
Photo by Unsplash user @foodiesfeed

BBM406

Fundamentals of Machine Learning

Lecture 22:

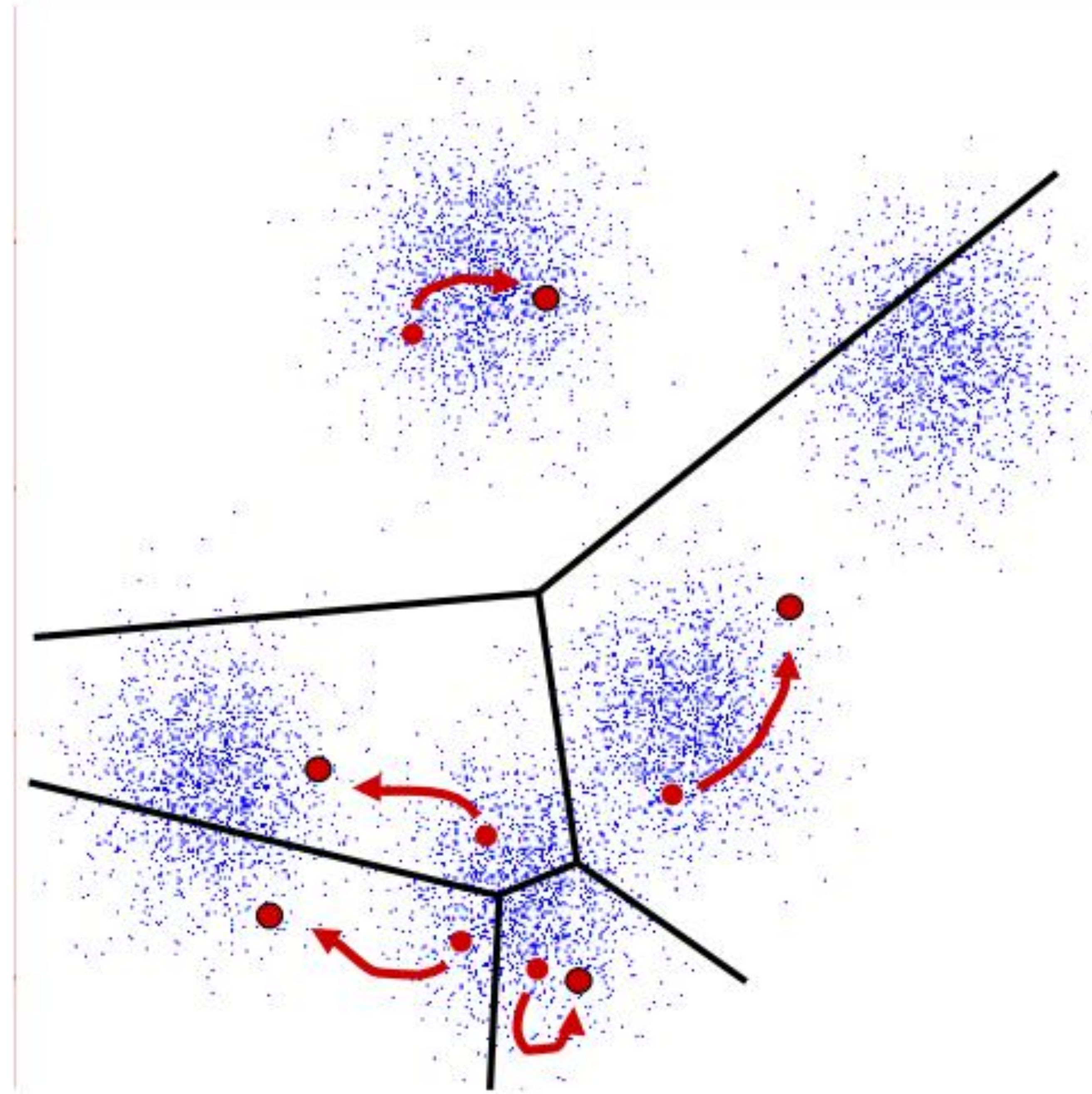
K-Means Example Applications
Spectral clustering
Hierarchical clustering
What is a good clustering?

HACETTEPE UNIVERSITY COMPUTER VISION LAB

Aykut Erdem // Hacettepe University // Fall 2019

Last time… **K-Means**

- An iterative clustering algorithm
  - Initialize: Pick *K* random points as cluster centers (means)
  - Alternate:
    - Assign data instances to closest mean
    - Assign each mean to the average of its assigned points
  - Stop when no points' assignments change



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Today

- K-Means Example Applications
- Spectral clustering
- Hierarchical clustering
- What is a good clustering?

K-Means
Example Applications

Example: K-Means for Segmentation

K=2

Original

Goal of Segmentation is to partition an image into regions each of which has reasonably homogenous visual appearance.

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Example: K-Means for Segmentation

K=2

K=3

Original

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Example: K-Means for Segmentation

K=2 K=3 K=10 Original

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Example: Vector quantization

FIGURE 14.9. *Sir Ronald A. Fisher (1890 – 1962) was one of the founders of modern day statistics, to whom we owe maximum-likelihood, sufficiency, and many other fundamental concepts. The image on the left is a* 1024×1024 *grayscale image at* 8 *bits per pixel. The center image is the result of* 2×2 *block VQ, using* 200 *code vectors, with a compression rate of* 1.9 *bits/pixel. The right image uses only four code vectors, with a compression rate of* 0.50 *bits/pixel*

[Figure from Hastie *et al.* book]

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Example: Simple Linear Iterative Clustering (SLIC) superpixels

$$\Psi(x, y) = \begin{bmatrix} \lambda x \\ \lambda y \\ I(x, y) \end{bmatrix}$$

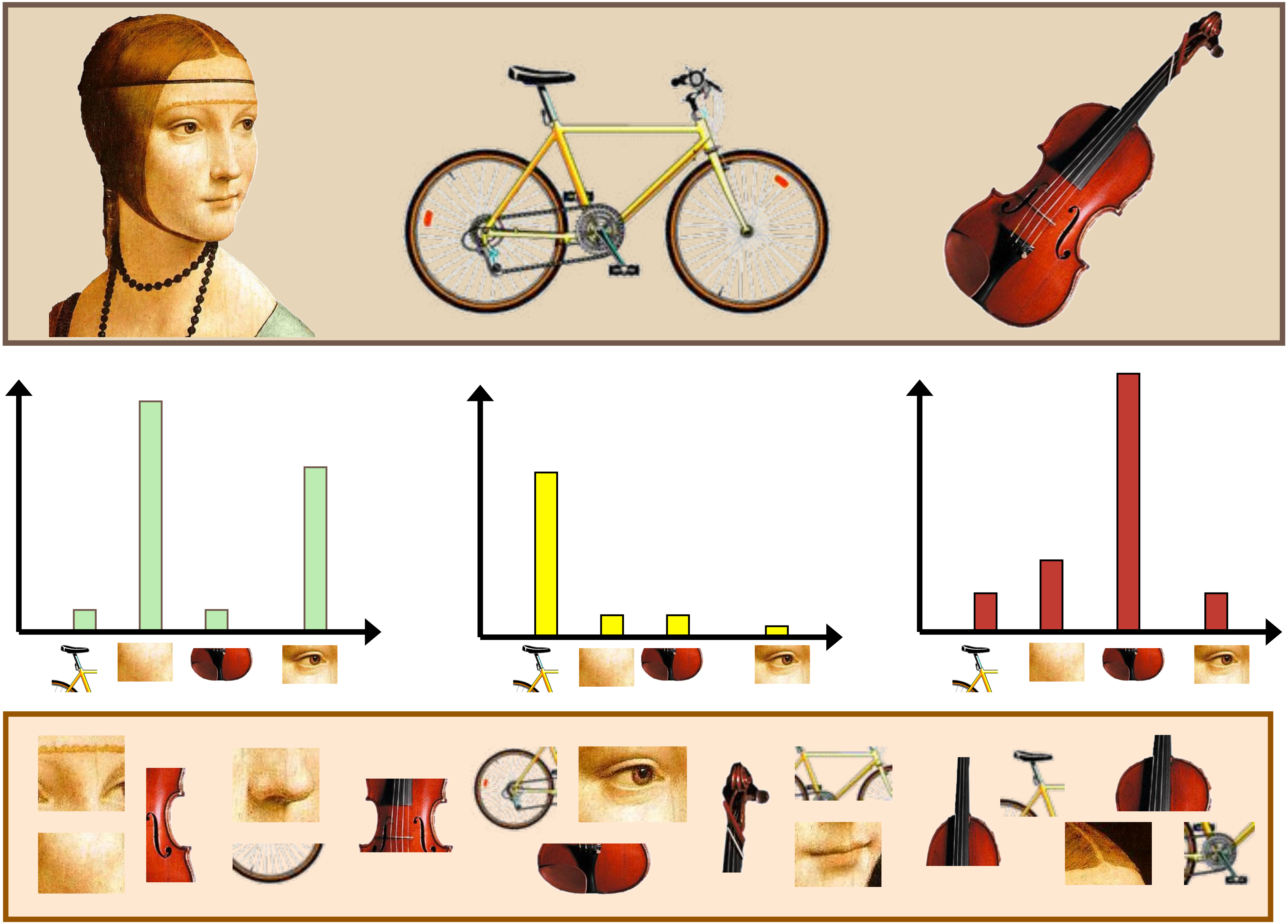
λ: spatial regularization parameter

R. Achanta, A. Shaji, K. Smith, A. Lucchi, P. Fua, and S. Susstrunk SLIC Superpixels Compared to State-of-the-art Superpixel Methods, IEEE T-PAMI, 2012

Bag of Words model

aardvark	0
about	2
all	2
Africa	1
apple	0
anxious	0
...	
gas	1
...	
oil	1
…	
Zaire	0

slide by Carlos Guestrin



slide by Fei Fei Li

Object → Bag of 'words'

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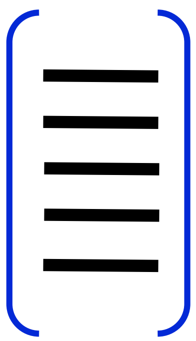
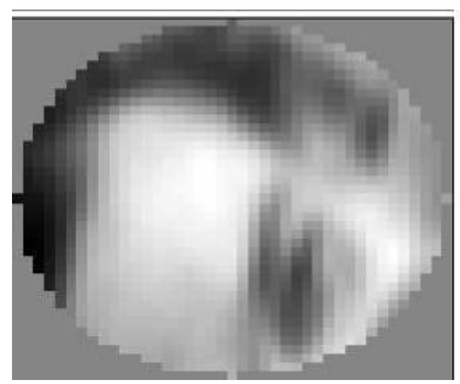
Interest Point Features

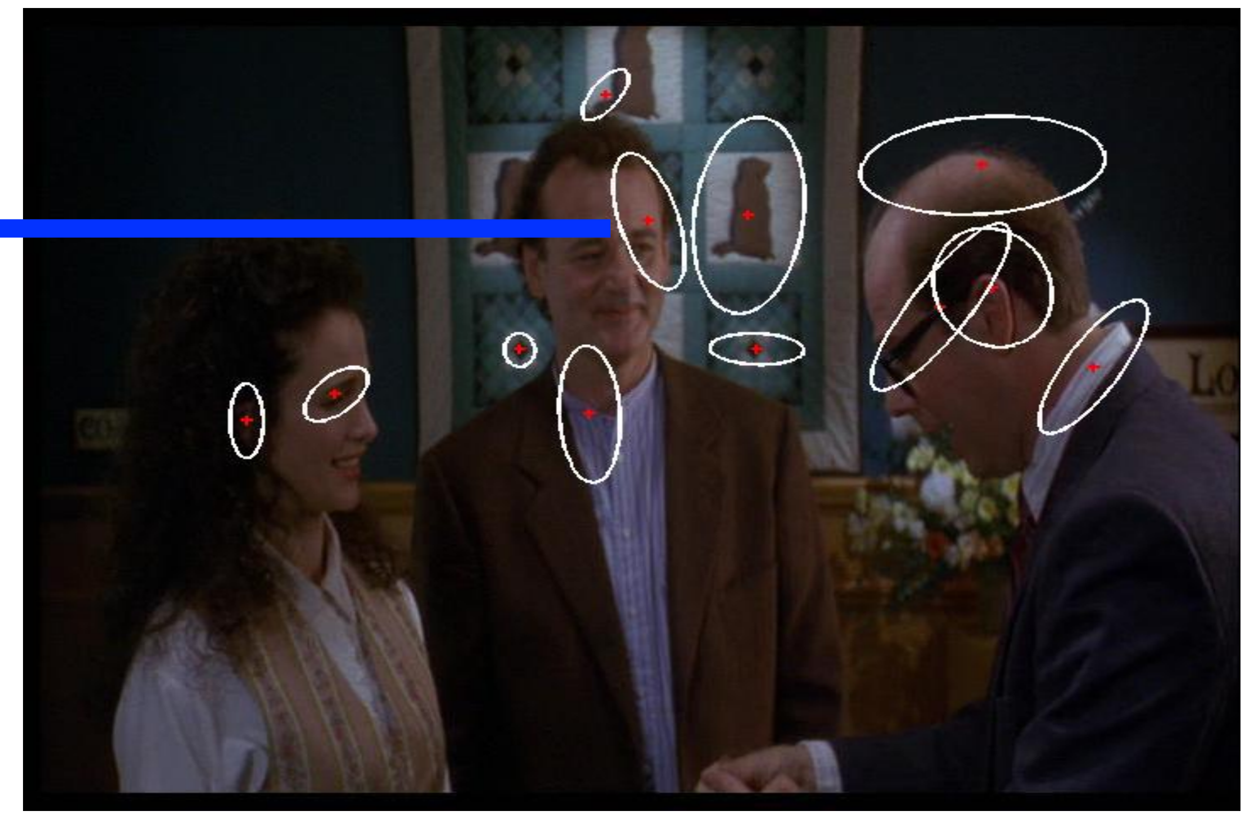


Compute SIFT descriptor

[Lowe'99]



