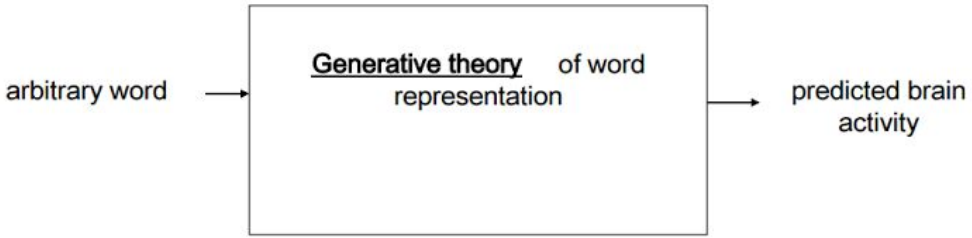

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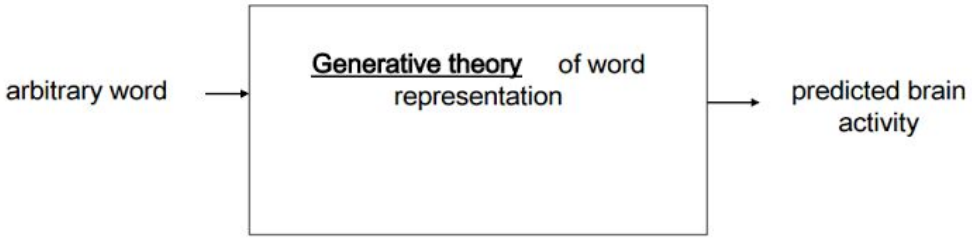
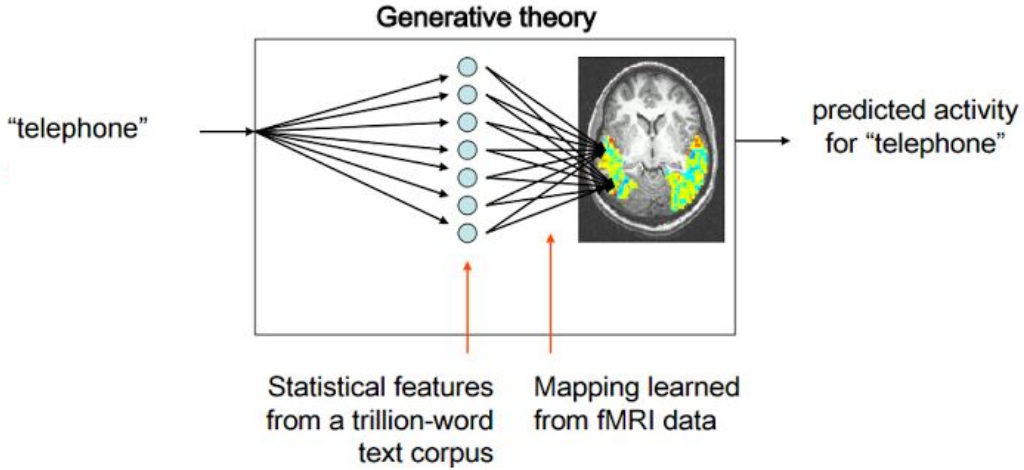


- In an fMRI, we present words to subjects, one at a time
- We aim to use the fMRI data, along with its corresponding word label to train a general model that can predict brain activity for an arbitrary word (even a word that was never presented to the subject)

Let’s consider semantics within one person first



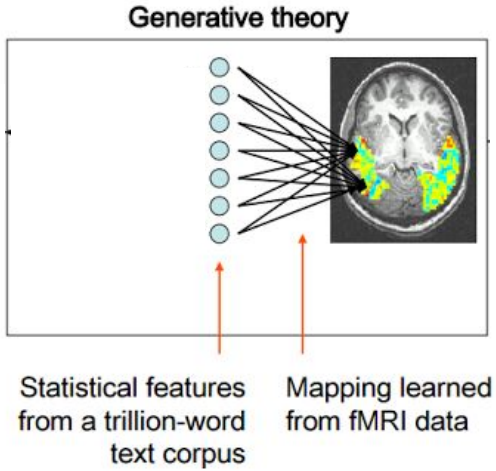
Mitchell et al., Science 2008

Semantic features for 2 presented words

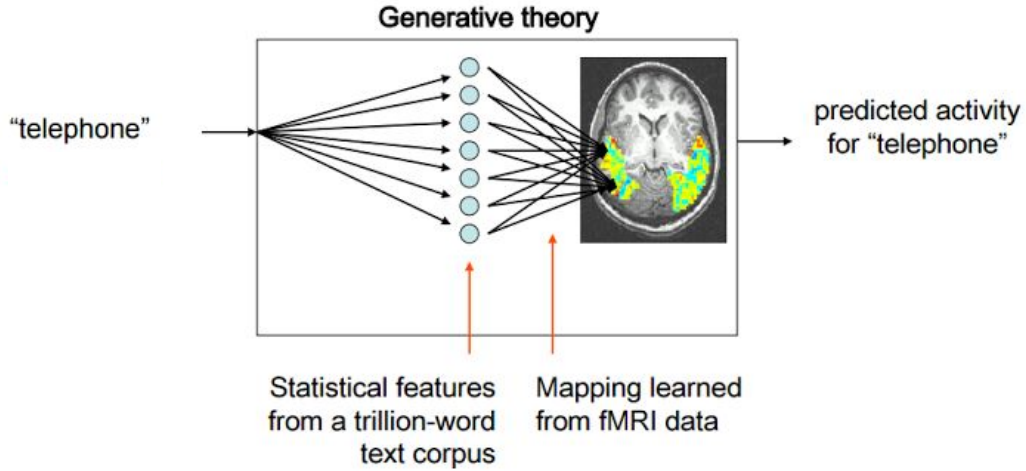
Semantic feature values:
"**celery**"
0.8368, eat
0.3461, taste
0.3153, fill
0.2430, see
0.1145, clean
0.0600, open
0.0586, smell
0.0286, touch
…
…
0.0000, drive
0.0000, wear
0.0000, lift
0.0000, break
0.0000, ride

Semantic feature values:
"**airplane**"
0.8673, ride
0.2891, see
0.2851, say
0.1689, near
0.1228, open
0.0883, hear
0.0771, run
0.0749, lift
…
…
0.0049, smell
0.0010, wear
0.0000, taste
0.0000, rub
0.0000, manipulate

Training the model: learn a regression between semantic vectors and fMRI data for all words in training set



Applying the model: for any given word, look up semantic vector, then apply learned regression weights to generate corresponding fMRI image



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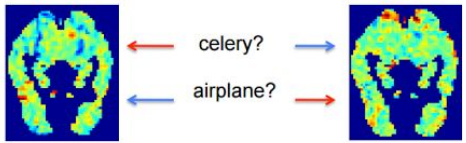

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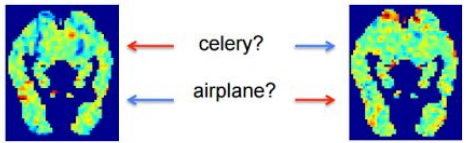

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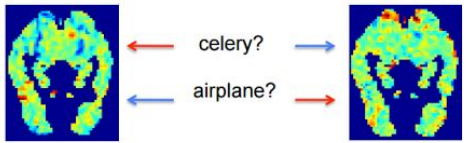

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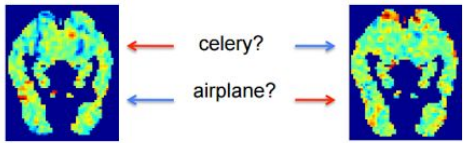

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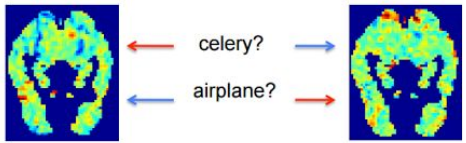

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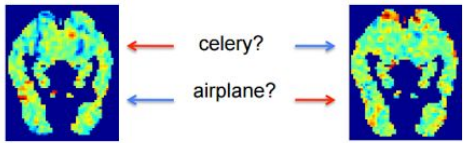

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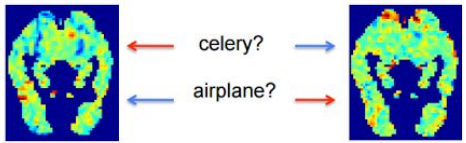
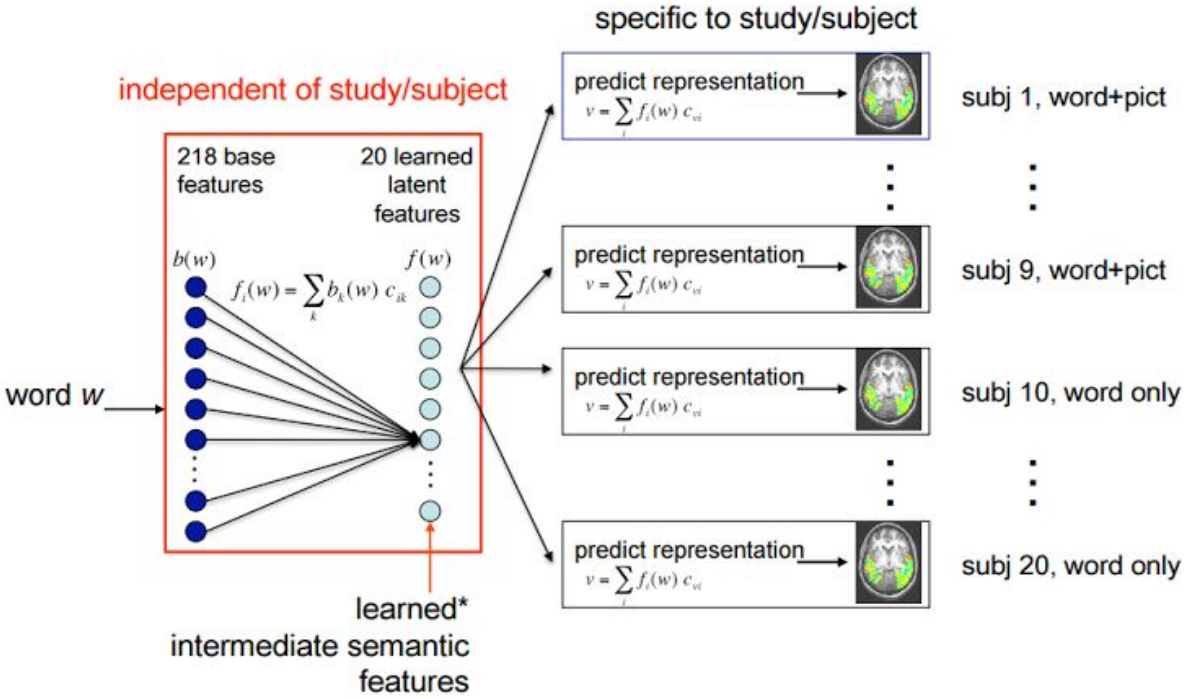


- We can predict the fMRI activation corresponding to a word the model has never seen before

CCA: extending the model to multiple subjects and experiments improves accuracy to 87% (by 8%)



CCA takeaways

- CCA learns linear transformations of multiple data sets, such that these transformations are maximally correlated

CCA takeaways

- CCA learns linear transformations of multiple data sets, such that these transformations are maximally correlated
- In neuroscience, it can be used to extend models to multiple subjects or experiments

Beyond linear transformation: laplacian eigenmaps

- Linear methods find lower-dimensional linear projects that preserves distances between **all** points

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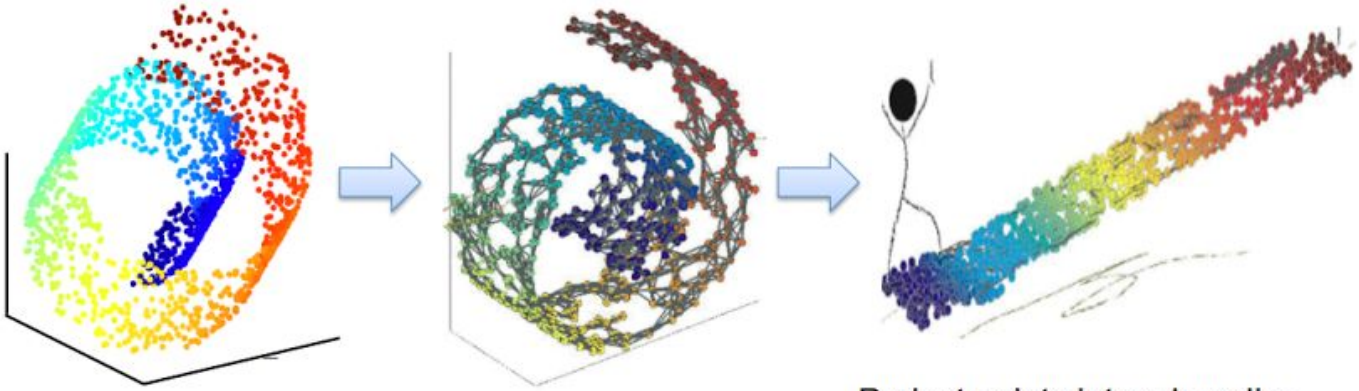

Construct graph from data points (capture local information)

Project points into a low-dim space using “eigenvectors of the graph”

Laplacian eigenmaps: 3 main steps

- ❏ Construct graph

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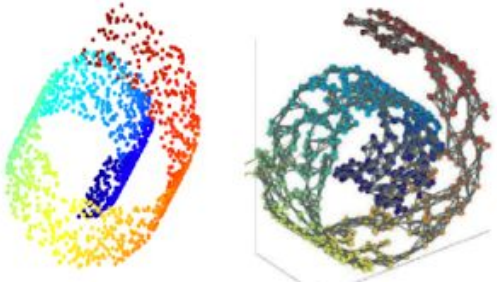
- ❏ Embed points using graph Laplacian

Step 1: constructing a similarity graph

- Similarity graphs model local neighborhood relations between data points



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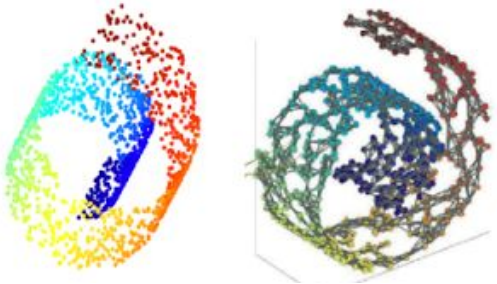

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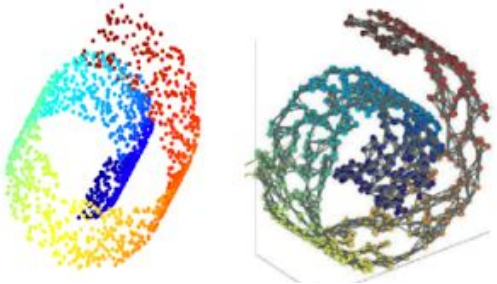

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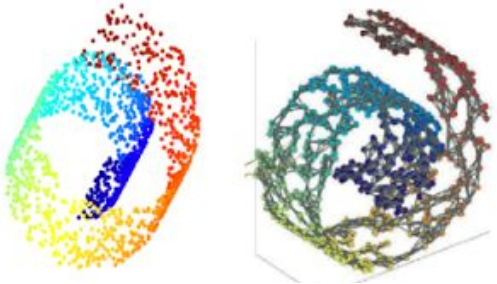

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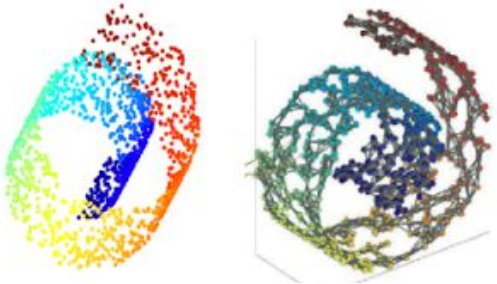

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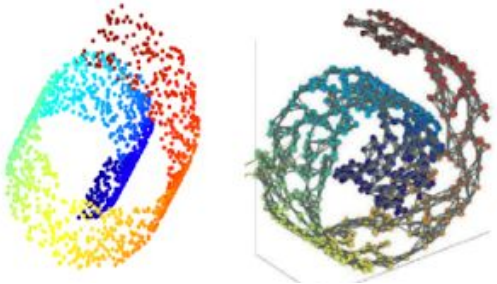

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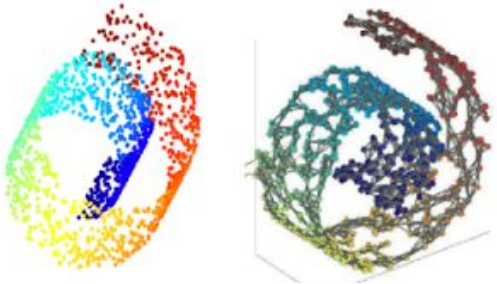

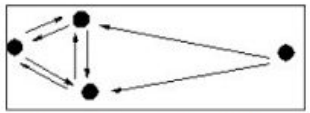

Directed nearest neighbors

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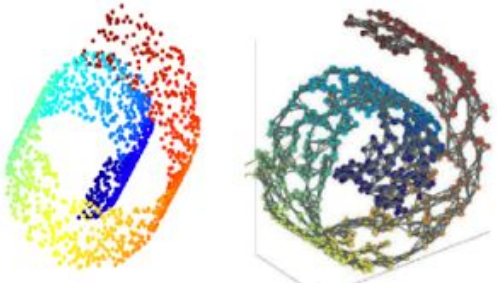

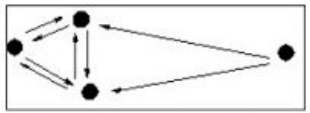

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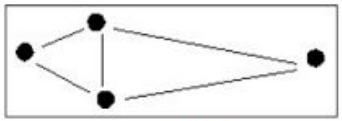

(symmetric) kNN graph

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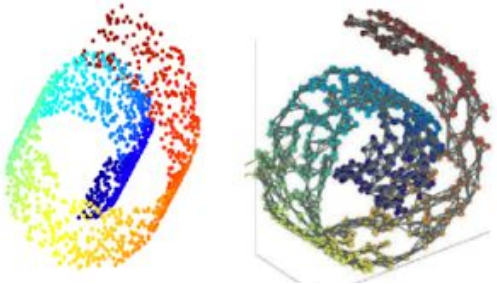
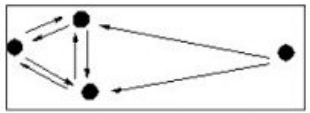
          - mutual: edge A-B if A is k-NN of B AND B is k-NN of A





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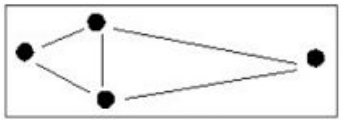

(symmetric) kNN graph

mutual kNN graph

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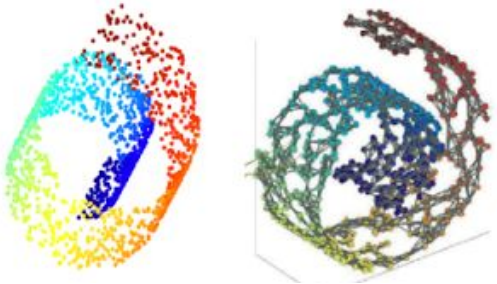

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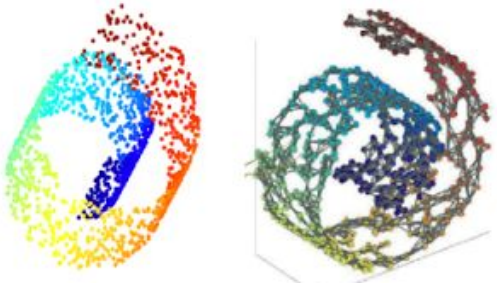

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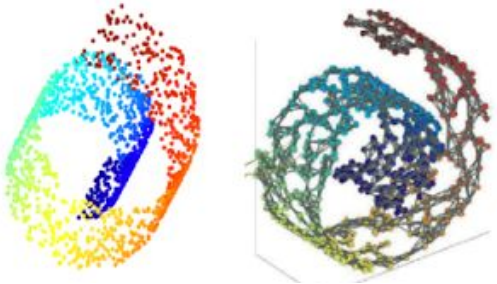

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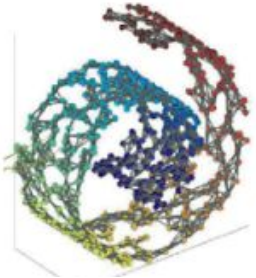
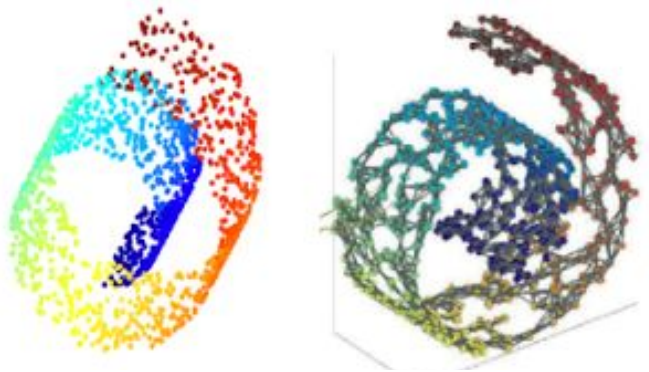
      - $W_{ij}= e^{-\frac{\|x_i - x_j\|^2}{2\sigma^2}}$, Gaussian kernel similarity function (aka heat kernel)



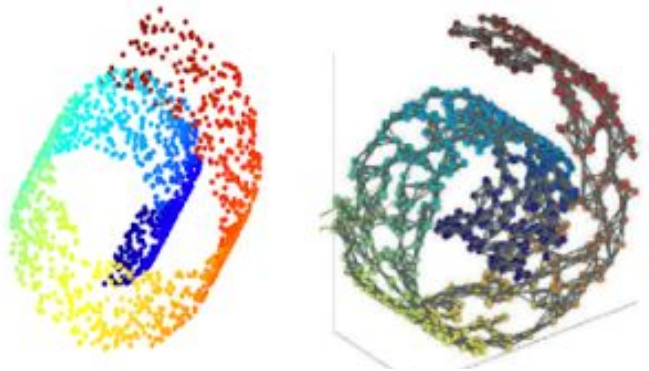
How do we choose k, ε?

- The goal is to preserve local information so we don't want to choose neighborhood sizes that are too large



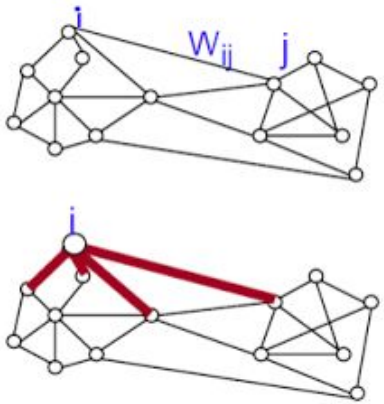
How do we choose k, ε?

- The goal is to preserve local information so we don't want to choose neighborhood sizes that are too large
- Mostly dependent on the data, but want to avoid "shortcuts" that connect different arms of the swiss roll



Step 2: compute the graph Laplacian of the constructed graph

- Graph Laplacian = D - W



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- W = weight matrix from the constructed graph
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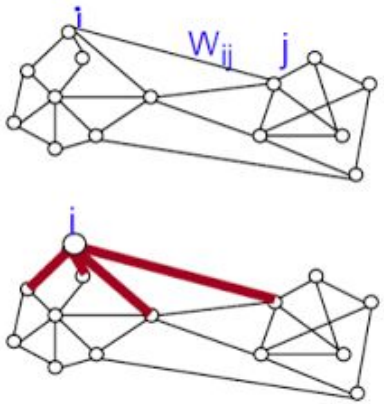

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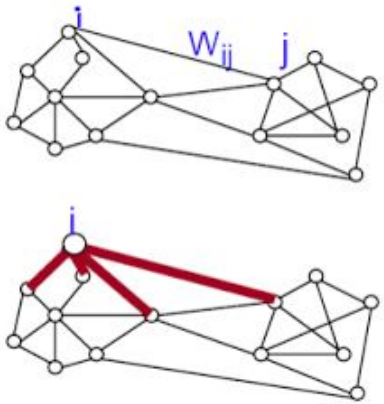
- D = degree matrix = diag(d_1,...,d_n)
  - d_i = degree of vertex i = sum of all weights that connect to vertex i
  - For n data points, D is size n x n



Step 3: embed data points using graph Laplacian

Original Representation		Transformed representation
data point		projections
x_i	→	$(f_1(i), \ldots, f_d(i))$
(D-dimensional vector)		(d-dimensional vector)

- Intuition = find vector f such that, if x_i is close to x_j in the graph (i.e. W_{ij} is large), then the projections f(i) and f(j) are also close

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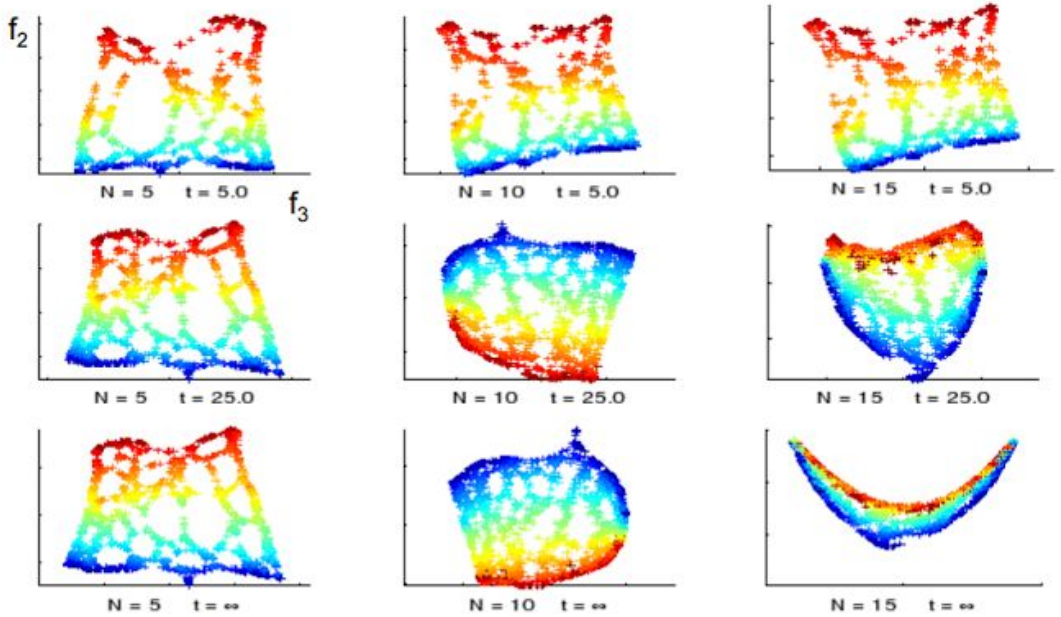
- Find eigenvectors of graph Laplacian and corresponding eigenvalues
- To embed data points in d-dimensional space, we project data into eigenvectors associated with the d smallest eigenvalues

Unrolling the swiss roll with Laplacian eigenmaps



N=number of nearest neighbors, t = the heat kernel parameter (Belkin & Niyogi'03)

Laplacian eigenmaps takeaways

- A way to do nonlinear dimensionality reduction

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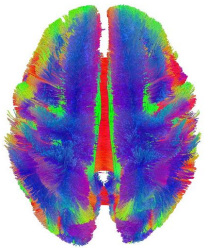
Laplacian eigenmaps takeaways

- A way to do nonlinear dimensionality reduction
- Aim to preserve local information
- Require 3 main steps:
  - Construct a similarity graph between data points
  - Compute the graph Laplacian
  - Use graph Laplacian to embed data points

Supervised vs unsupervised learning

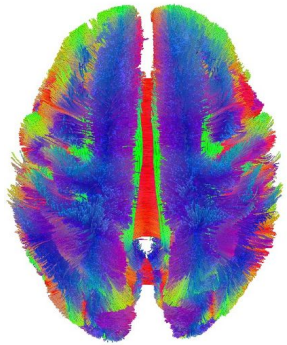
- So far we've only looked at supervised learning methods
  - Supervised methods require labels for each training data instance
    - classification
    - regression
  - Example: kNN classifier for DTI fibers assignments to anatomical bundles
- But what if we have a lot of unlabeled data and acquiring labels is expensive, or not even possible?
  - expensive labels: DTI fibers assignments to anatomical bundles
  - unknown labels: "brain states" assignments of resting state fMRI



- Unsupervised learning! We'll discuss two such methods today
  - dimensionality reduction
  - **clustering**

Clustering: motivation

- We talked about using kNN to classify individual DTI fibers into anatomical bundles



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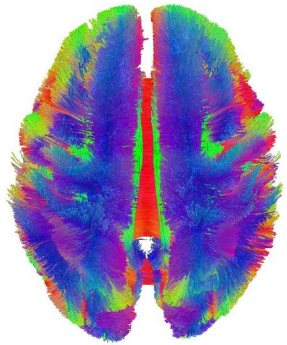

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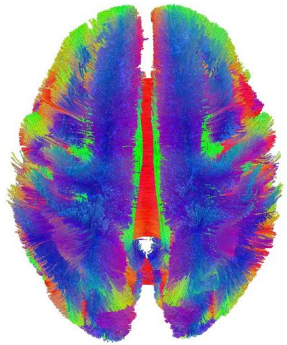

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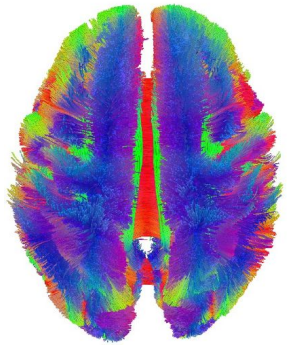
- Can we free the human?