Normalize patch



Detect patches

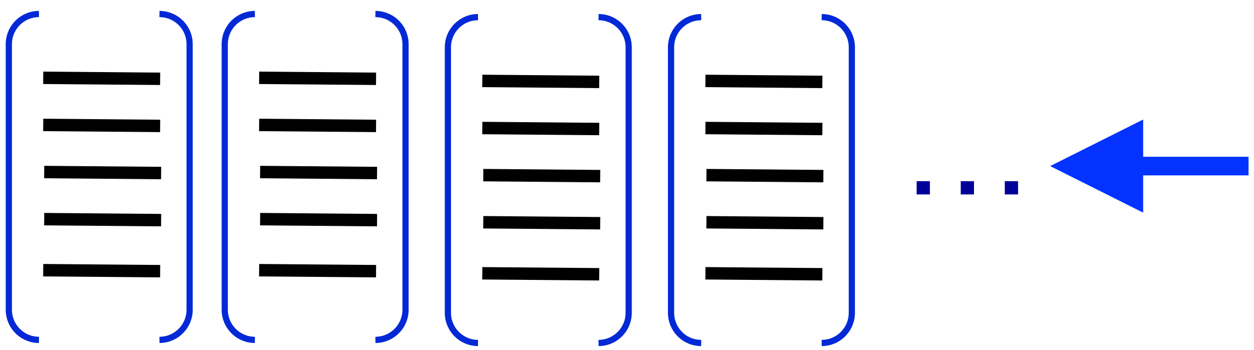
[Mikojaczyk and Schmid '02]

[Matas et al. '02]

[Sivic et al. '03]

slide by Josef Sivic

Patch Features



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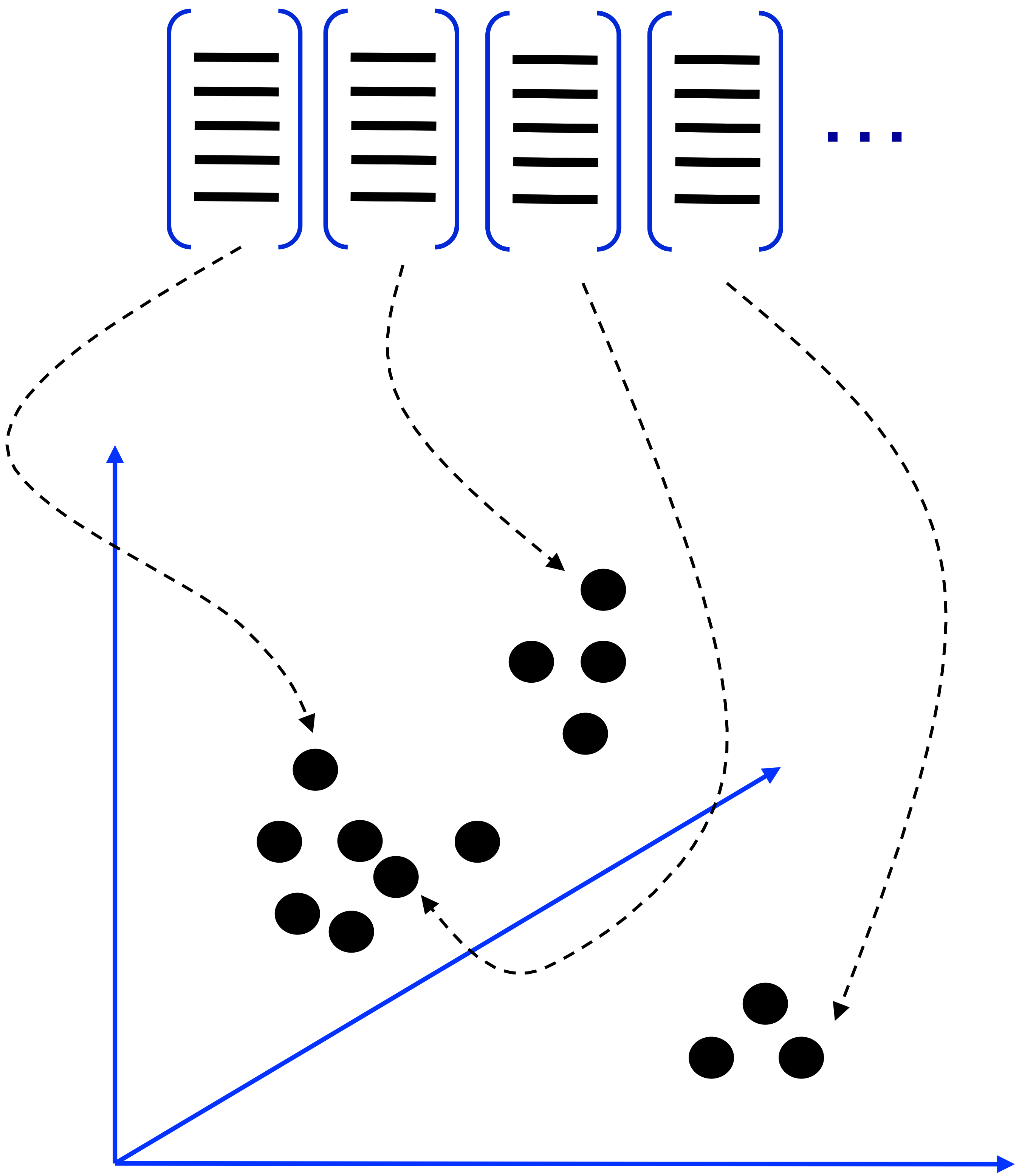
Dictionary Formation



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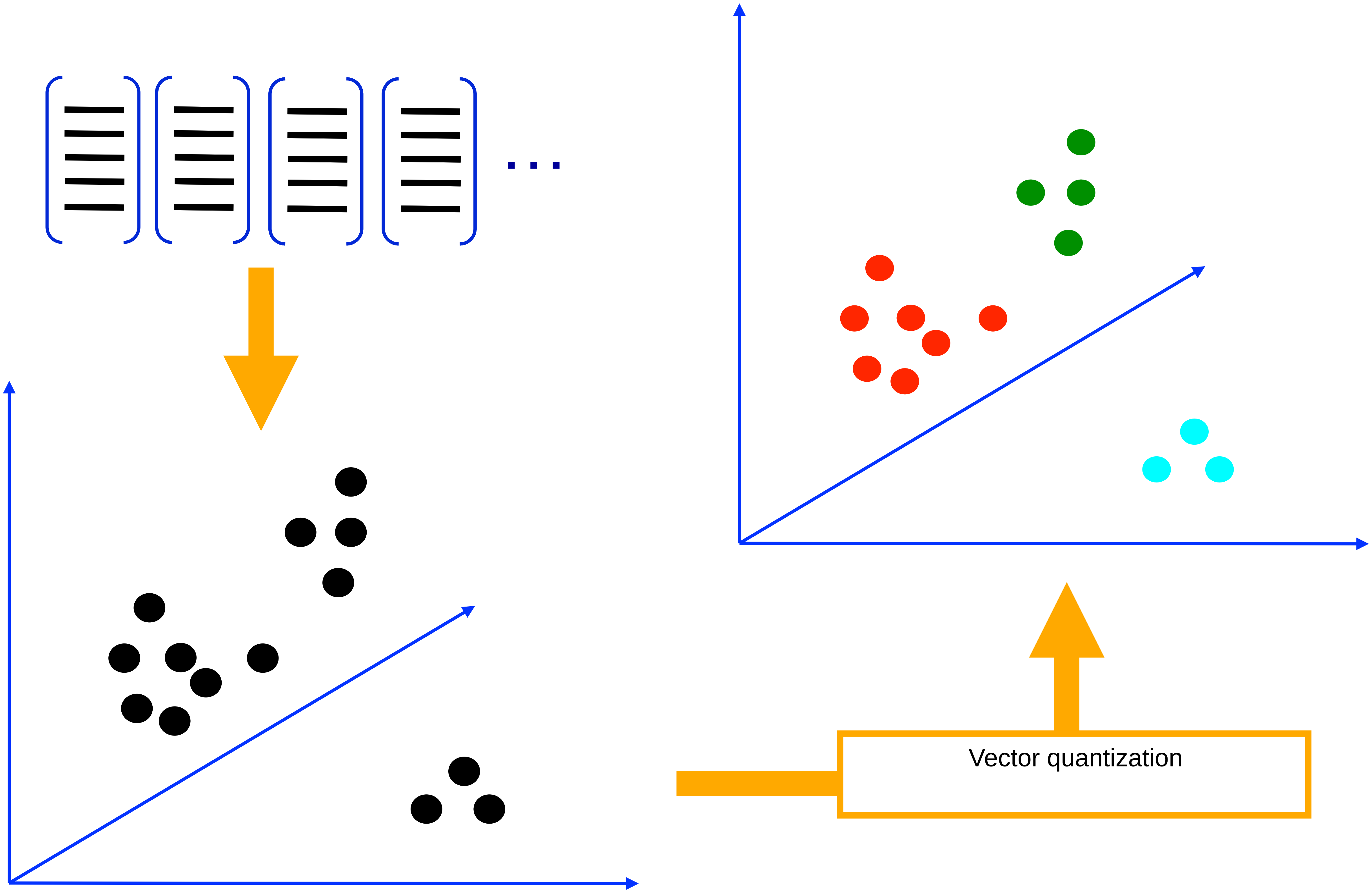
Clustering (usually K-means)



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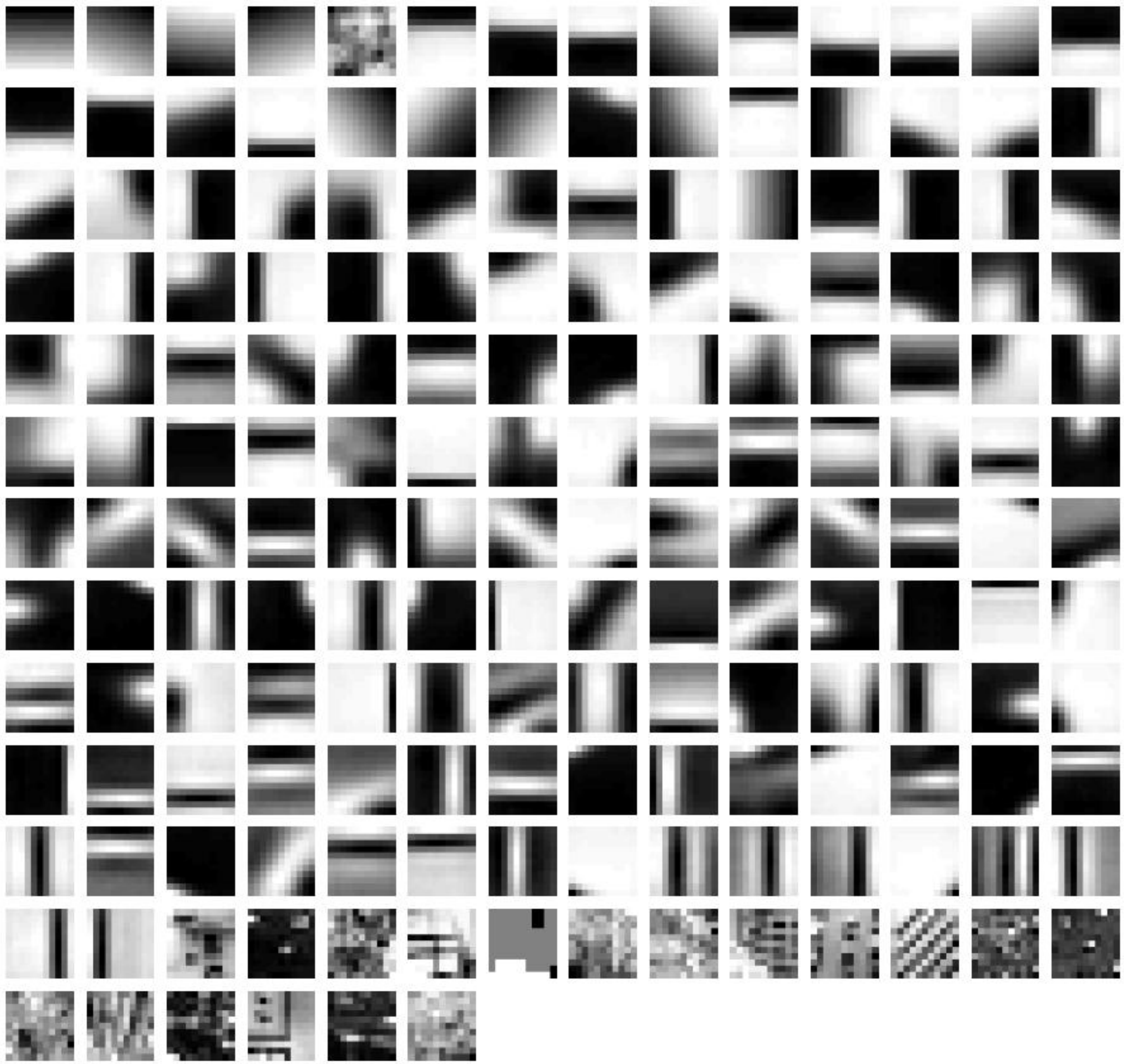
Clustered Image Patches



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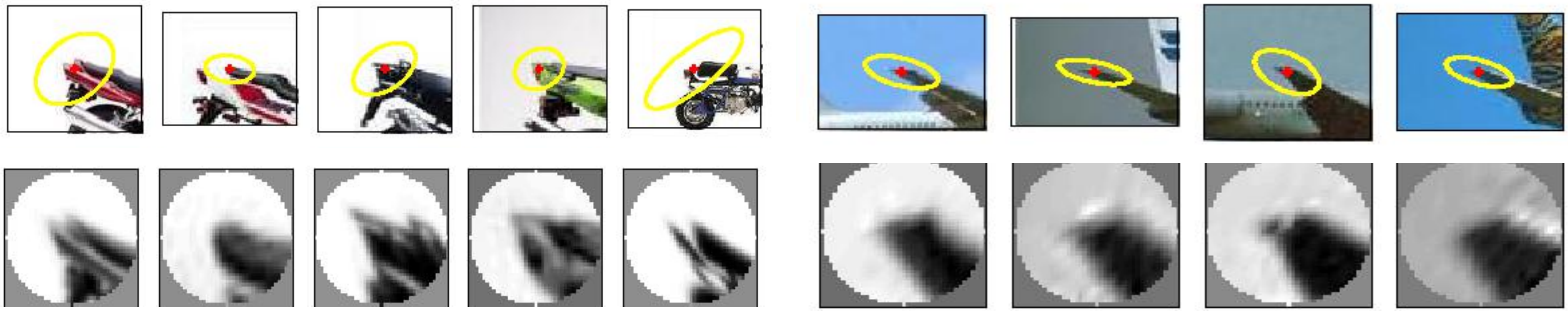
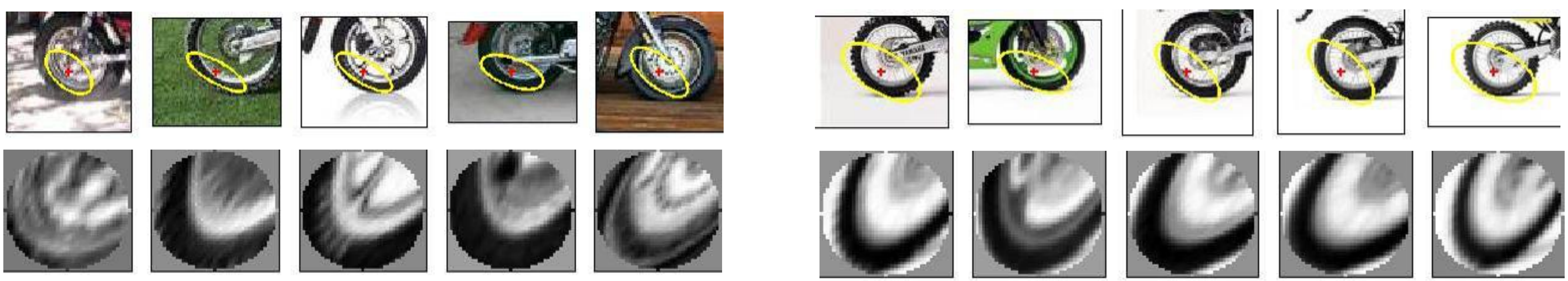
Visual synonyms and polysemy



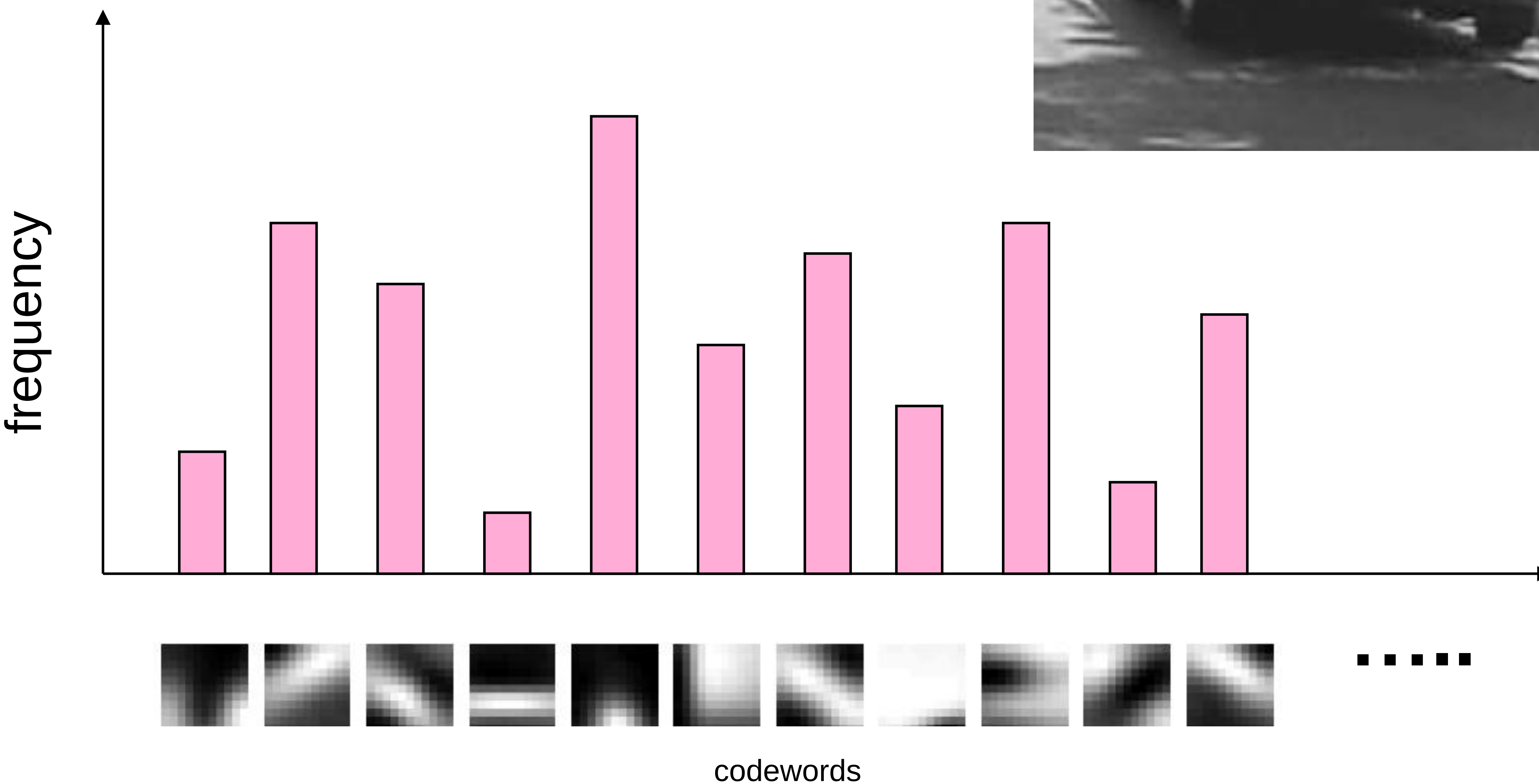
Visual Polysemy. Single visual word occurring on different (but locally similar) parts on different object categories.



Visual Synonyms. Two different visual words representing a similar part of an object (wheel of a motorbike).

slide by Andrew Zisserman

Image Representation



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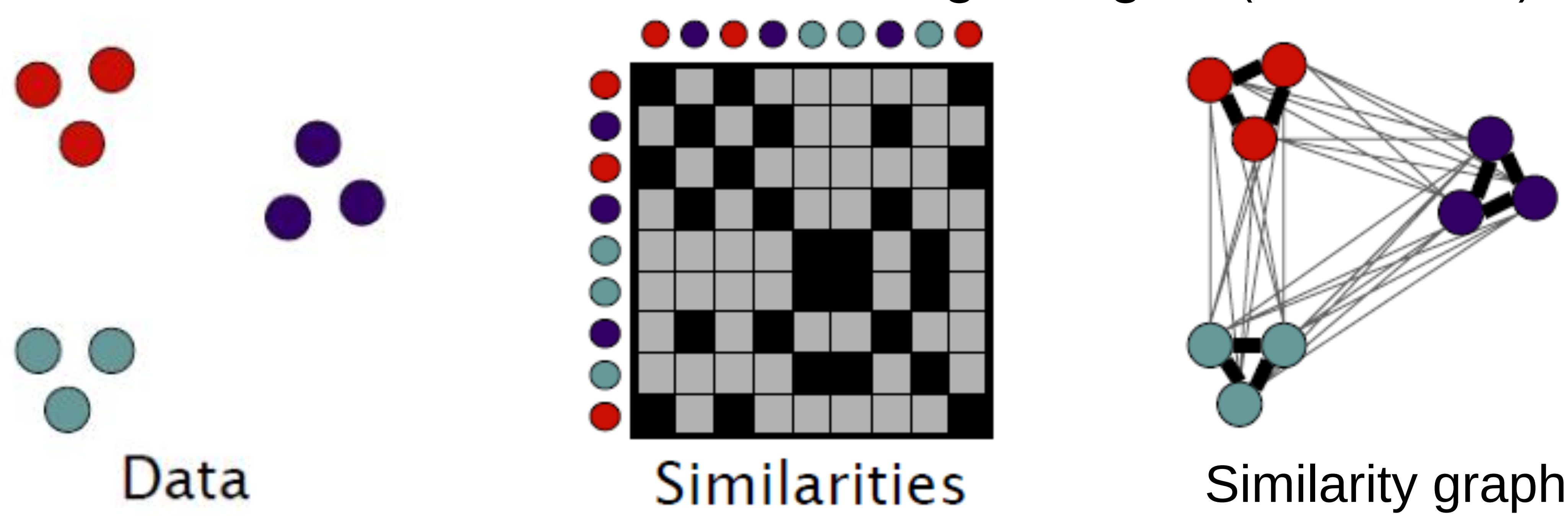
Spectral clustering

Graph-Theoretic Clustering

Goal: Given data points $X_1, \ldots, X_n$ and similarities $W(X_i, X_j)$, partition the data into groups so that points in a group are similar and points in different groups are dissimilar.

Similarity Graph: G(V,E,W)

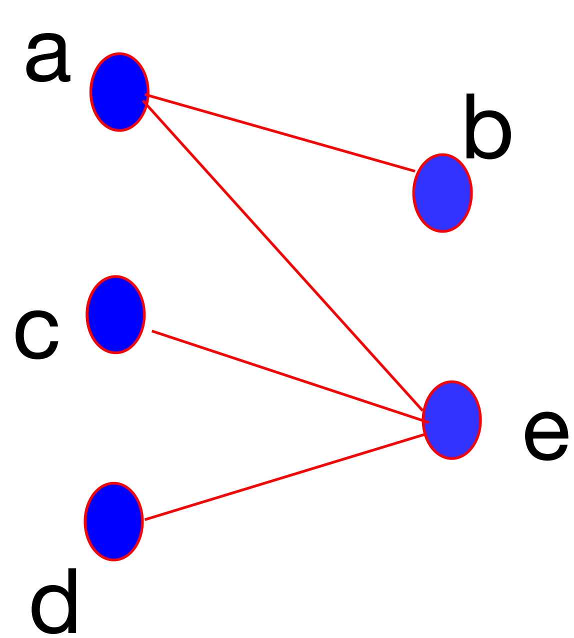
V – Vertices (Data points)
E – Edge if similarity > 0
W - Edge weights (similarities)



Partition the graph so that edges within a group have large weights and edges across groups have small weights.

slide by Aarti Singh

Graphs Representations



$$
\begin{array}{c|ccccc}
 & a & b & c & d & e \\
a & 0 & 1 & 0 & 0 & 1 \\
b & 1 & 0 & 0 & 0 & 0 \\
c & 0 & 0 & 0 & 0 & 1 \\
d & 0 & 0 & 0 & 0 & 1 \\
e & 1 & 0 & 1 & 1 & 0
\end{array}
$$

Adjacency Matrix

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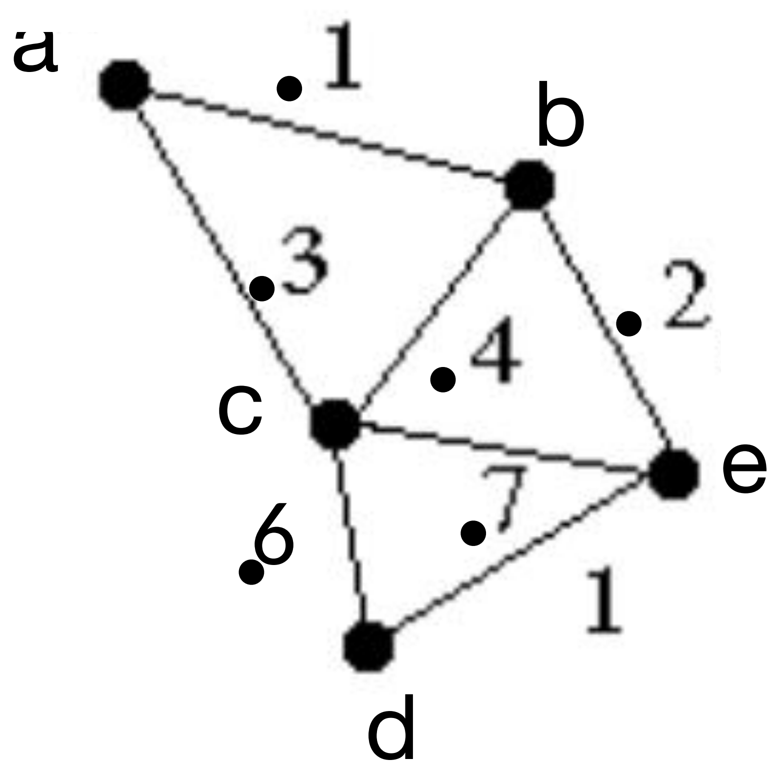
A Weighted Graph and its Representation



Affinity Matrix

$$W = \begin{bmatrix} 1 & .1 & .3 & 0 & 0 \\ .1 & 1 & .4 & 0 & .2 \\ .3 & .4 & 1 & .6 & .7 \\ 0 & 0 & .6 & 1 & 1 \\ 0 & .2 & .7 & 1 & 1 \end{bmatrix}$$