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What is clustering?

- Organizing data into groups, or clusters, such that there is:
  - High similarity within groups
  - Low similarity between groups
- Unsupervised, so no labels to rely on for clustering

How to measure “similarity” between/within clusters?

- Any function that takes two data points as input and produces a real number as output

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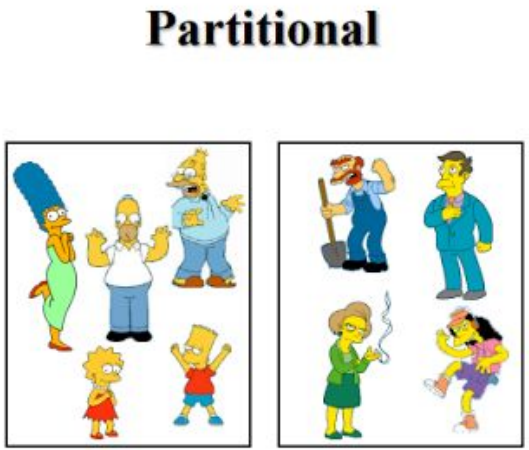
  - Correlation coefficient: $s(x,y) = \frac{\sum_i (x_i - \mu_x)(y_i - \mu_y)}{\sigma_x \sigma_y}$

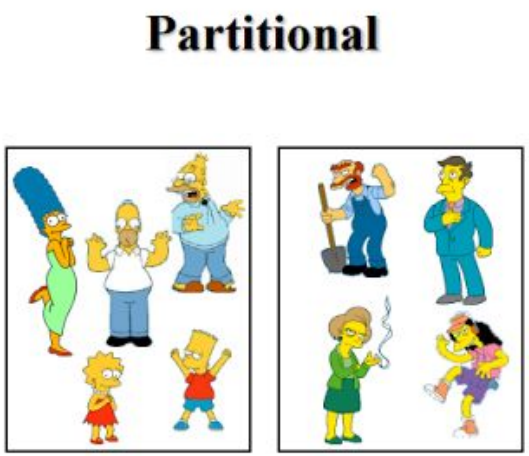
Clustering algorithms divide into 2 main types

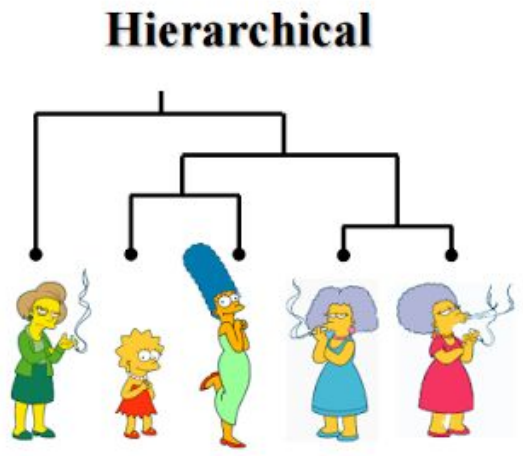
- Partitional algorithms
  - Construct various partitions and then evaluate the partitions by some criterion



Clustering algorithms divide into 2 main types

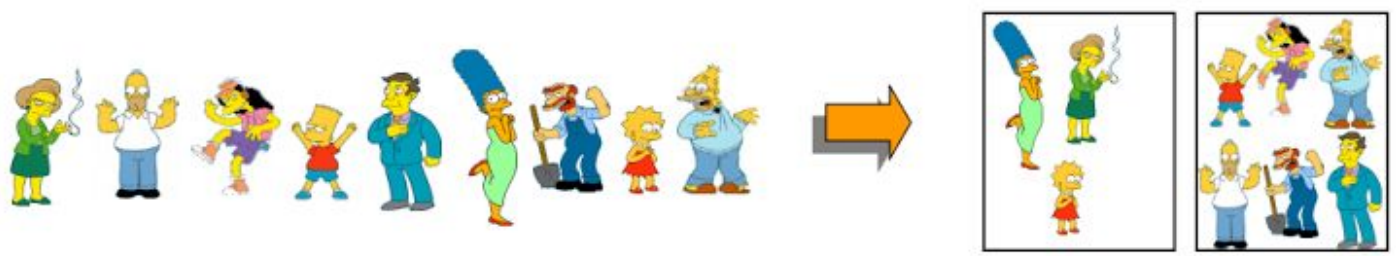
- Partitional algorithms
  - Construct various partitions and then evaluate the partitions by some criterion
- Hierarchical algorithms
  - Create a hierarchical decomposition of the set of objects using some criterion





Partitional clustering

- Each data instance is placed in exactly one of K non-overlapping clusters



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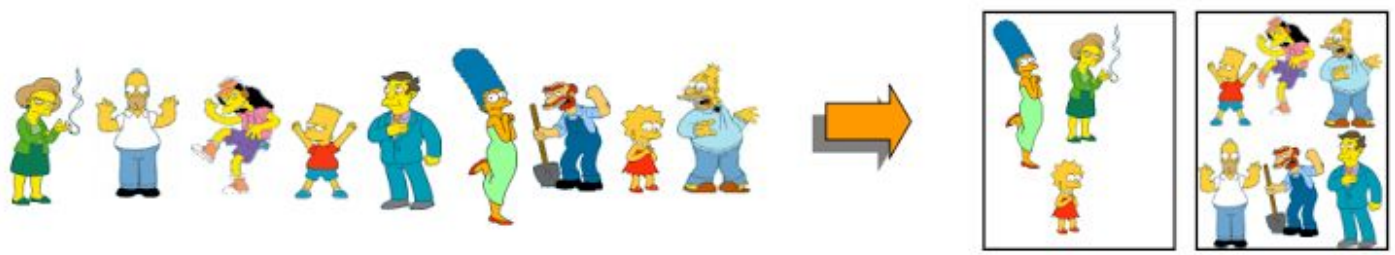

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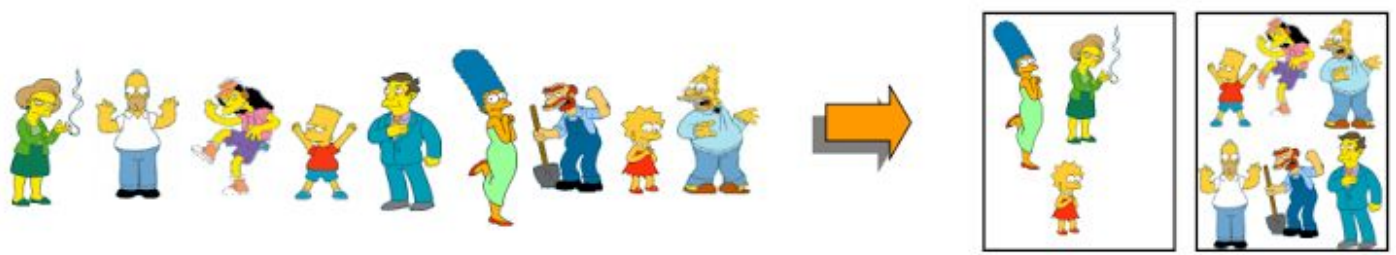
- The user must specify the number of clusters K
- We'll discuss 2 such algorithms:
  - k-means
  - spectral clustering



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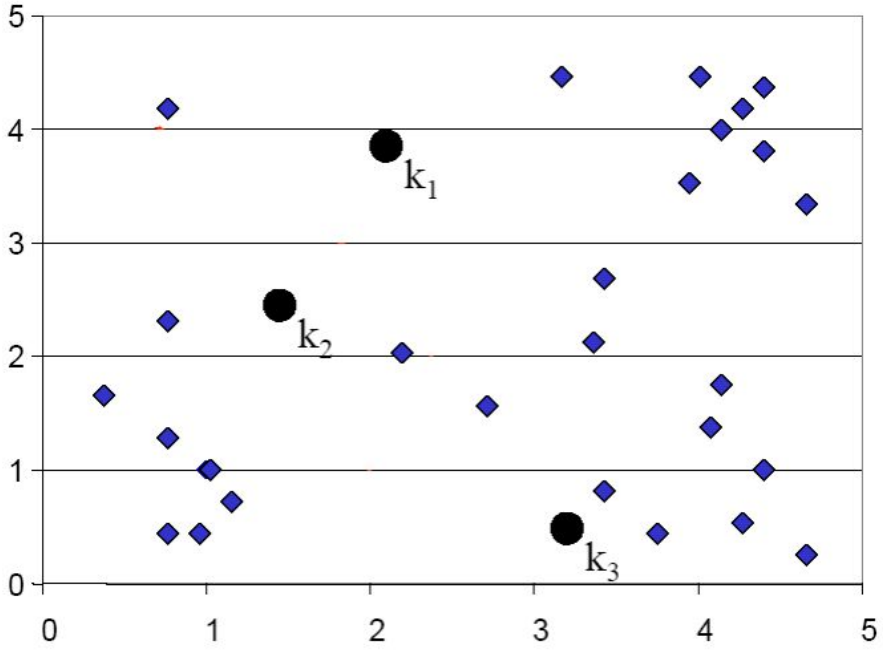
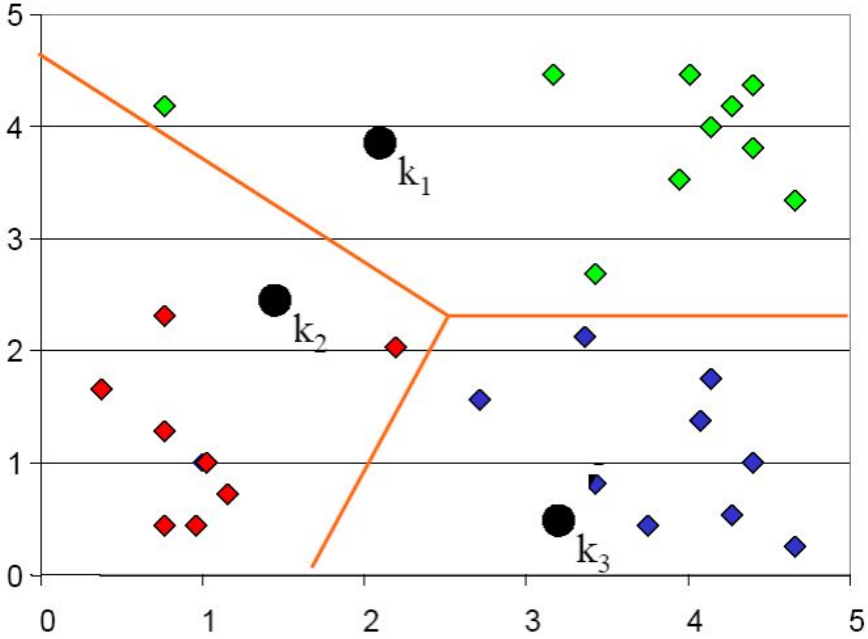
- Terminate if none of the assignments changed in the last iteration

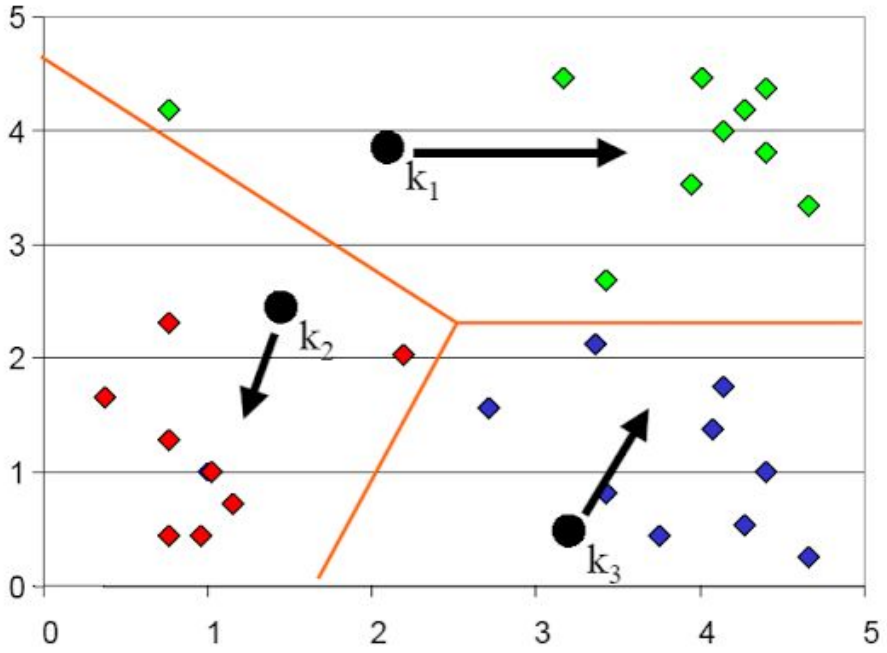
Step 1 + 2: input number of clusters k, initialize their positions