W_{ij} : probability that i &j belong to the same cluster

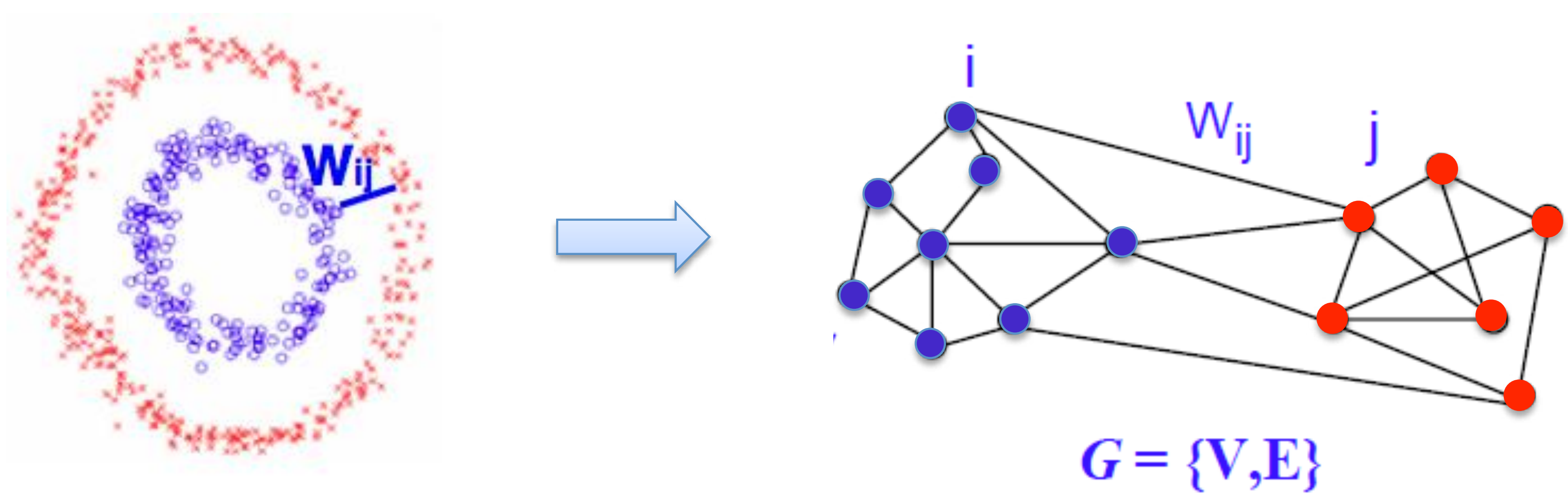
Similarity graph construction

- Similarity Graphs: Model local neighborhood relations between data points
- E.g. epsilon-NN

$$W_{ij} = \begin{cases} 1 & \|x_i - x_j\| \le \epsilon \\ 0 & \text{otherwise} \end{cases}$$

Controls size of neighborhood

or mutual k-NN graph (W_{ij} = 1 if x_i or x_j is k nearest neighbor of the other)



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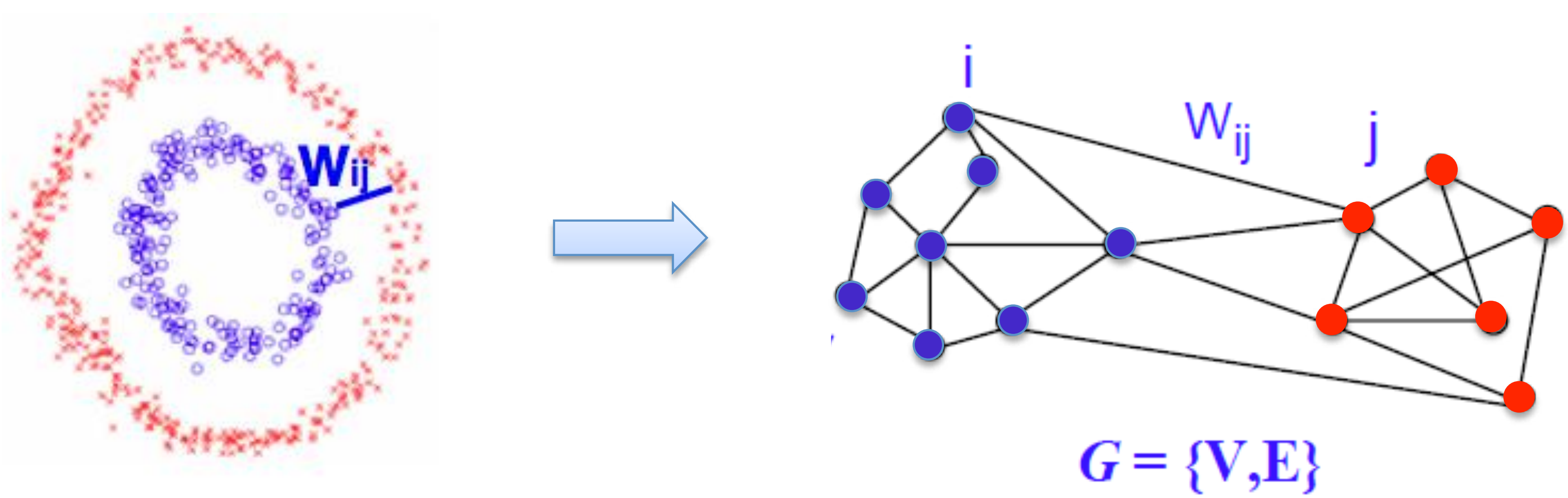
Similarity graph construction

- Similarity Graphs: Model local neighborhood relations between data points
- E.g. Gaussian kernel similarity function

$$W_{ij} = e^{\frac{\|x_i - x_j\|^2}{2\sigma^2}}$$

→ Controls size of neighborhood



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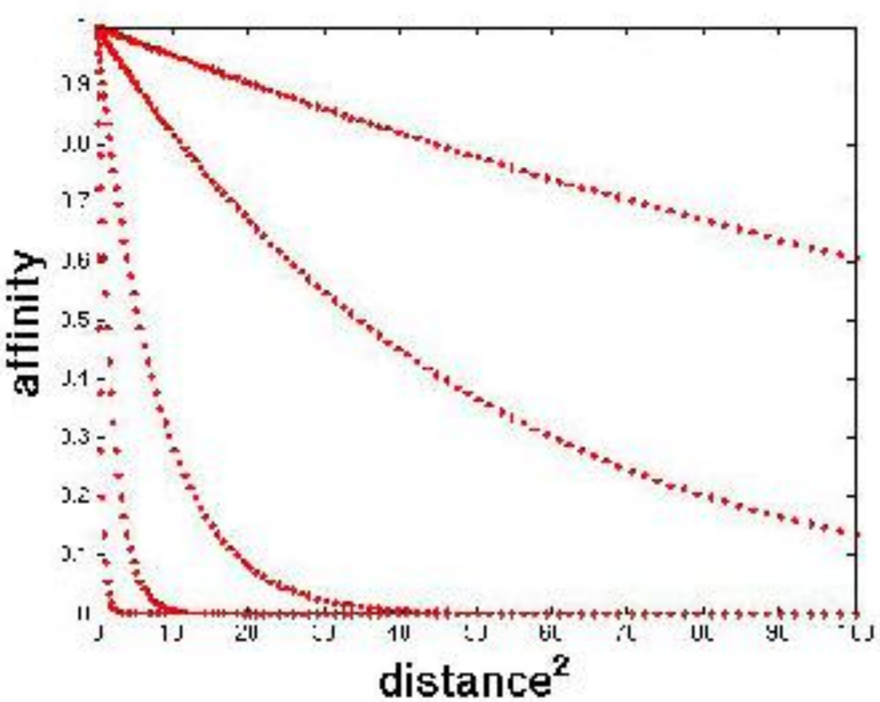
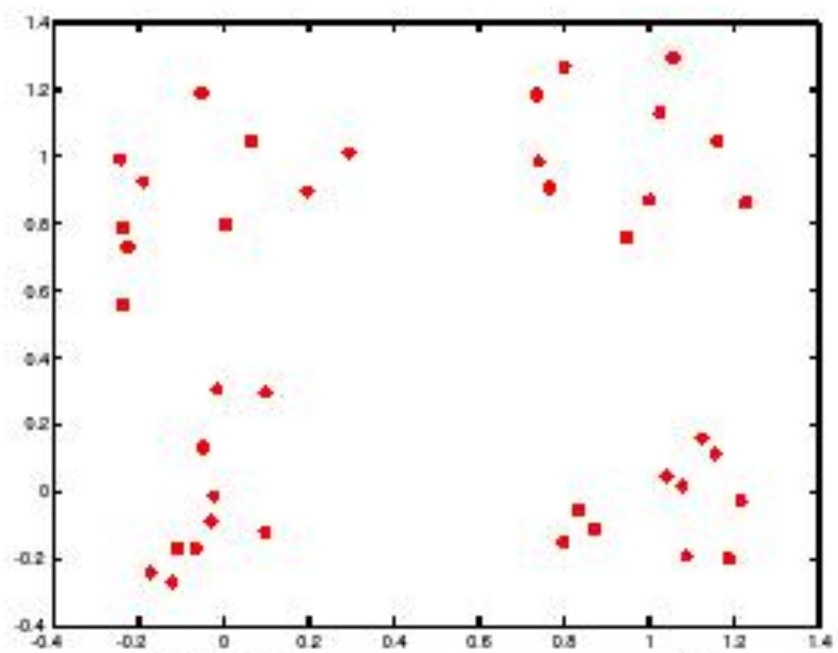
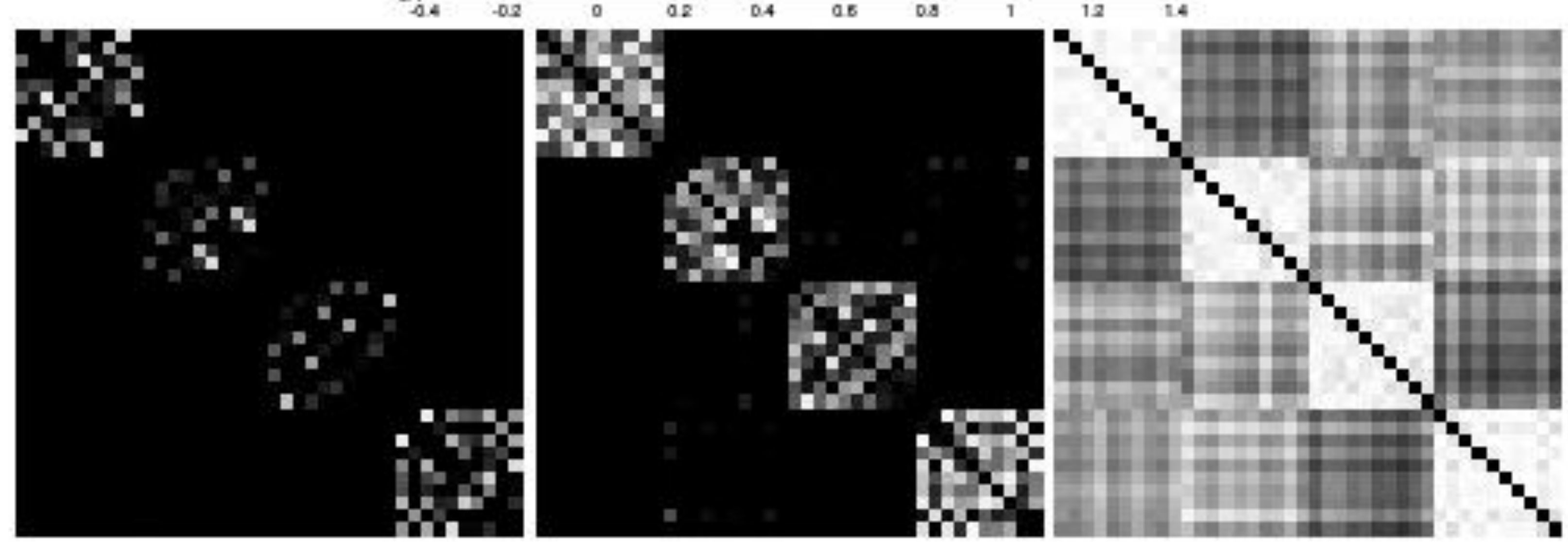
Scale affects affinity

- Small σ: group only nearby points
- Large σ: group far-away points





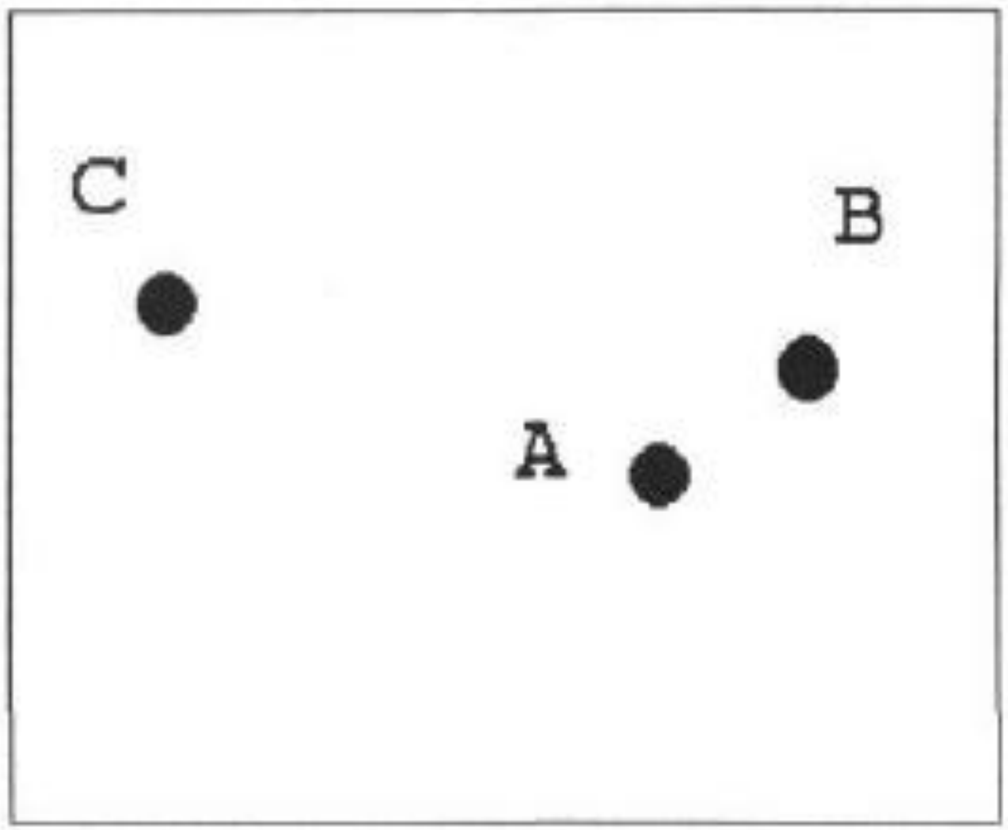


Feature grouping by "relocalisation" of eigenvectors of the proximity matrix

British Machine Vision Conference, pp. 103-108, 1990

Guy L. Scott
Robotics Research Group
Department of Engineering Science
University of Oxford