Step 3.1: assign all data to nearest cluster



Step 3.2: re-estimate k cluster means



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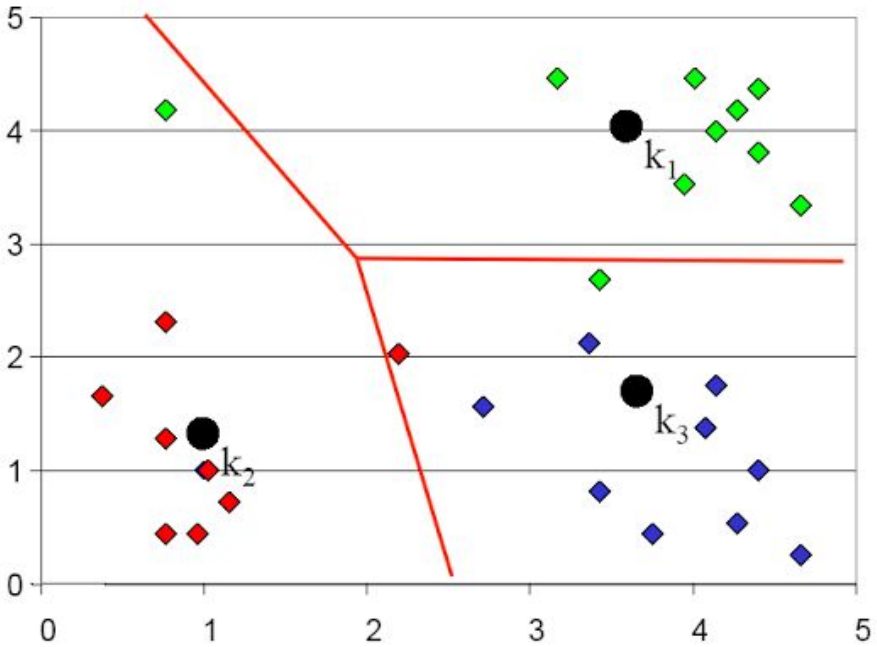
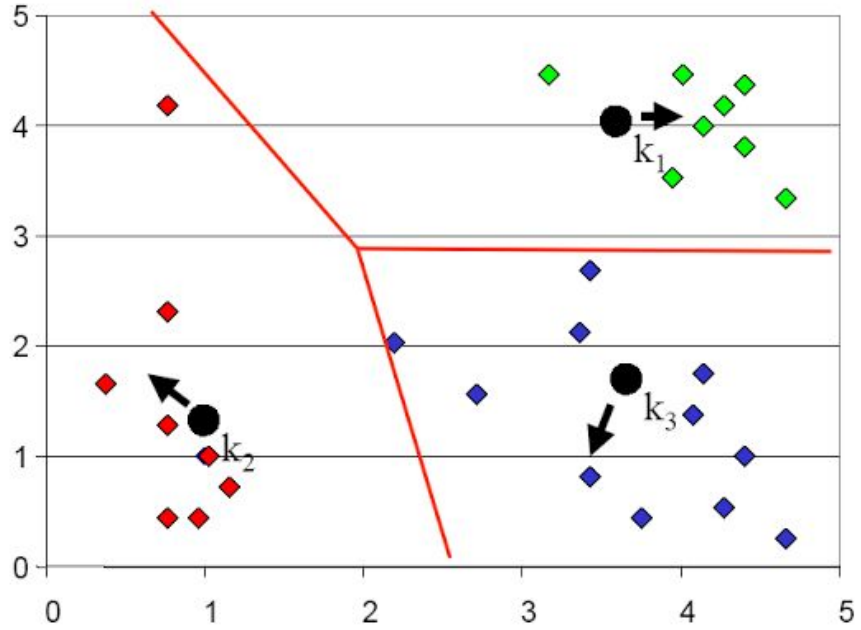


Step 3.1 again: assign all data to nearest cluster



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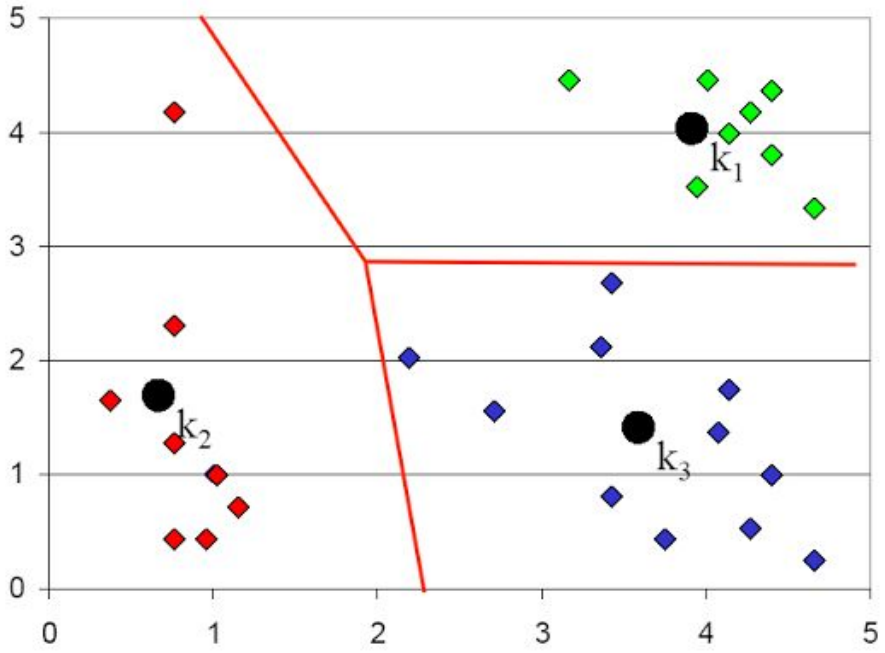
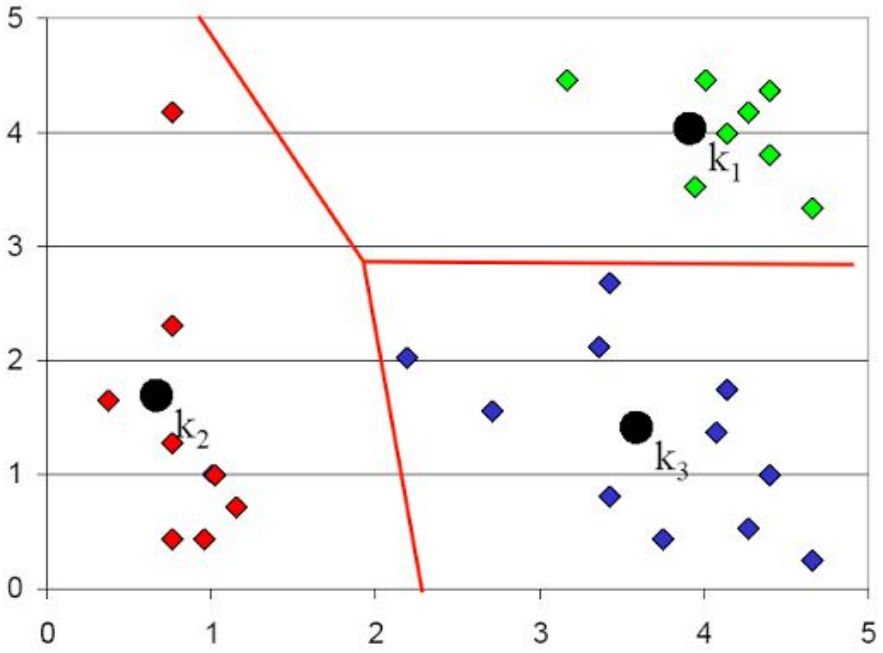
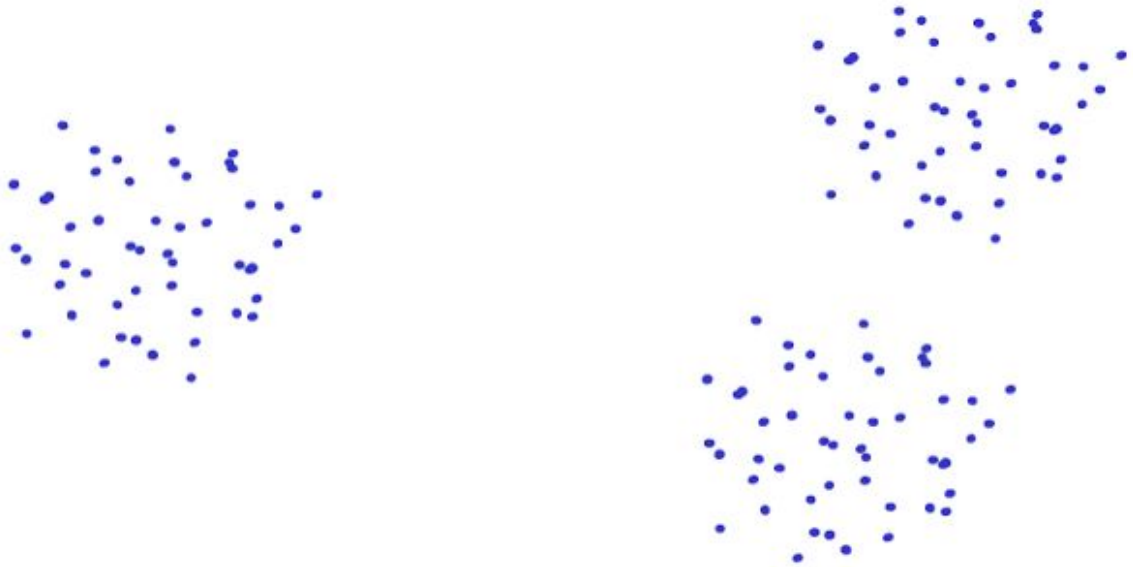


Step 4: terminate when cluster assignments don't change



K-means problems: sensitive to cluster initialization



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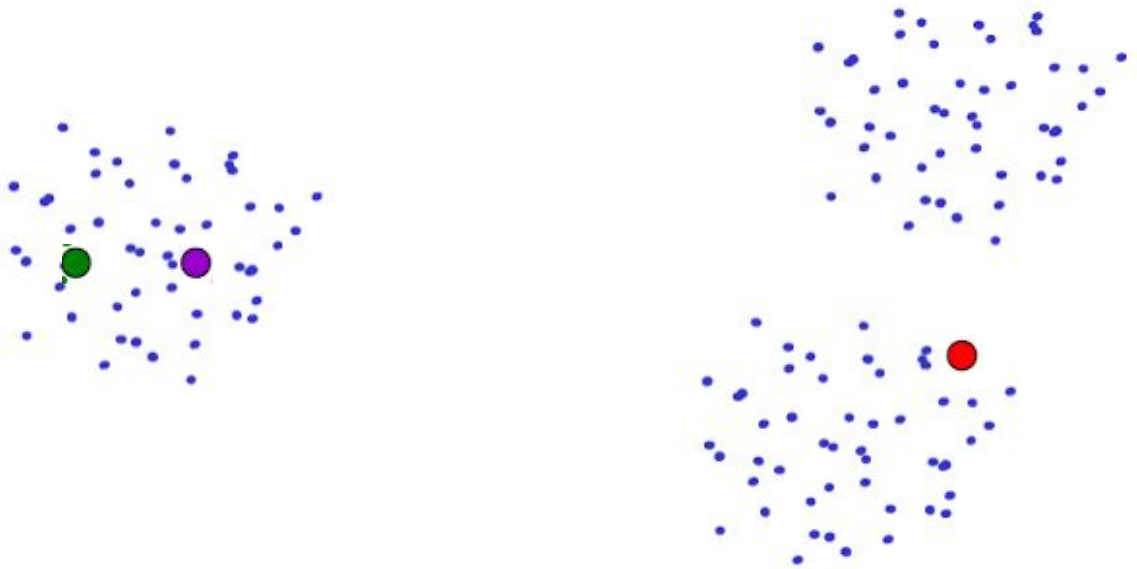

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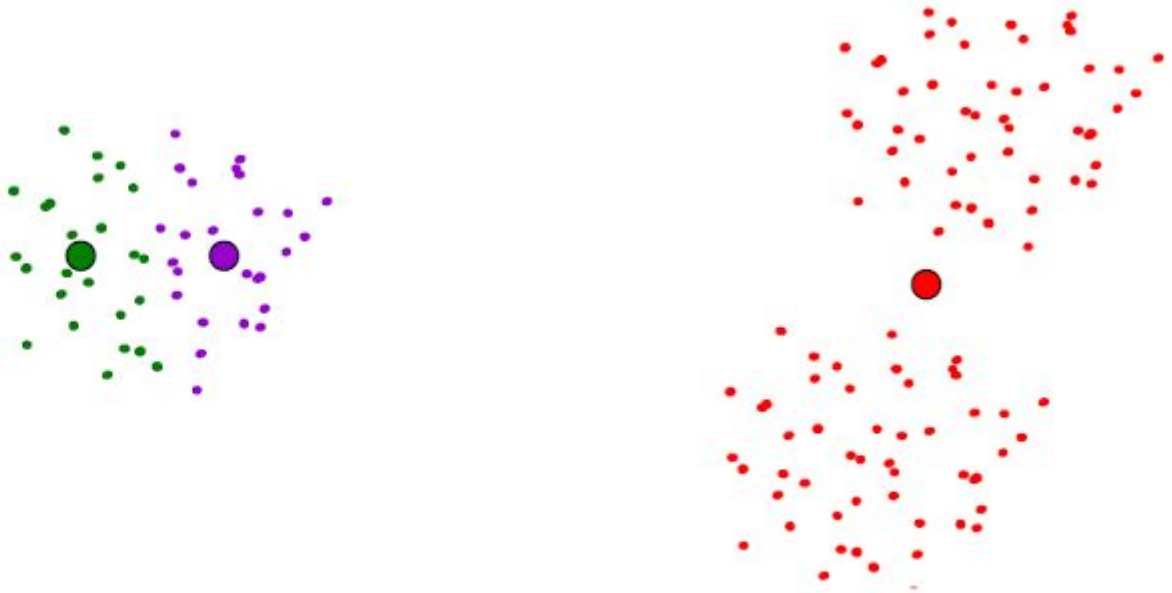

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K-means problems: sensitive to cluster initialization

- Very important to try multiple starting points for the initialization of cluster means
- Consider using k-means++ initialization
  - initializes cluster means to be generally distant from each other
  - provably better results than random initialization

K-means problems: choosing k

- Objective function: $\sum_{j=1}^{m} ||\mu_{C(j)} - x_j||^2$

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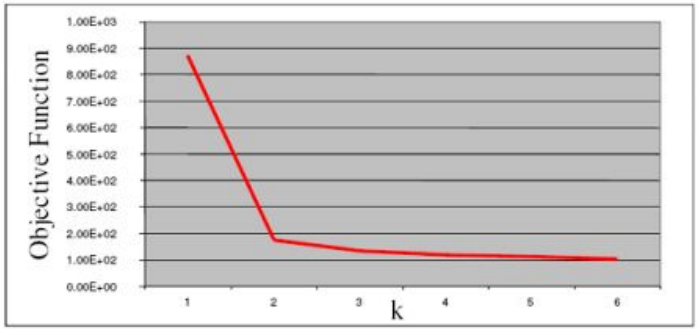

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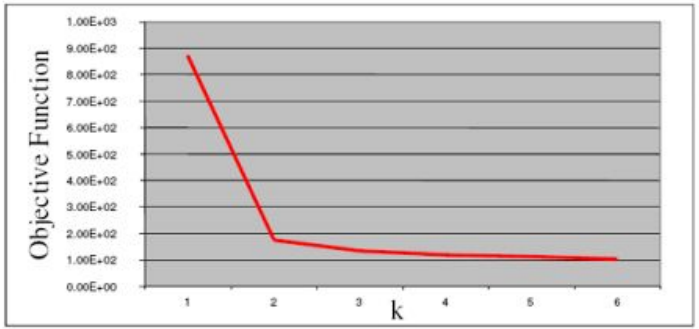

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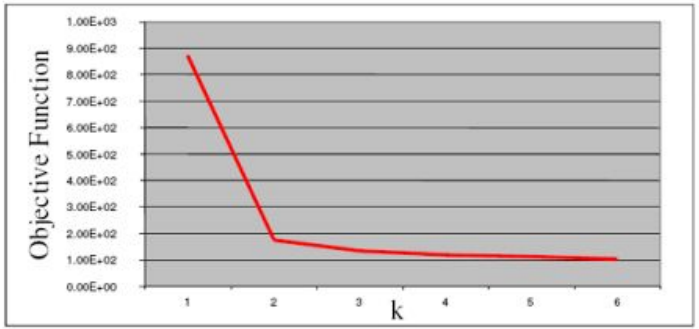
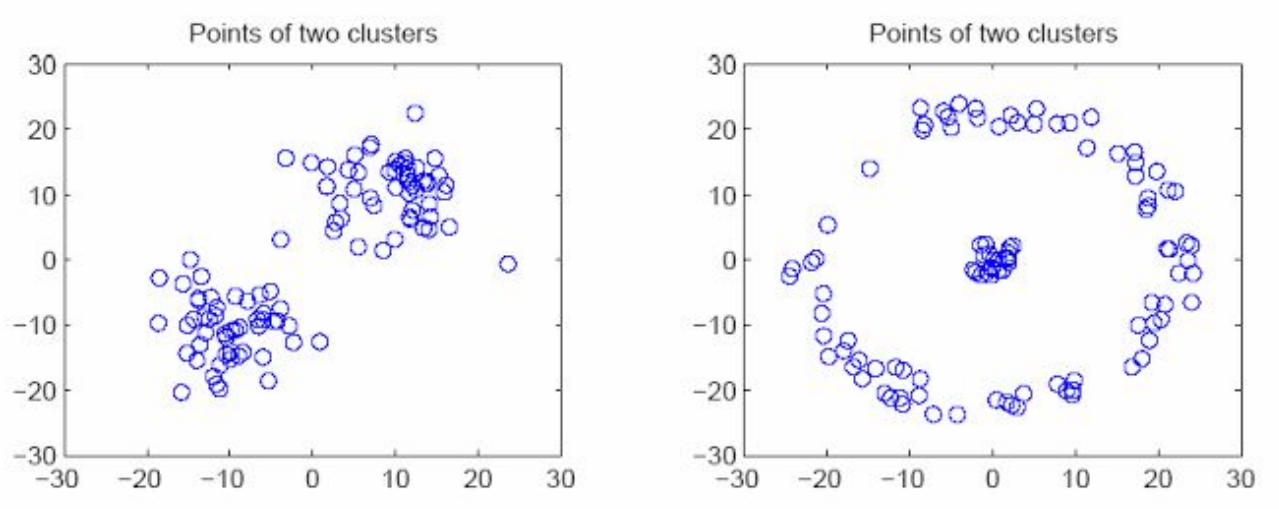


- Can we choose k by minimizing the objective over k? No! The objective will go to 0 as the number of clusters approaches the number of centers!

K-means problems: shape of clusters

- Assumes convex clusters



K-means takeaways

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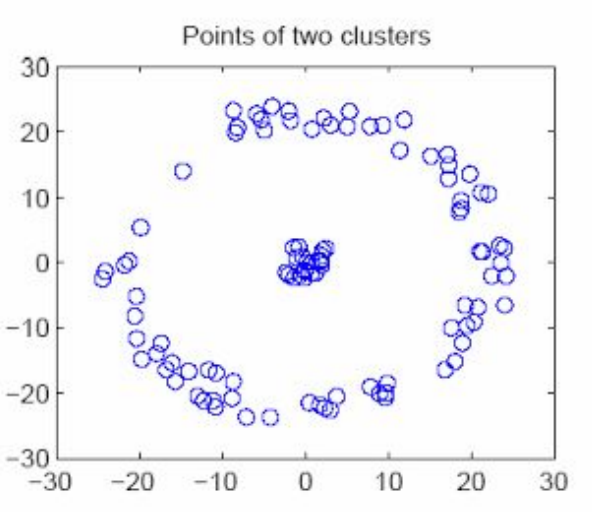
What if clusters aren’t convex?

- We can first do laplacian eigenmaps to reduce dimensionality



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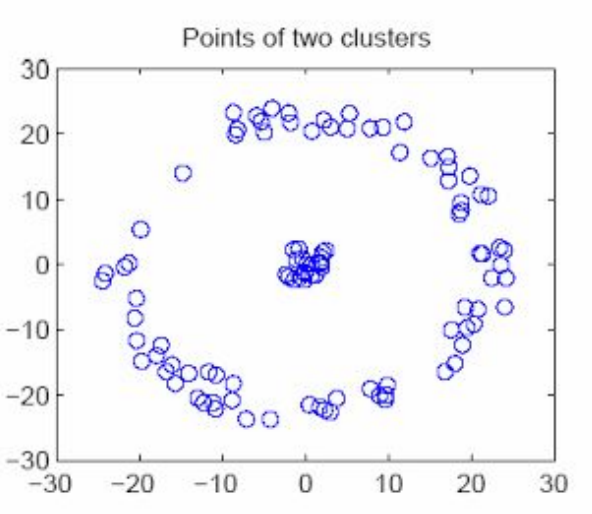
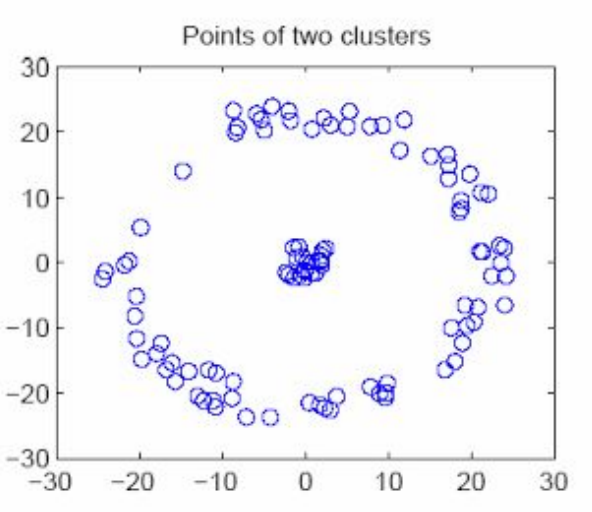


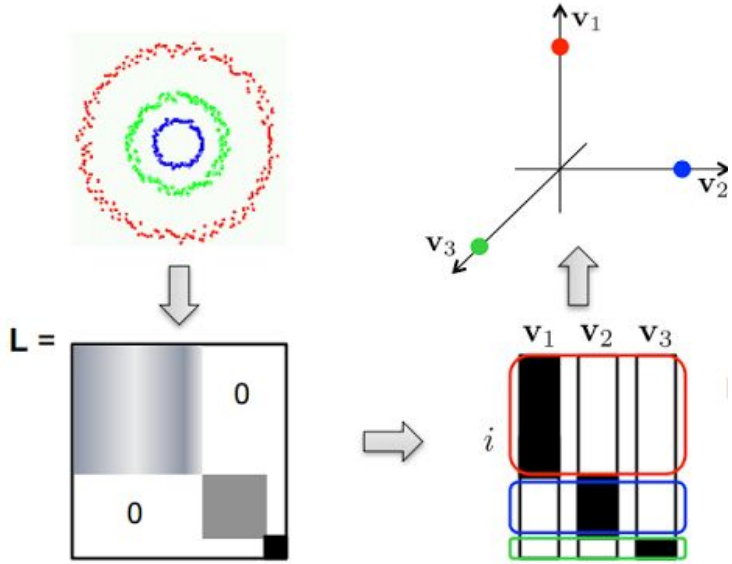
What if clusters aren’t convex?

- ❏ We can first do laplacian eigenmaps to reduce dimensionality
- ❏ Then we can do k-means on the embedded points in lower-dimension
- ❏ This is called spectral clustering



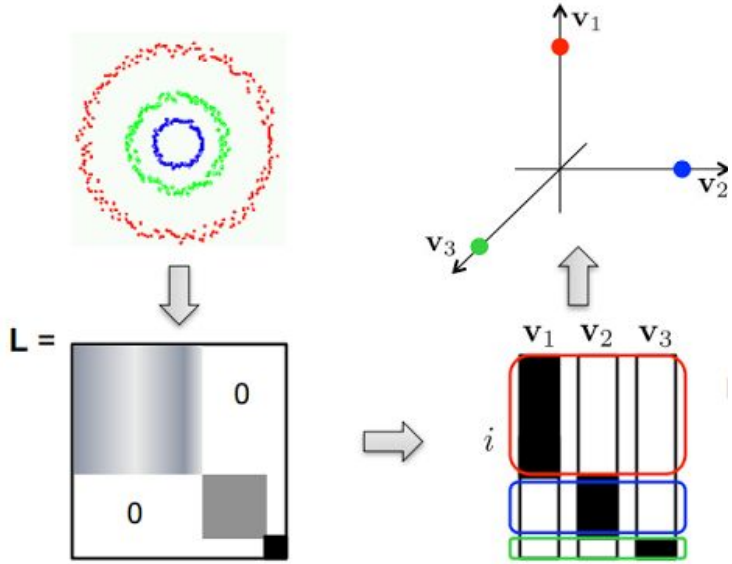
Spectral clustering: intuition

- Laplacian eigenmaps constructs a graph. If there are separable clusters, the corresponding graph should have disconnected subgraphs



Spectral clustering: intuition

- Laplacian eigenmaps constructs a graph. If there are separable clusters, the corresponding graph should have disconnected subgraphs
- Points are easy to cluster in the embedded space using k-means



Spectral clustering problems

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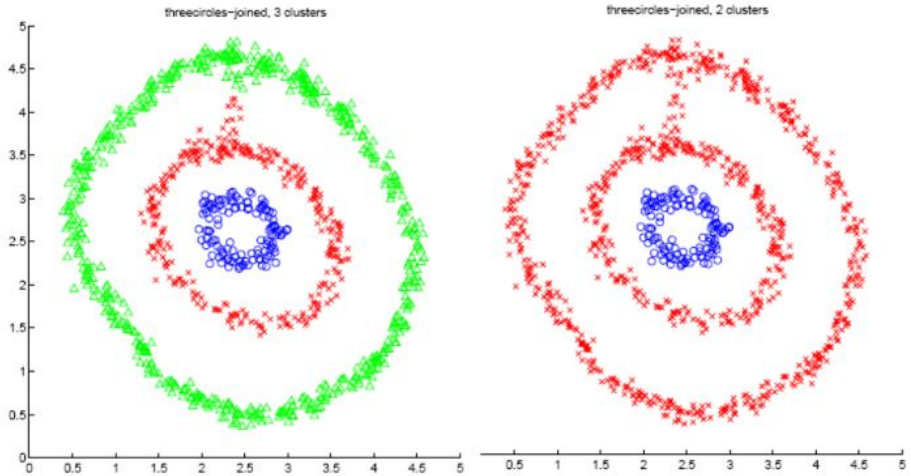
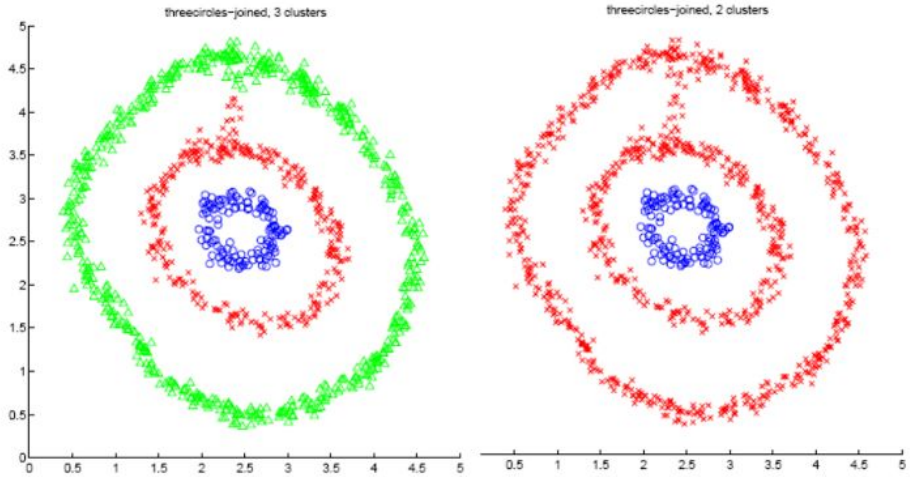


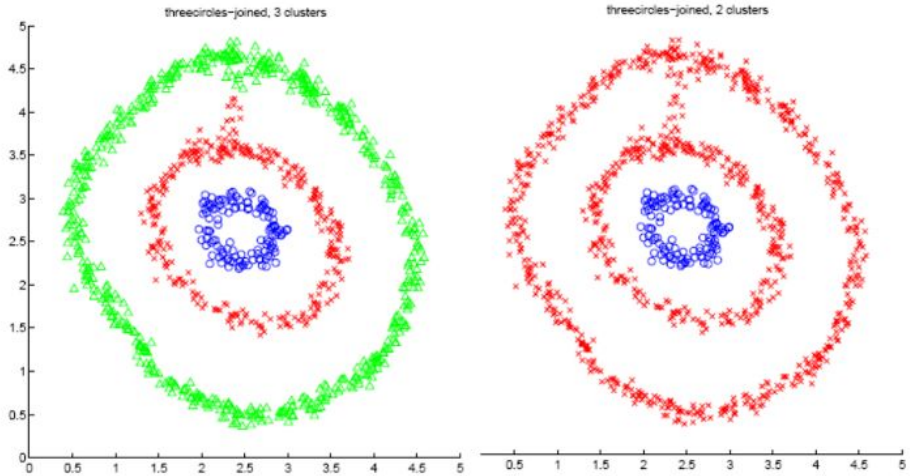
Spectral clustering problems

- ❏ Same problems as laplacian eigenmaps (choice of k for k-NN, or ε)
- ❏ Also need a way to choose number of clusters k