H. Christopher Longuet-Higgins
University of Sussex
Falmer
Brighton



Three points in feature space

$$W_{ij} = \exp(-\| z_i - z_j \|^2 / s^2)$$

With an appropriate s

W=

	A	B	C
A	1.00	0.63	0.03
B	0.63	1.00	0.0
C	0.03	0.0	1.00

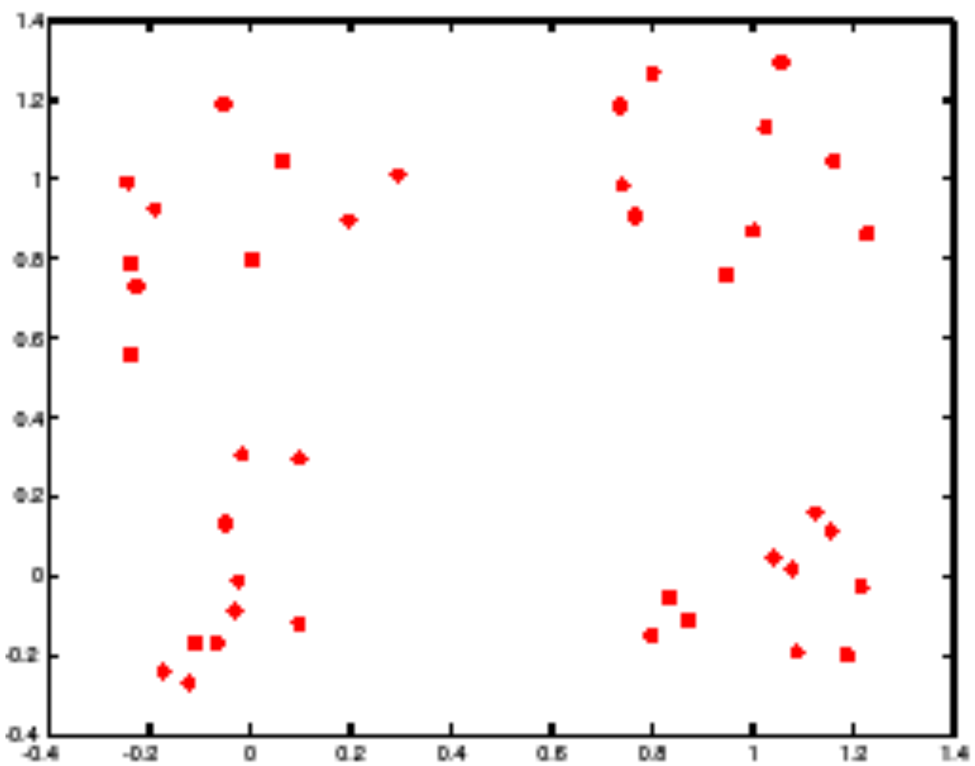
The eigenvectors of W are:

	E_1	E_2	E_3
Eigenvalues	1.63	1.00	0.37
A	-0.71	-0.01	0.71
B	-0.71	-0.05	-0.71
C	-0.04	1.00	-0.03

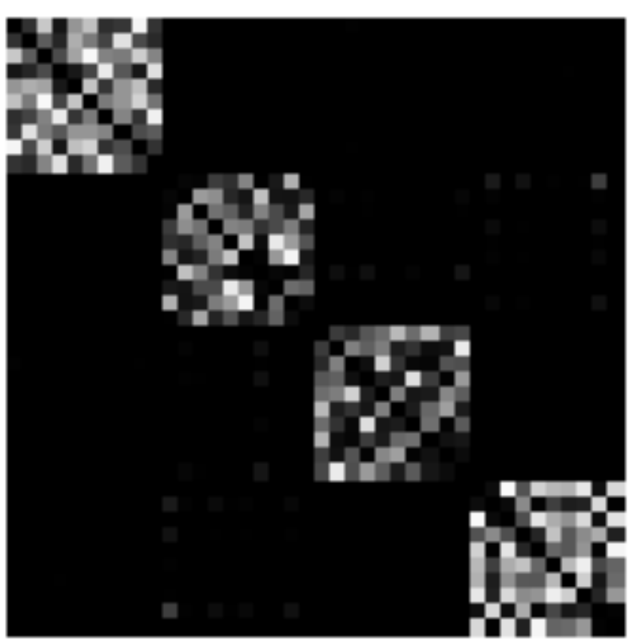
The first 2 eigenvectors group the points as desired…

slide by Bill Freeman and Antonio Torralba

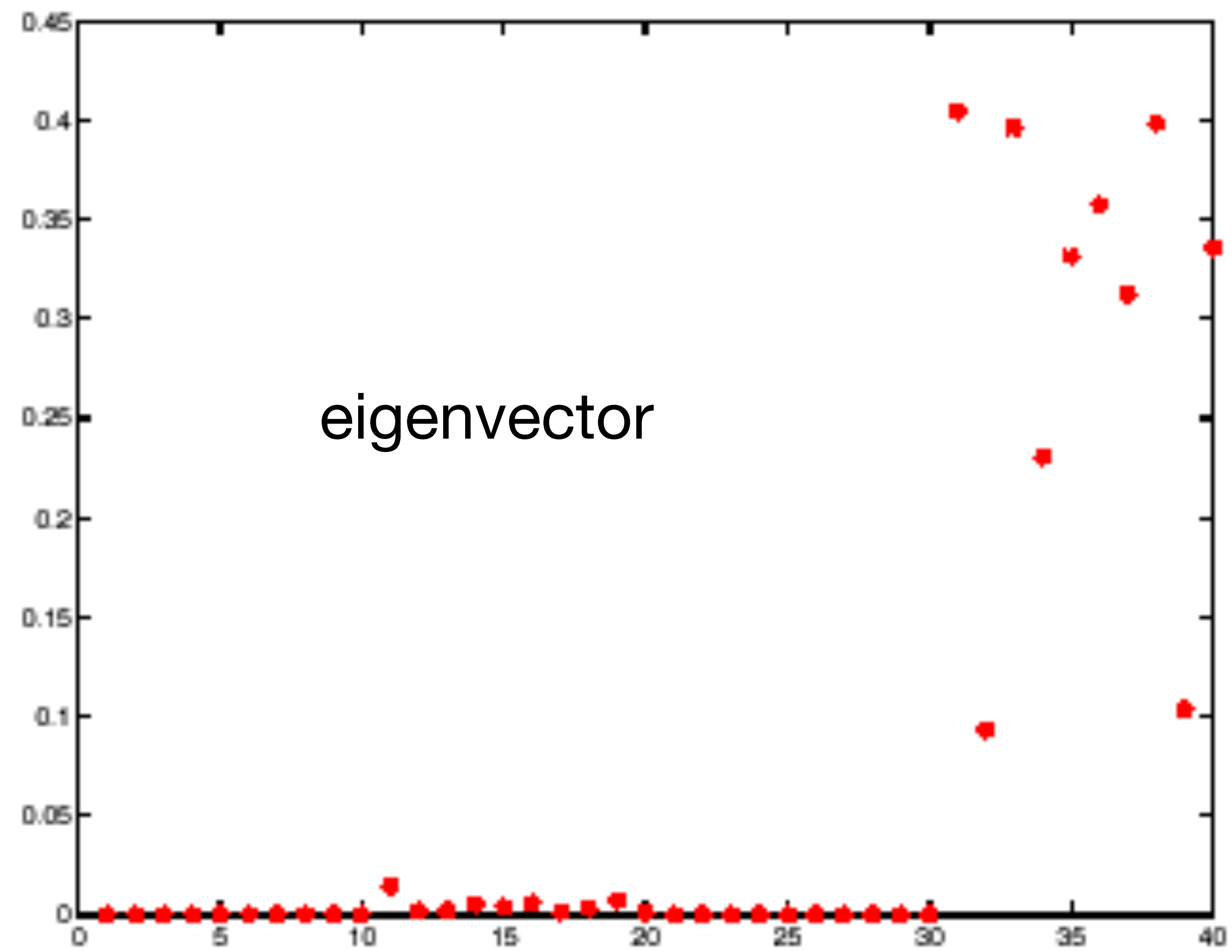
Example eigenvector



points



Affinity matrix



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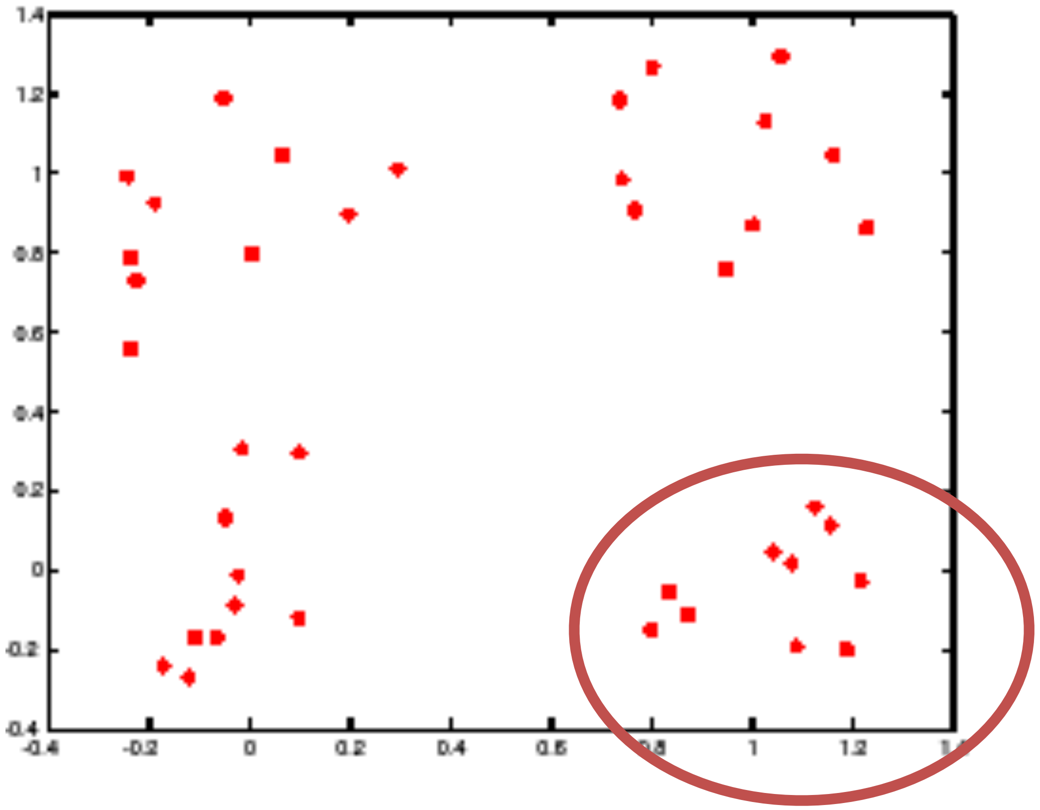
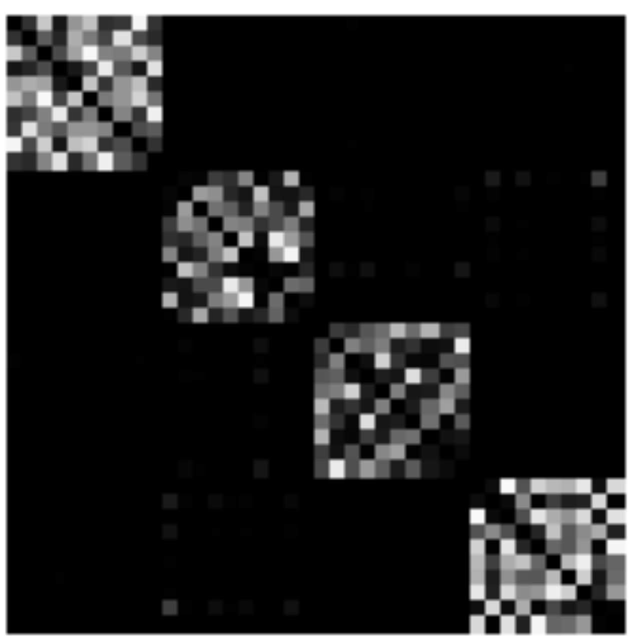
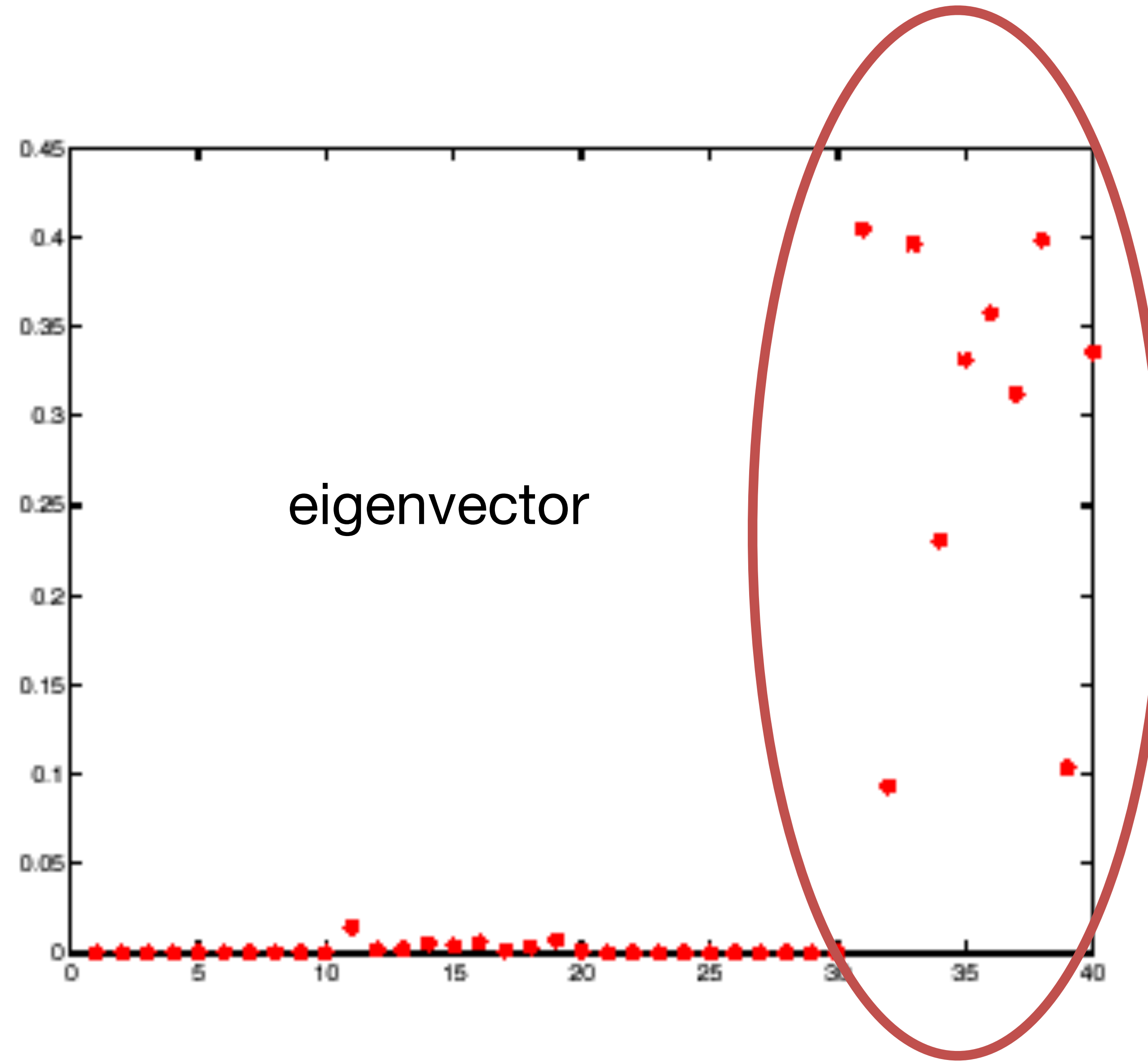
Example eigenvector