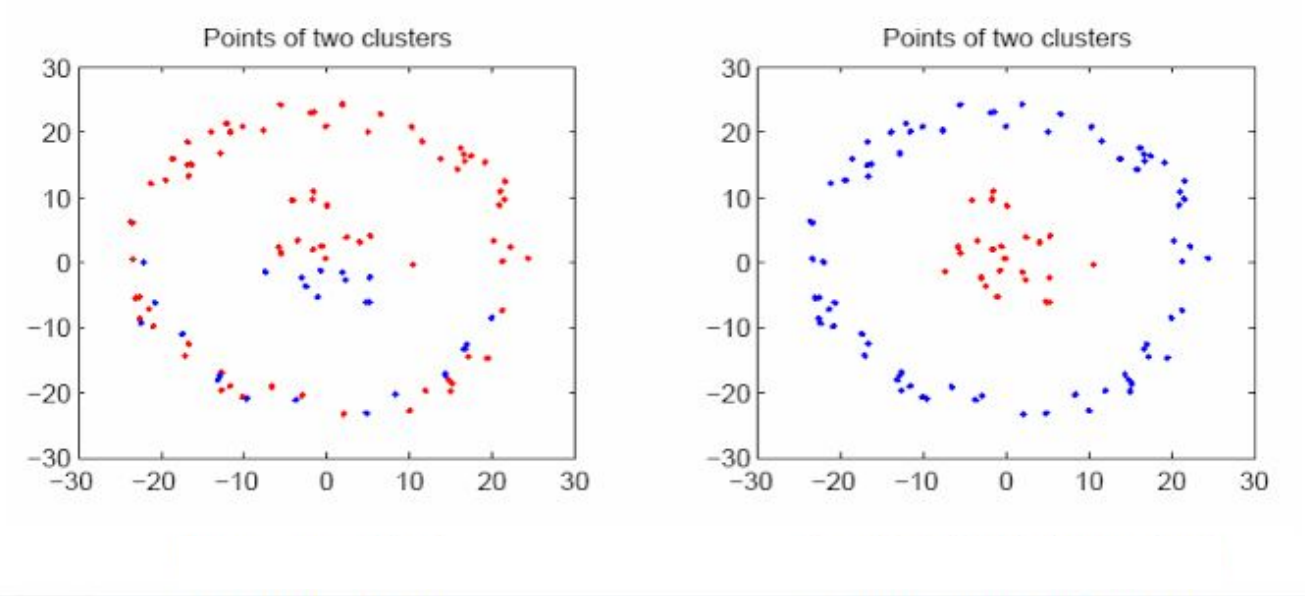


Spectral clustering problems

- Same problems as laplacian eigenmaps (choice of k for k-NN, or ε)
- Also need a way to choose number of clusters k
  - Most stable clustering is usually given by the value of k that maximizes the eigengap between consecutive eigenvalues



Spectral clustering vs k-means



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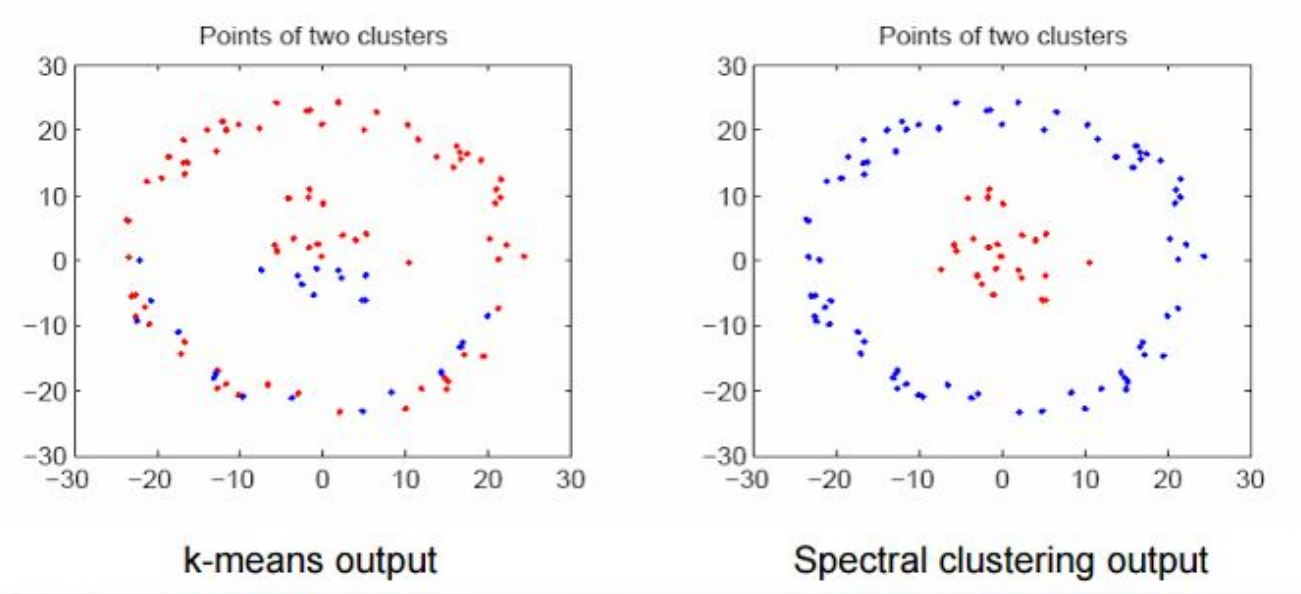

Spectral clustering takeaways

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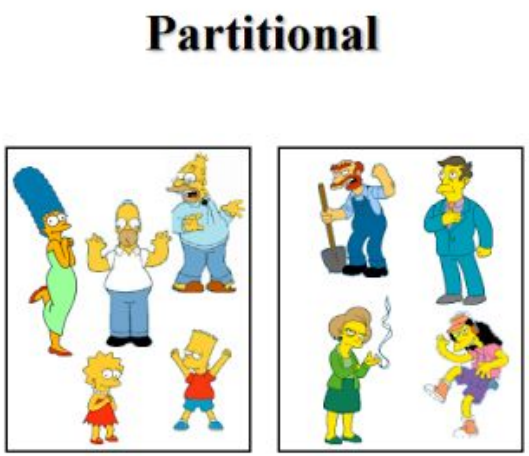
- First performs laplacian eigenmaps, and then clusters the embedded points using k-means

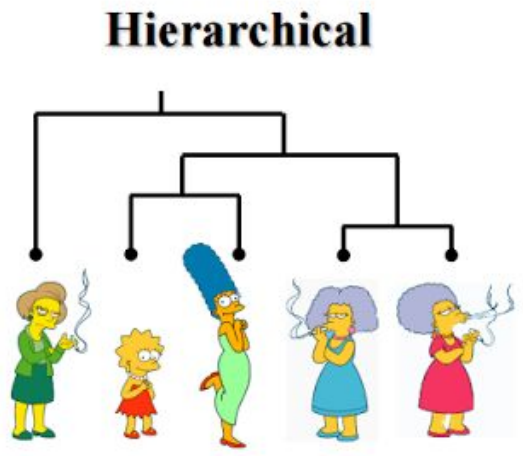
Spectral clustering takeaways

- Another type of partitional clustering
- Can deal with non-convex clusters
- First performs laplacian eigenmaps, and then clusters the embedded points using k-means
- Still need to choose the number of clusters k

Clustering algorithms divide into 2 main types

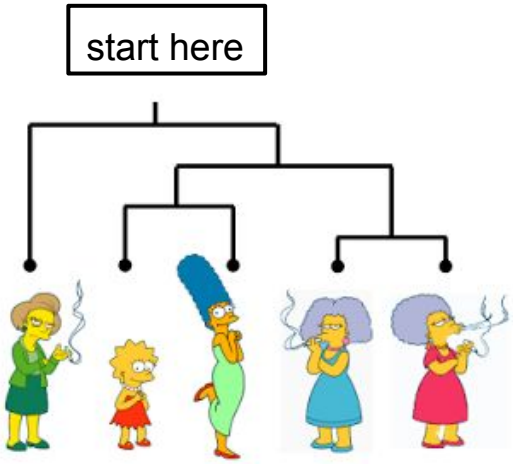
- Partitional algorithms
  - Construct various partitions and then evaluate the partitions by some criterion
- **Hierarchical algorithms**
  - **Create a hierarchical decomposition of the set of objects using some criterion**





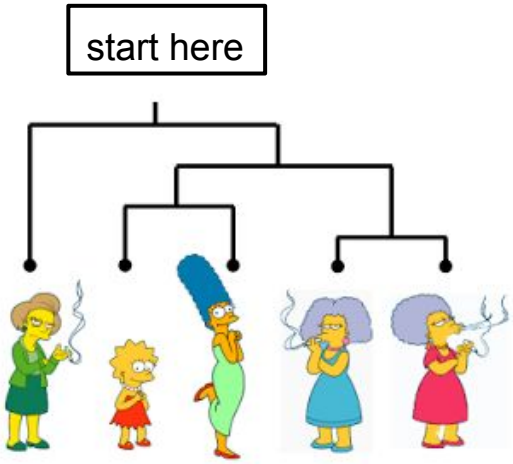
Hierarchical clustering: 2 types

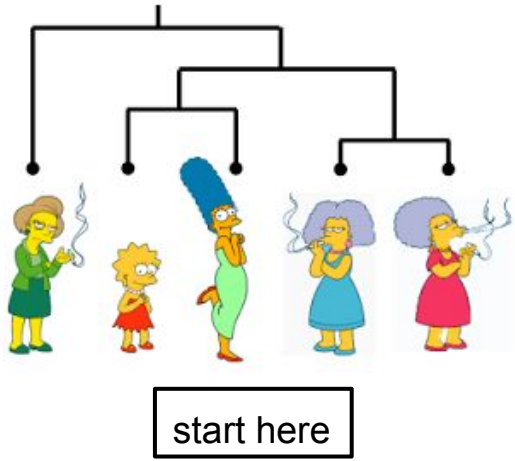
- Divisive (top-down)



Hierarchical clustering: 2 types

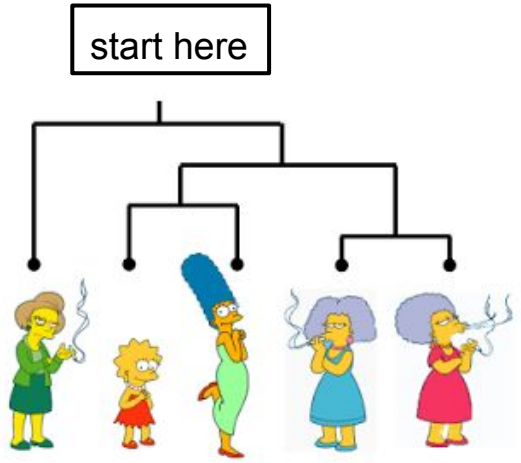
- Divisive (top-down)
- Agglomerative (bottom-up)





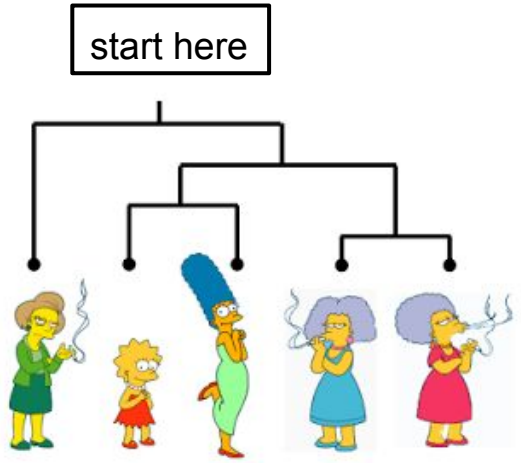
Divisive hierarchical clustering (top-down)

- Step 1: start with all data in one cluster



Divisive hierarchical clustering (top-down)

- Step 1: start with all data in one cluster
- Step 2: split cluster using a partitional clustering method



Divisive hierarchical clustering (top-down)

- Step 1: start with all data in one cluster
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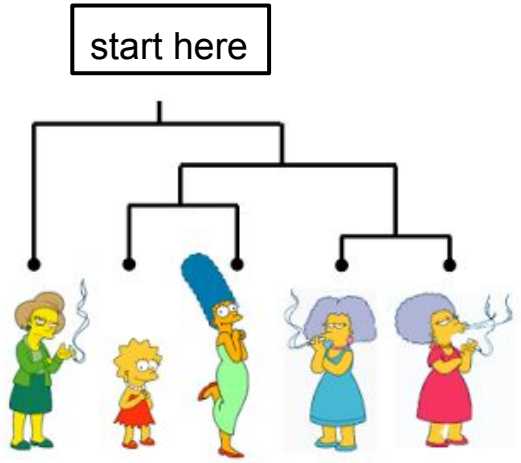

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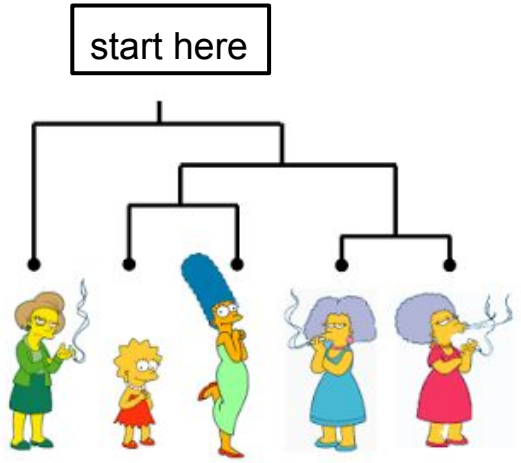

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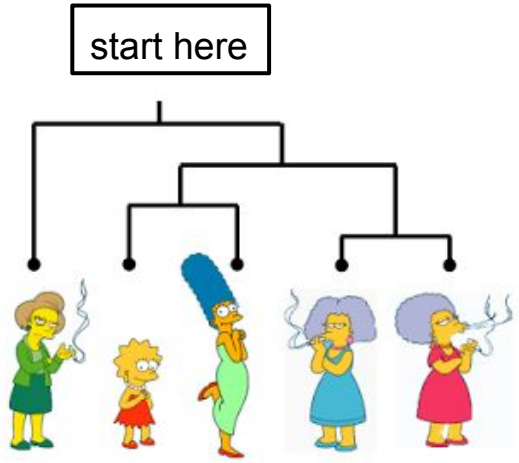

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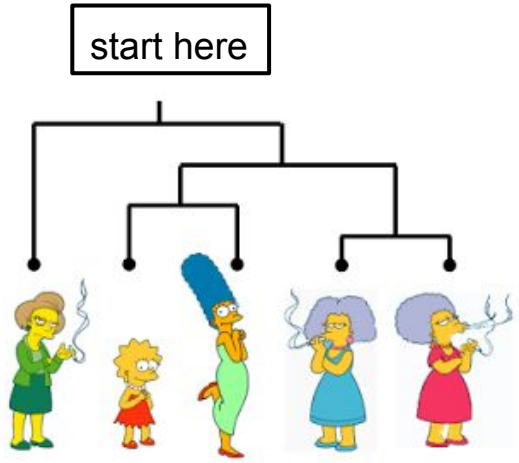