points



Affinity matrix



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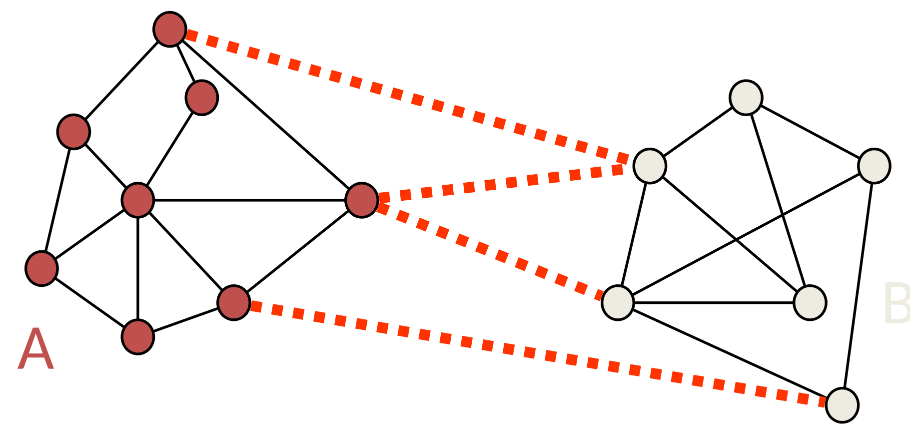
Graph cut

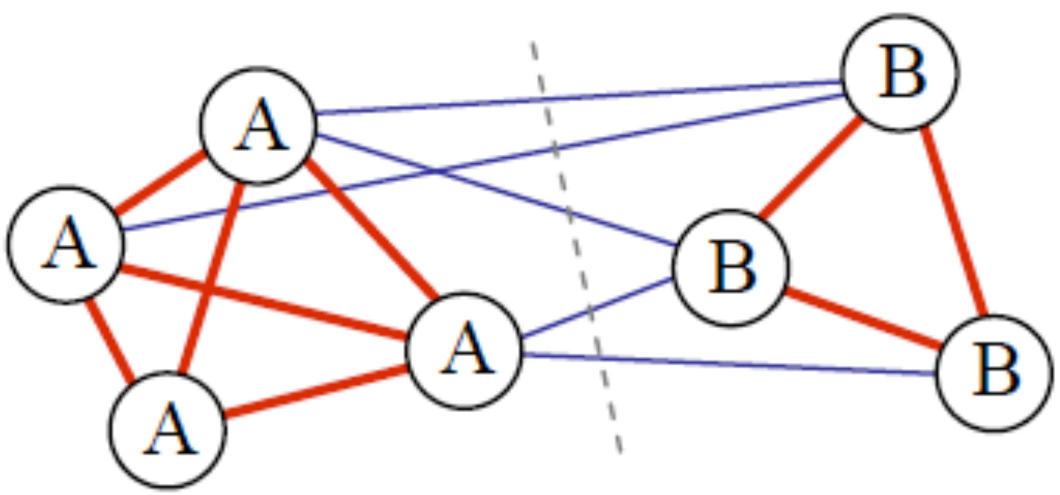


- Set of edges whose removal makes a graph disconnected
- Cost of a cut: sum of weights of cut edges
- A graph cut gives us a partition (clustering)
  - What is a "good" graph cut and how do we find one?

slide by Steven Seitz

Minimum cut

- A cut of a graph *G* is the set of edges *S* such that removal of *S* from *G* disconnects *G*.



Cut: sum of the weight of the cut edges:

$$cut(\mathrm{A},\mathrm{B}) = \sum_{u \in \mathrm{A}, v \in \mathrm{B}} \mathrm{W}(u,v),$$

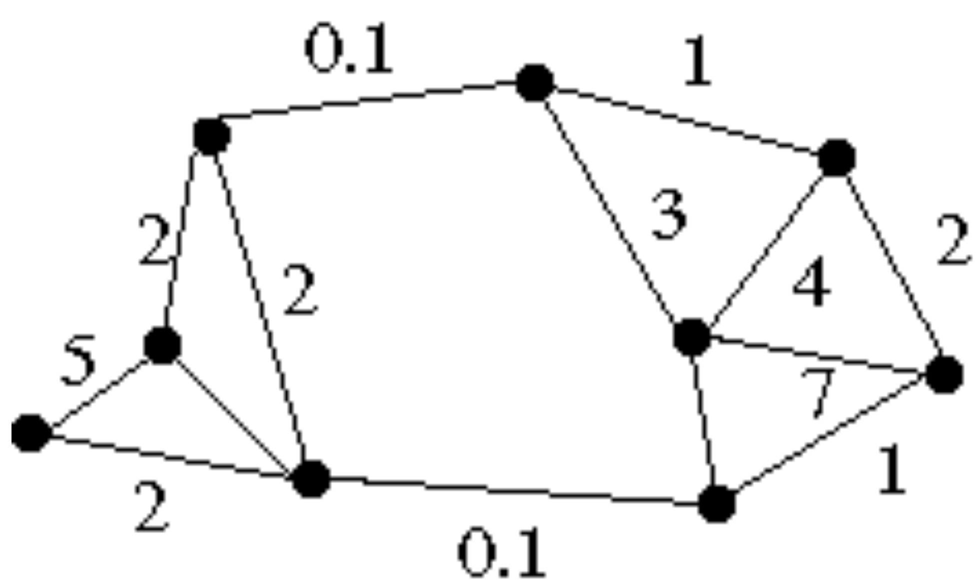
with $\mathrm{A} \cap \mathrm{B} = \varnothing$

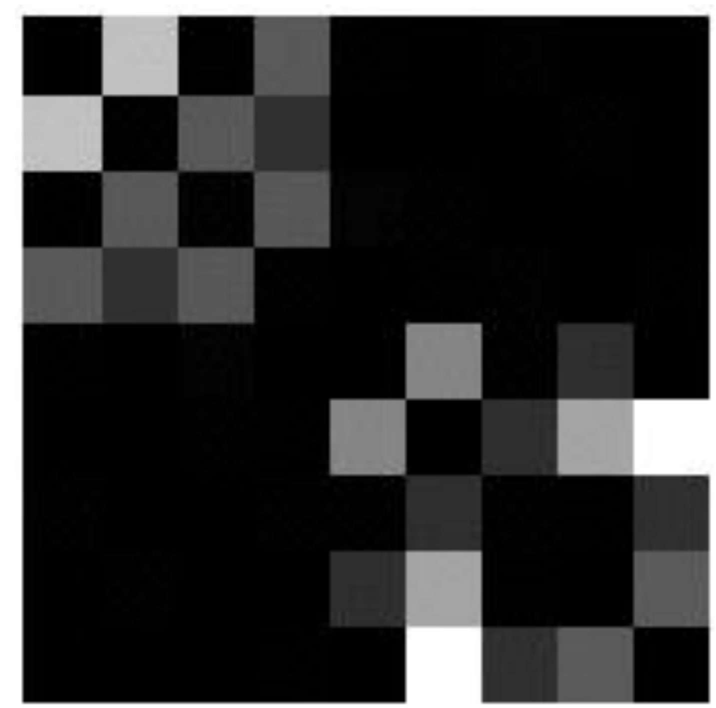
slide by Bill Freeman and Antonio Torralba

Minimum cut

- We can do clustering by finding the minimum cut in a graph
  - Efficient algorithms exist for doing this

Minimum cut example



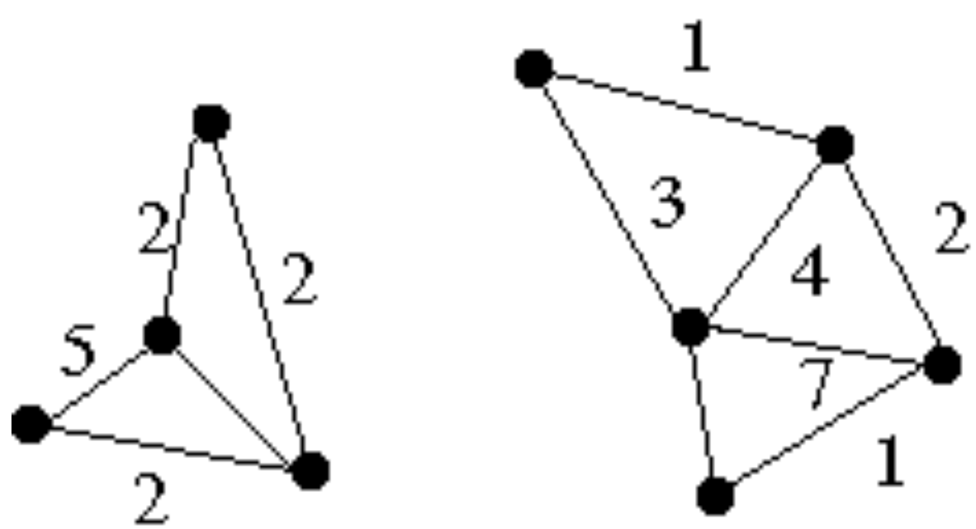


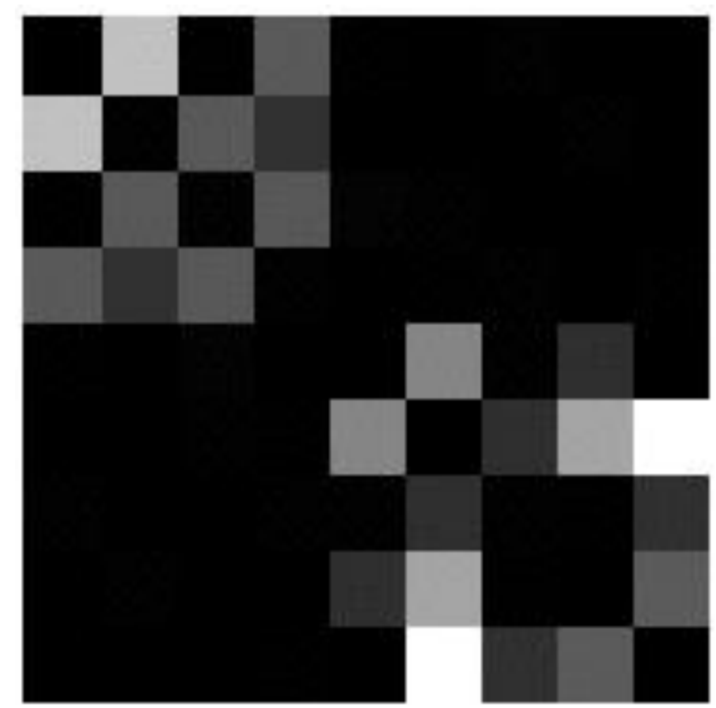
slide by Svetlana Lazebnik

Minimum cut

- We can do segmentation by finding the minimum cut in a graph
  - Efficient algorithms exist for doing this