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- Benefits from global information
- Can be efficient if:
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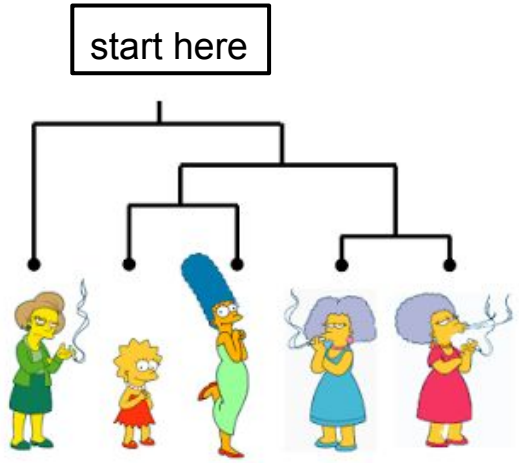
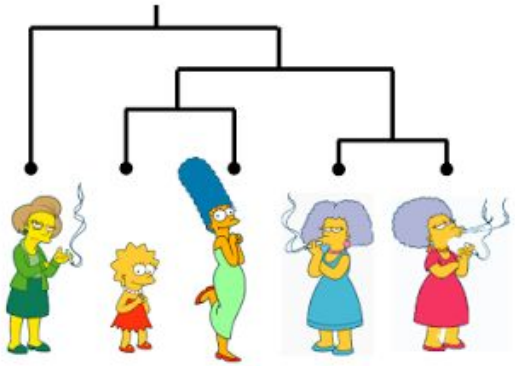
  - Use an efficient partitional method (like k-means)



Agglomerative clustering (bottom-up)

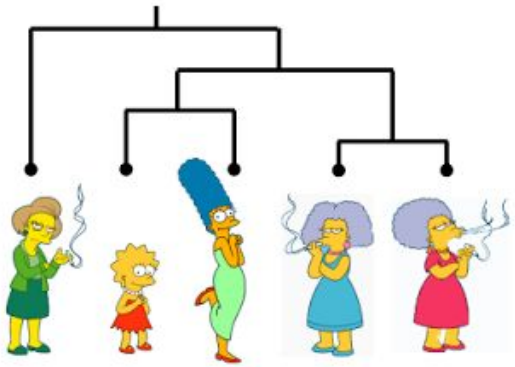
- Step 1: start with each item in own cluster



start here

Agglomerative clustering (bottom-up)

- Step 1: start with each item in own cluster
- Step 2: find best pair to merge into a new cluster



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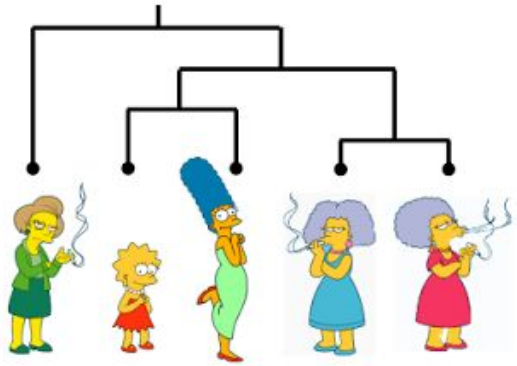
Agglomerative clustering (bottom-up)

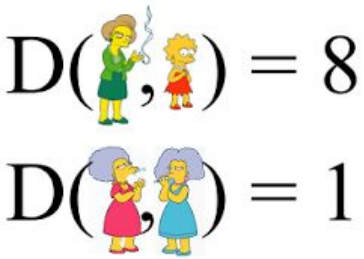
- Step 1: start with each item in own cluster
- Step 2: find best pair to merge into a new cluster
- Step 3: repeat step 2 until all clusters are fused together

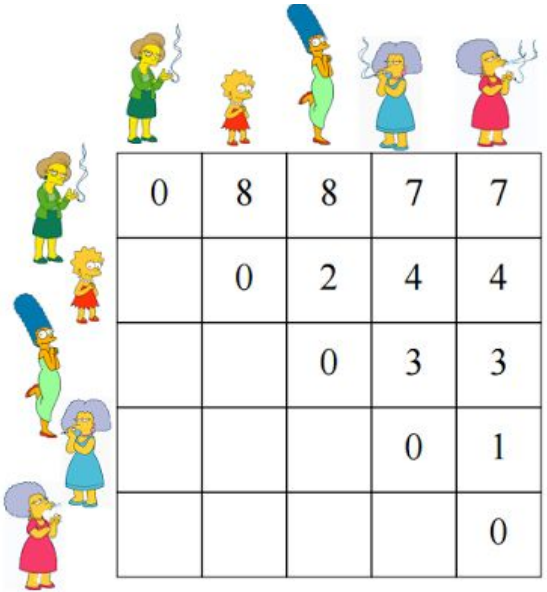


start here

But how do we find the best data points to merge?

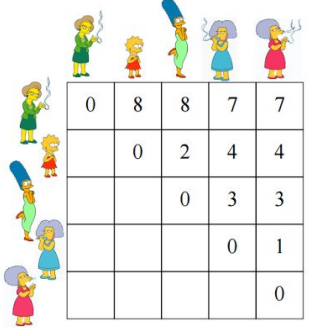
- Start with a distance matrix that contains the distances between every pair of data instances





0	8	8	7	7
	0	2	4	4
		0	3	3
			0	1
				0

Step 2: find the best pair to merge in a cluster



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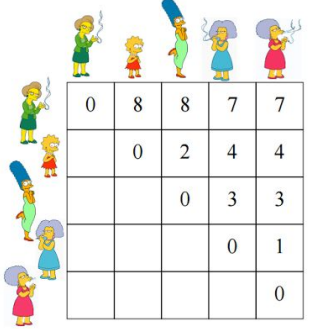

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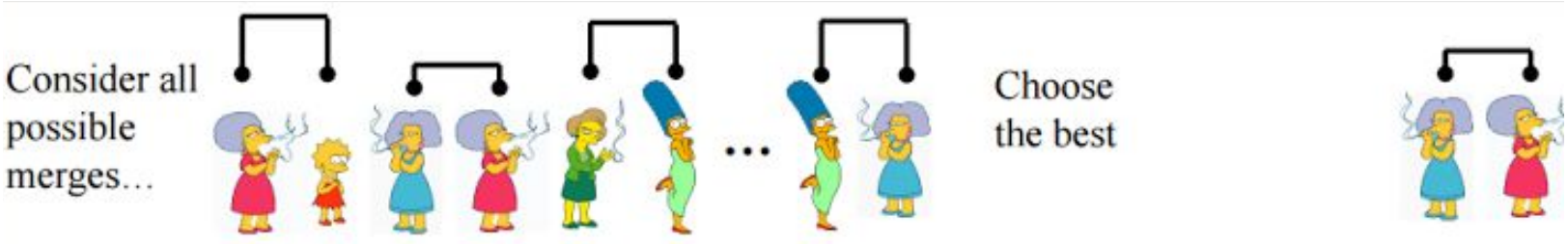
		0	3	3
			0	1
				0



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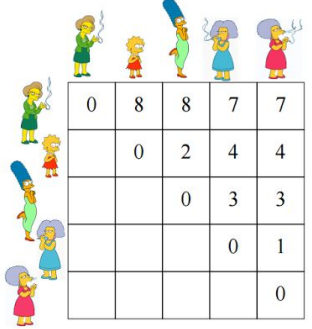

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	0	2	4	4
		0	3	3
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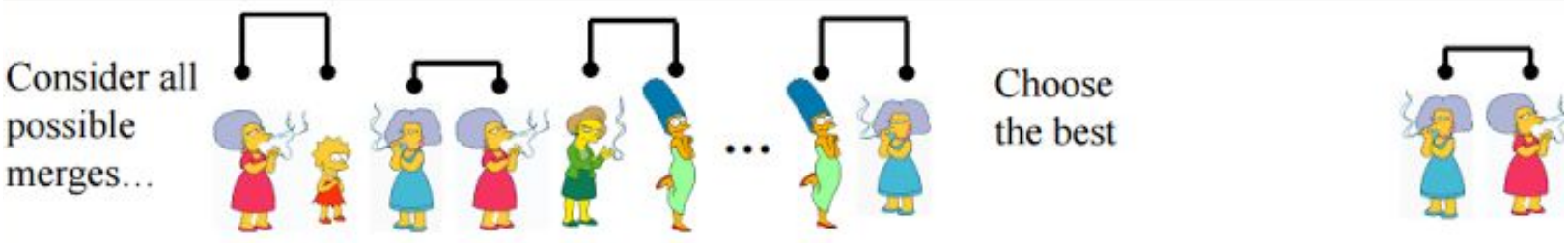

How do we compute distances between clusters?

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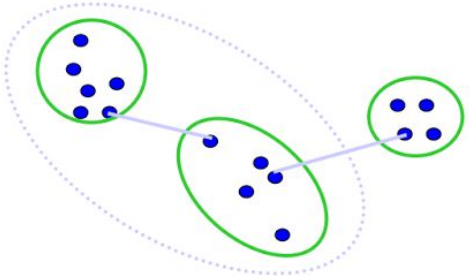

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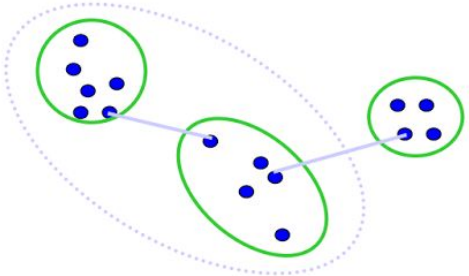
  - potentially long and skinny clusters



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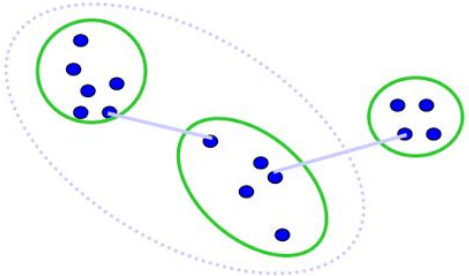

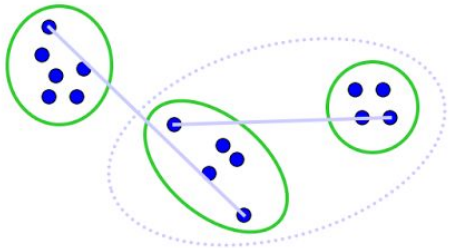

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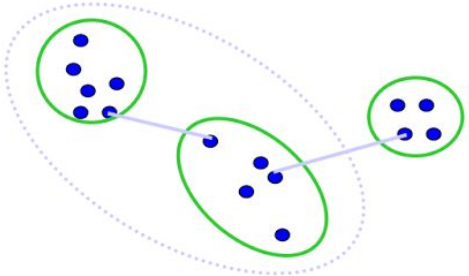
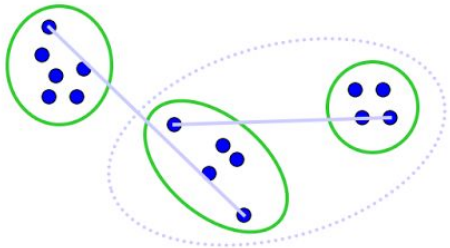
  - “complete link”
  - tight clusters





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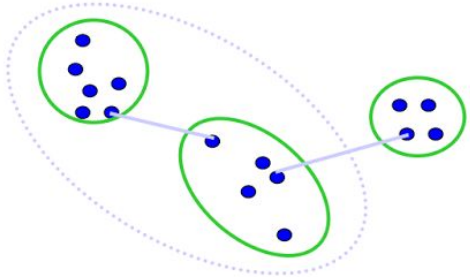
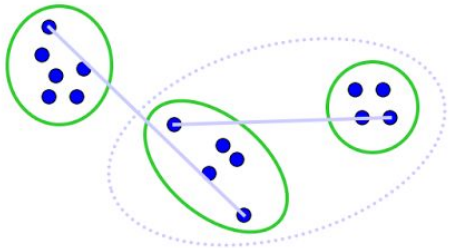
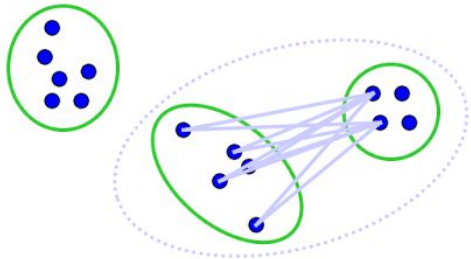
  - tight clusters
- Average distance of all pairs
  - “average link”







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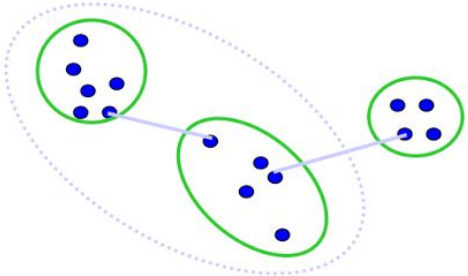

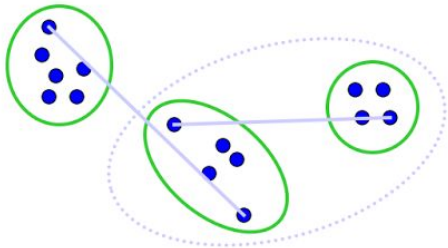

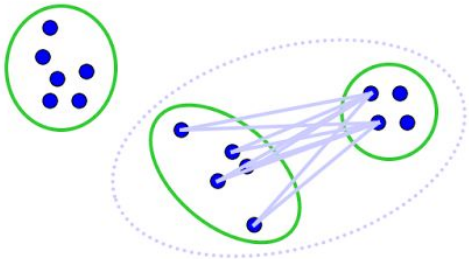

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  - “complete link”
  - tight clusters
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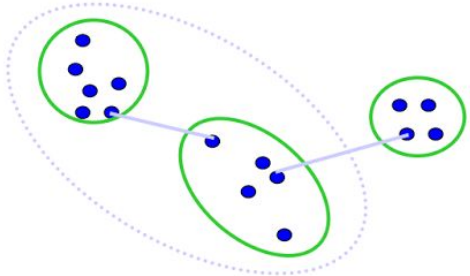
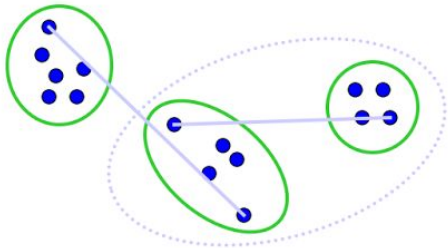
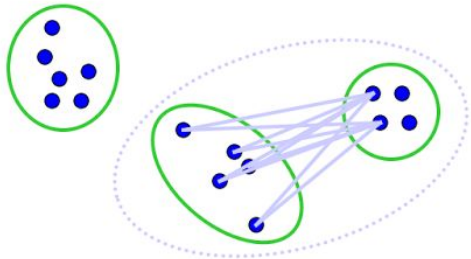
  - “average link”
  - robust against noise
  - most widely used







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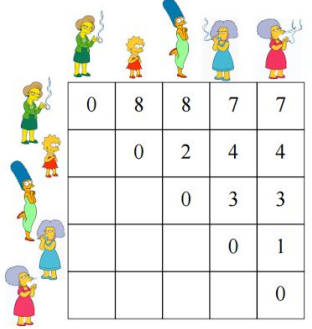

0	8	8	7	7
	0	2	4	4
		0	3	3
			0	1
				0

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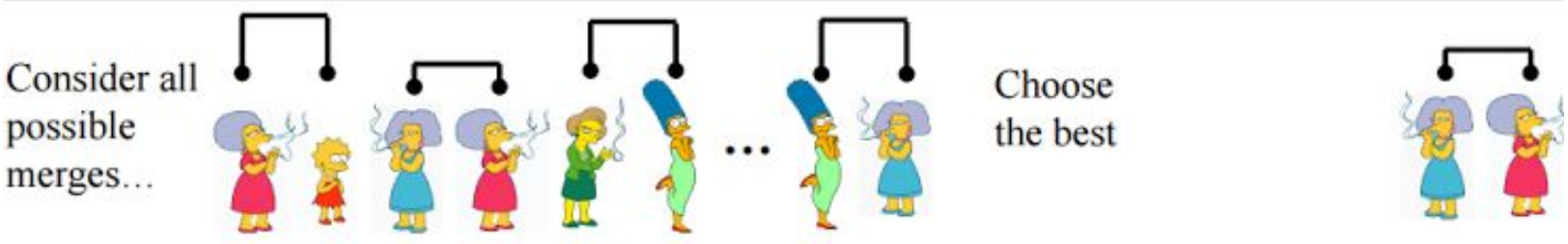

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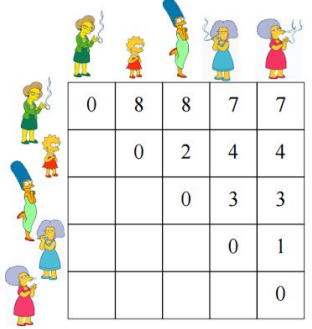

0	8	8	7	7
	0	2	4	4
		0	3	3
			0	1
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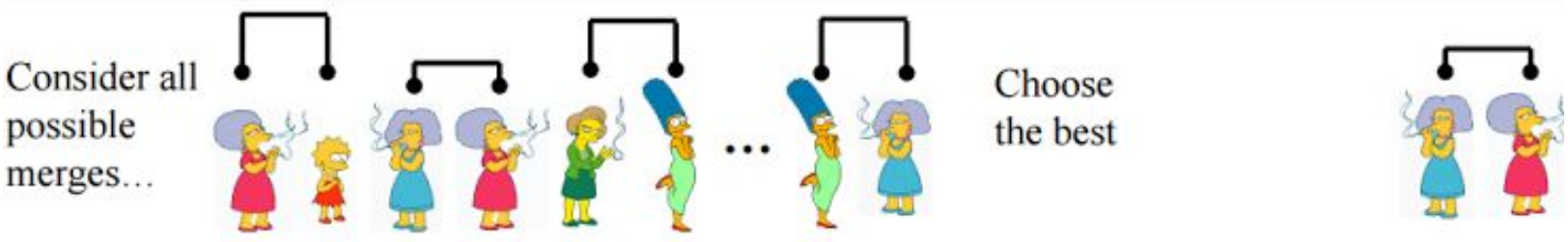
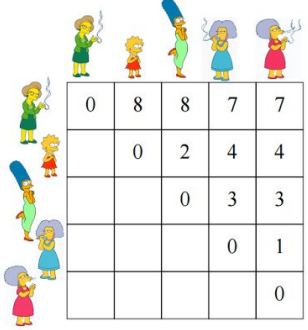
Now what? How do we compute distances between clusters with multiple data instances? => **use complete link!**





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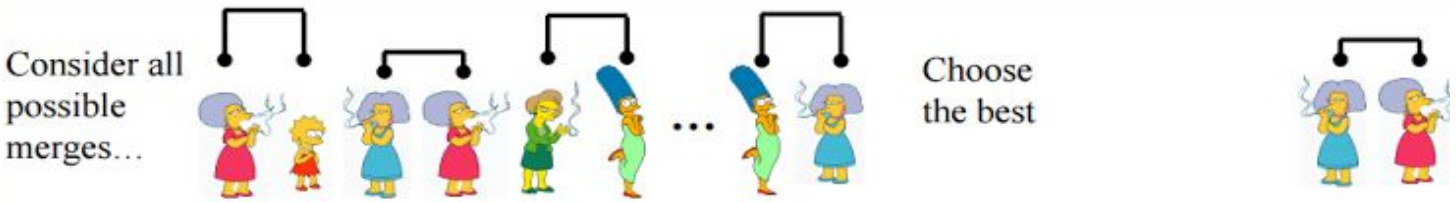

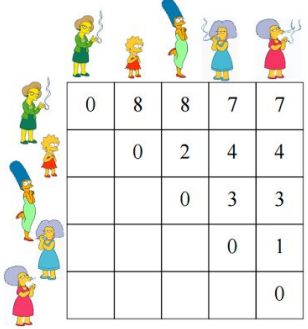

0	8	8	7	7
	0	2	4	4
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			0	1
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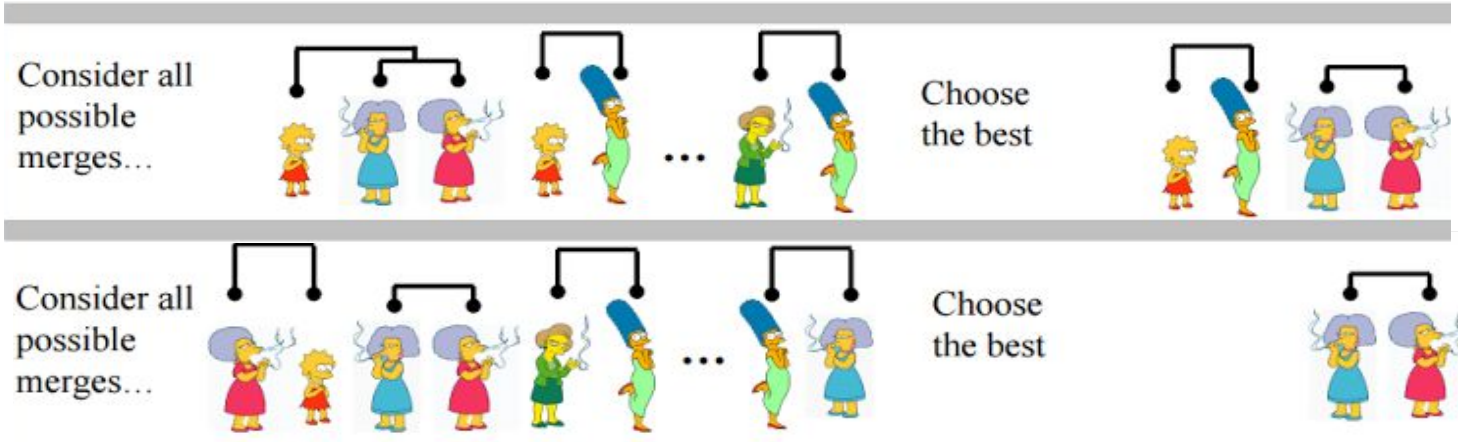

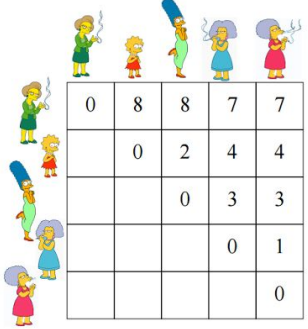

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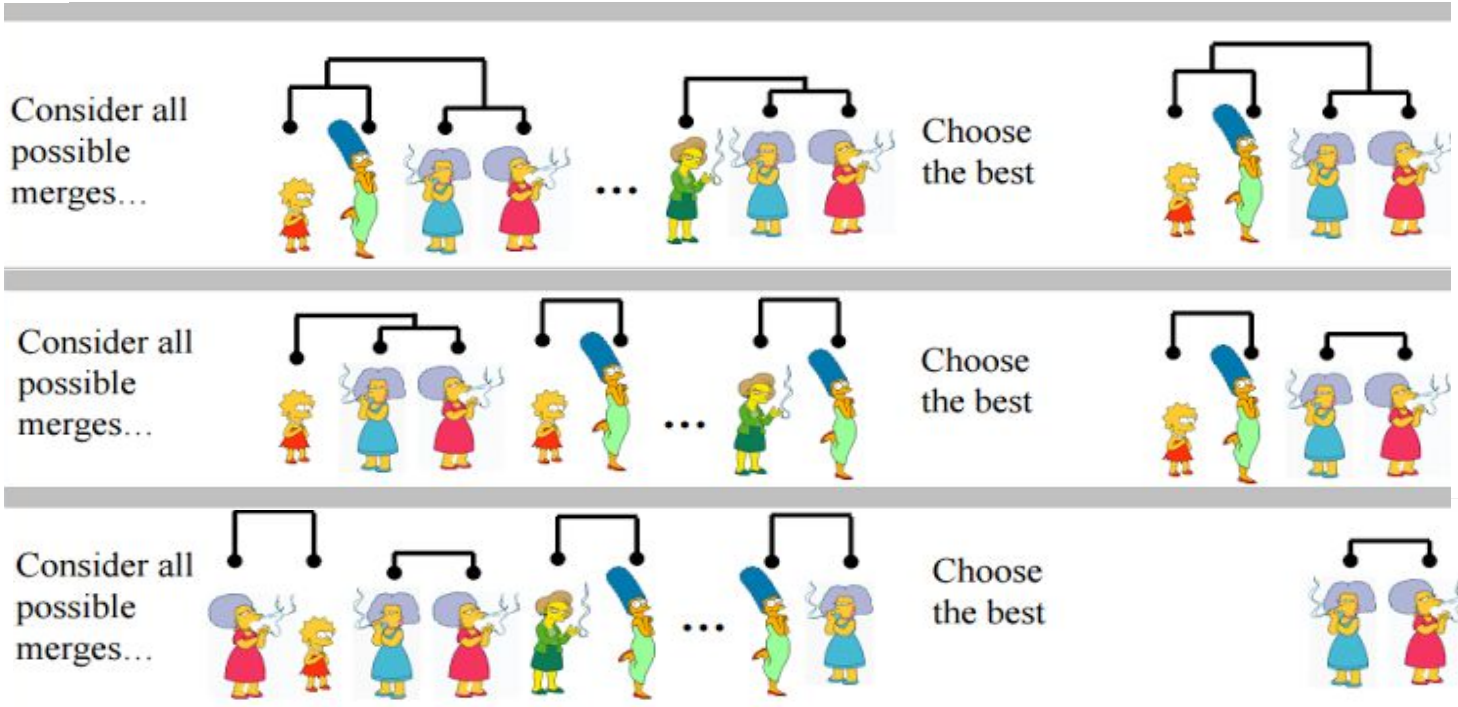

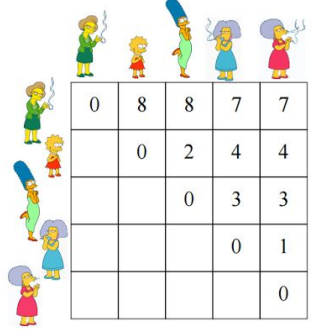

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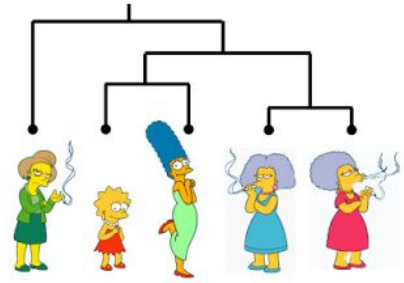
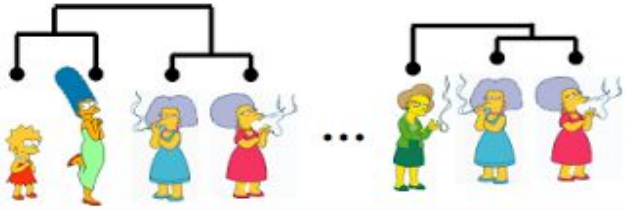
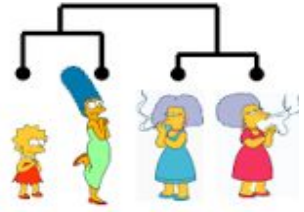


Consider all possible merges…



Choose the best



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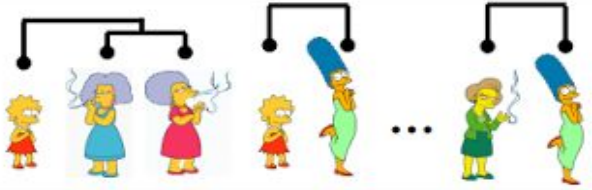

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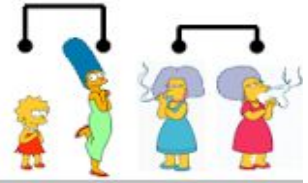

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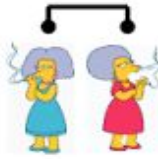

Hierarchical clustering takeaways

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- But we don’t have to specify number of clusters apriori

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- Both are unsupervised methods that can be used when no labeled data is available

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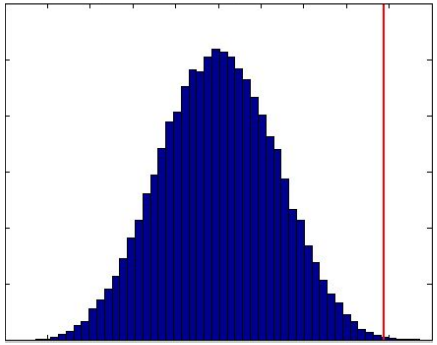
- Clustering can group different data instances without much domain knowledge

Next time: advanced topics!



- Evaluate results
  - cross validation (how generalizable are our results?)
  - nearly assumption-free significance testing (are the results different from chance?)
- **Complex data-driven hypotheses of brain processing**
  - **advanced topics: latent variable models, reinforcement learning, deep learning**