Minimum cut example





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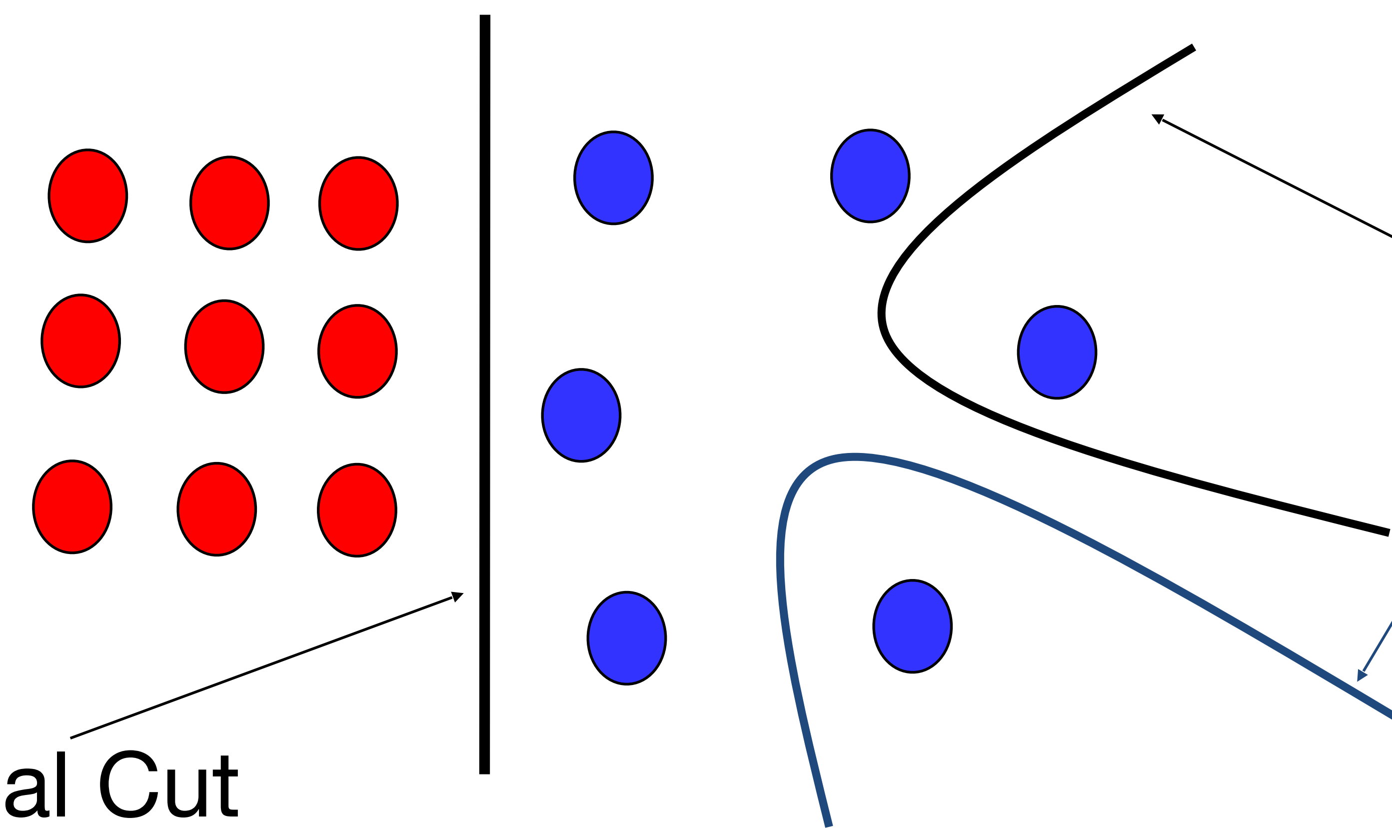
Drawbacks of Minimum cut

- Weight of cut is directly proportional to the number of edges in the cut.



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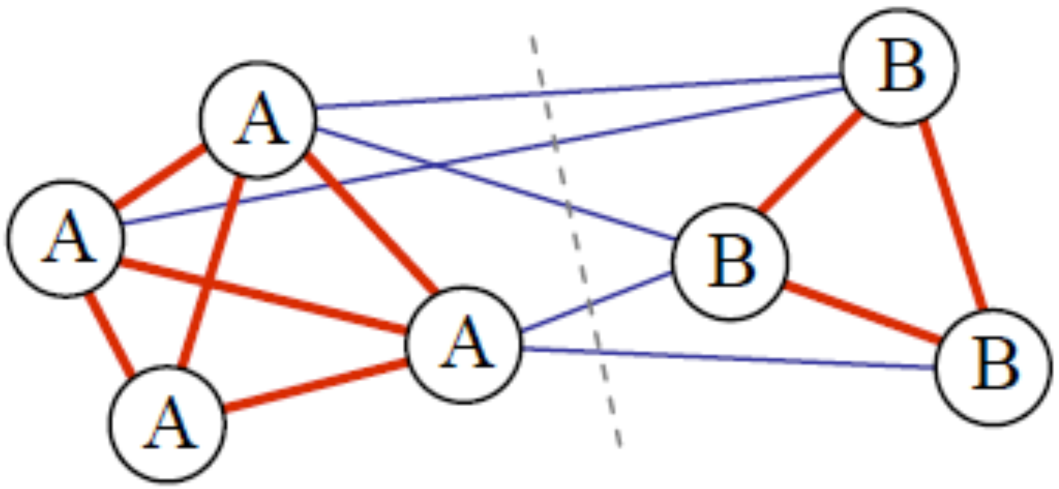
* Slide from Khurram Hassan-Shafique CAP5415 Computer Vision 2003

Normalized cuts

Write graph as V, one cluster as A and the other as B



$$\text{Ncut}(A,B) = \frac{\text{cut}(A,B)}{\text{assoc}(A,V)} + \frac{\text{cut}(A,B)}{\text{assoc}(B,V)}$$

cut(A,B) is sum of weights with one end in A and one end in B

$$cut(\mathrm{A},\mathrm{B}) = \sum_{u \in \mathrm{A}, v \in \mathrm{B}} \mathrm{W}(u,v),$$

with $\mathrm{A} \cap \mathrm{B} = \varnothing$

assoc(A,V) is sum of all edges with one end in A.

$$assoc(\mathrm{A},\mathrm{B}) = \sum_{u \in \mathrm{A}, v \in \mathrm{B}} \mathrm{W}(u,v)$$

A and B not necessarily disjoint

J. Shi and J. Malik. [Normalized cuts and image segmentation.] PAMI 2000

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Normalized cut

- Let W be the adjacency matrix of the graph
- Let D be the diagonal matrix with diagonal entries $D(i, i) = \Sigma_j W(i, j)$
- Then the normalized cut cost can be written as

$$\frac{y^T (D - W) y}{y^T D y}$$

where y is an indicator vector whose value should be 1 in the i-th position if the i-th feature point belongs to A and a negative constant otherwise

slide by Svetlana Lazebnik

J. Shi and J. Malik. Normalized cuts and image segmentation. PAMI 2000

Normalized cut

- Finding the exact minimum of the normalized cut cost is NP-complete, but if we *relax* y to take on arbitrary values, then we can minimize the relaxed cost by solving the **generalized eigenvalue problem**

  $(D - W)y = \lambda Dy$

- The solution y is given by the generalized eigenvector corresponding to the second smallest eigenvalue
- Intuitively, the i-th entry of y can be viewed as a "soft" indication of the component membership of the i-th feature
  - Can use 0 or median value of the entries as the splitting point (threshold), or find threshold that minimizes the Ncut cost

slide by Svetlana Lazebnik

J. Shi and J. Malik. [Normalized cuts and image segmentation.]() PAMI 2000

Normalized cut algorithm

1. Given an image or image sequence, set up a weighted graph $\mathbf{G} = (\mathbf{V}, \mathbf{E})$, and set the weight on the edge connecting two nodes being a measure of the similarity between the two nodes.

2. Solve $(\mathbf{D} - \mathbf{W})\boldsymbol{x} = \lambda \mathbf{D} \boldsymbol{x}$ for eigenvectors with the smallest eigenvalues.

3. Use the eigenvector with second smallest eigenvalue to bipartition the graph.

4. Decide if the current partition should be sub-divided, and recursively repartition the segmented parts if necessary.

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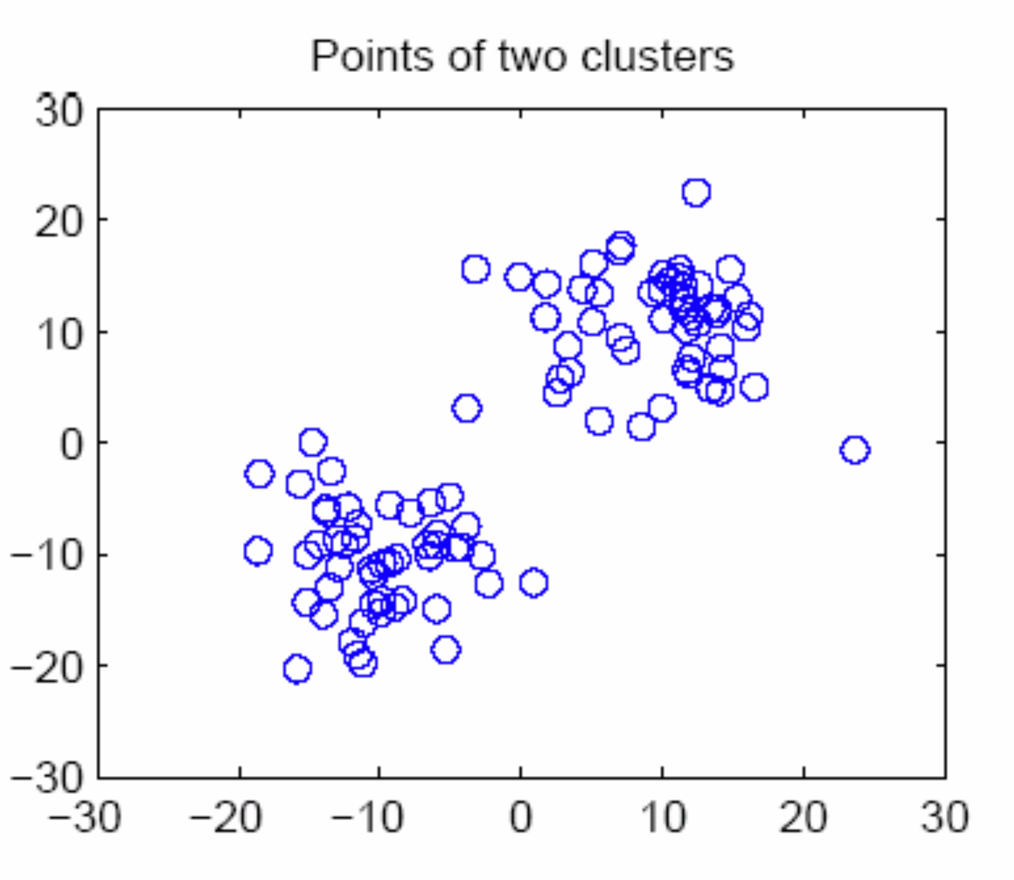
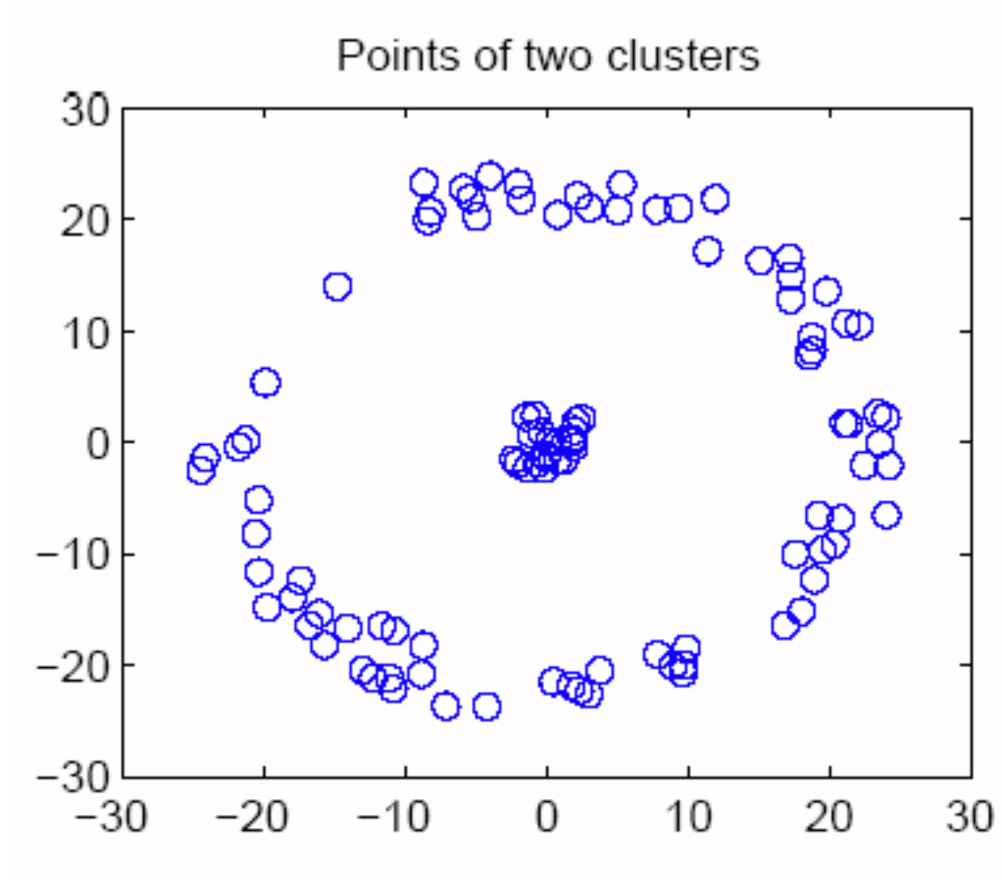
J. Shi and J. Malik. [Normalized cuts and image segmentation.] PAMI 2000

K-Means vs. Spectral Clustering

- Applying k-means to Laplacian eigenvectors allows us to find cluster with non-convex boundaries.



Both perform same



Spectral clustering is superior

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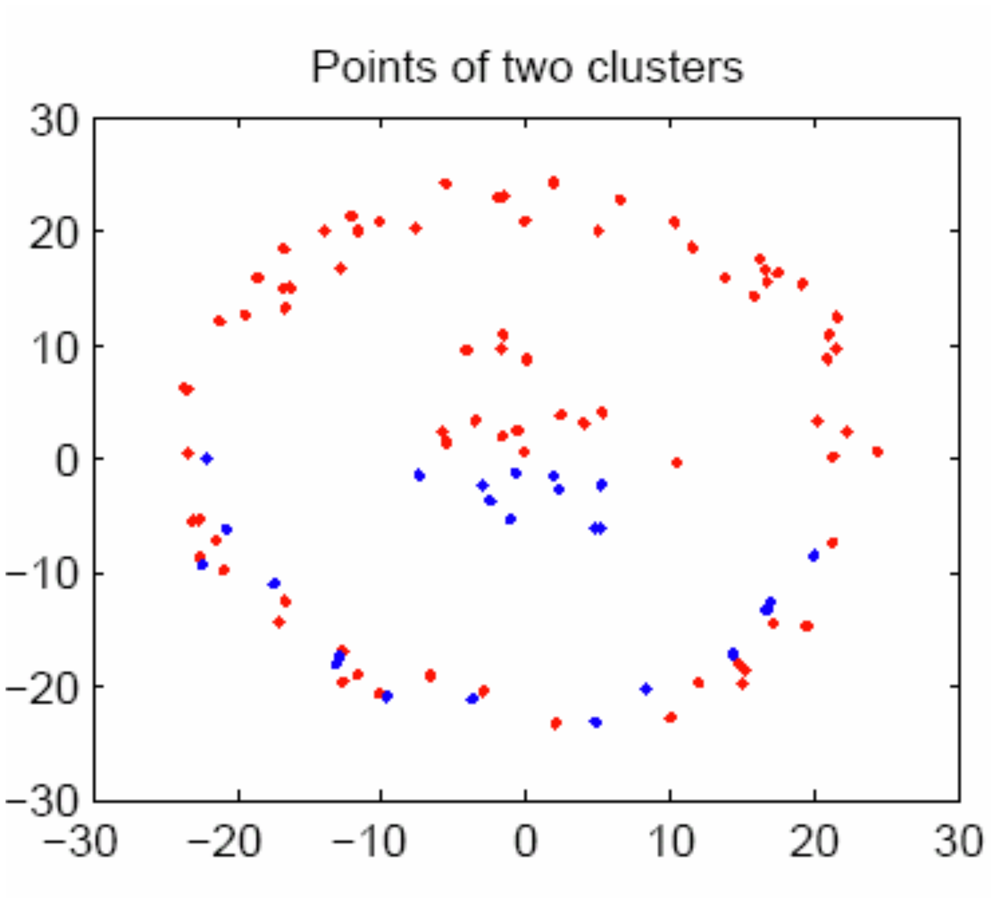
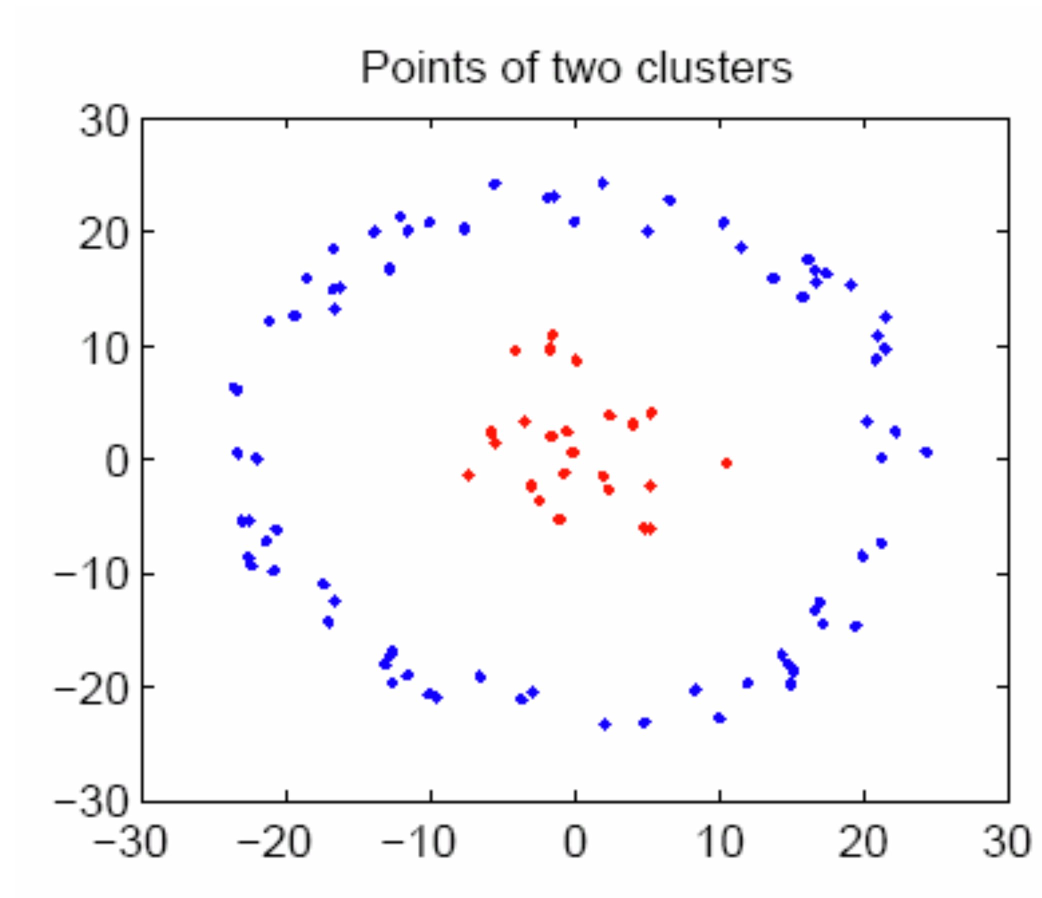
K-Means vs. Spectral Clustering

- Applying k-means to Laplacian eigenvectors allows us to find cluster with non-convex boundaries.



k-means output



Spectral clustering output

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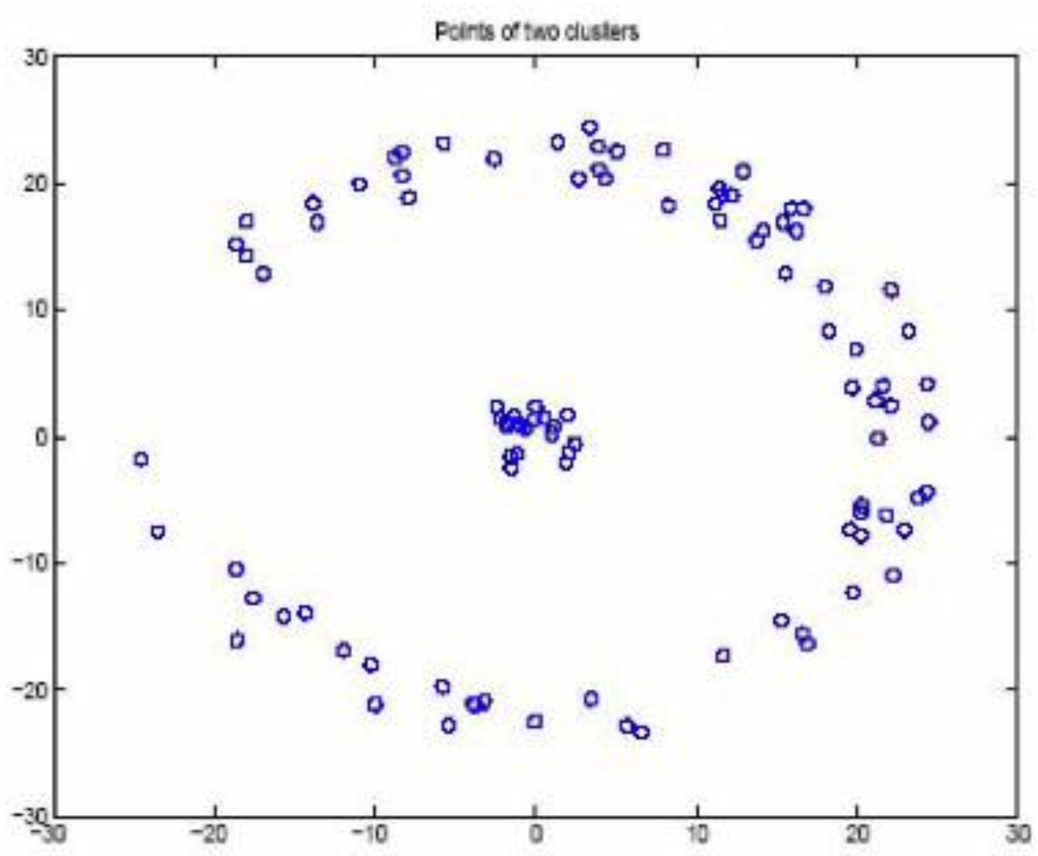
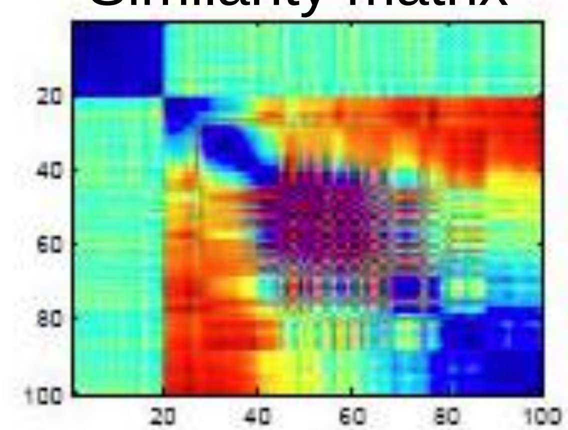
K-Means vs. Spectral Clustering

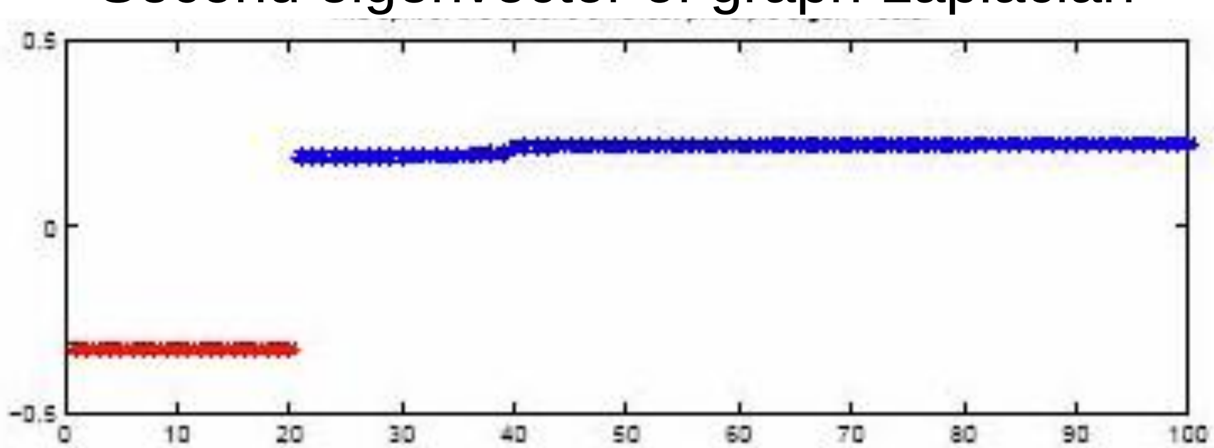
- Applying k-means to Laplacian eigenvectors allows us to find cluster with non-convex boundaries.



Similarity matrix



Second eigenvector of graph Laplacian



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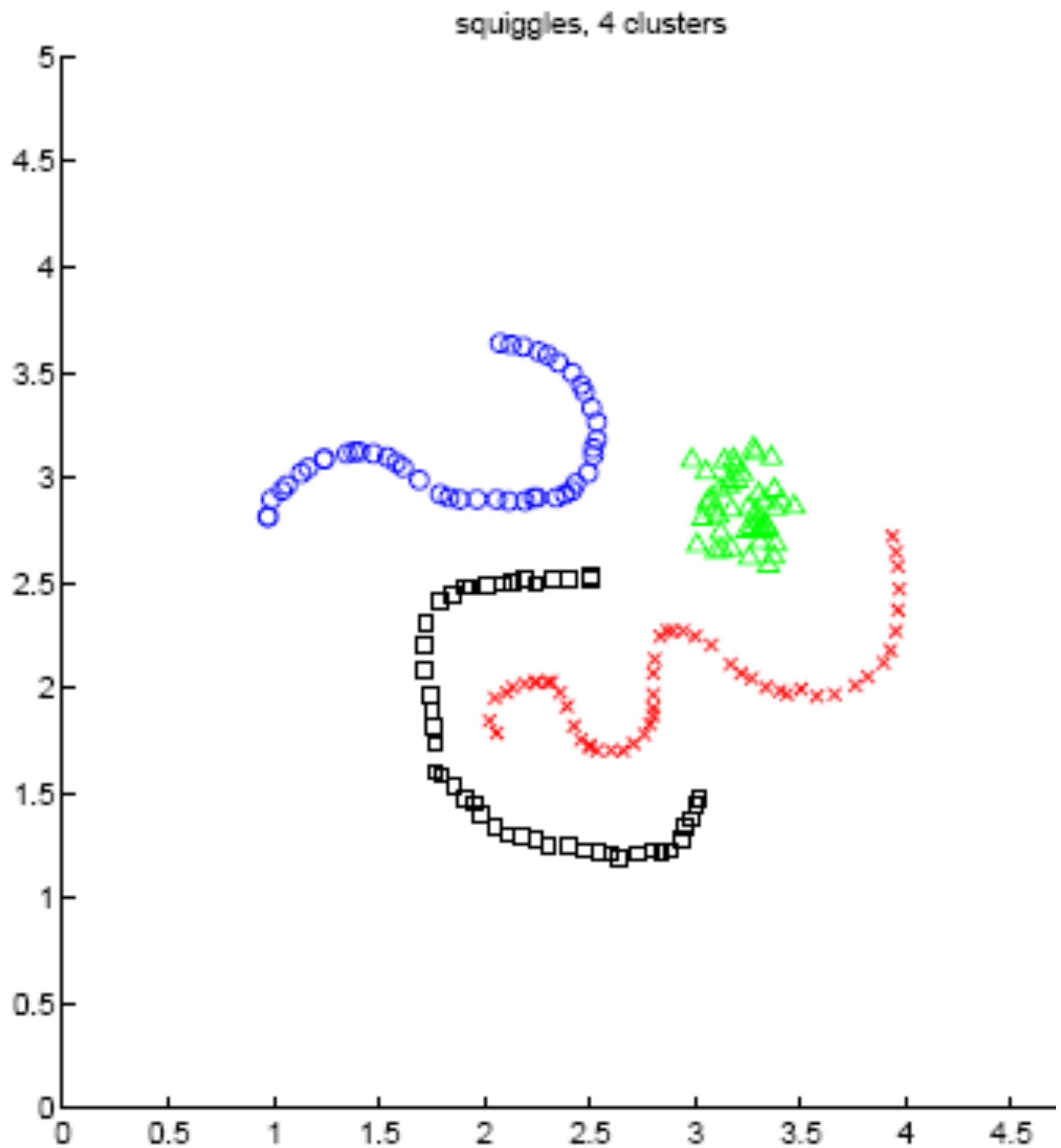
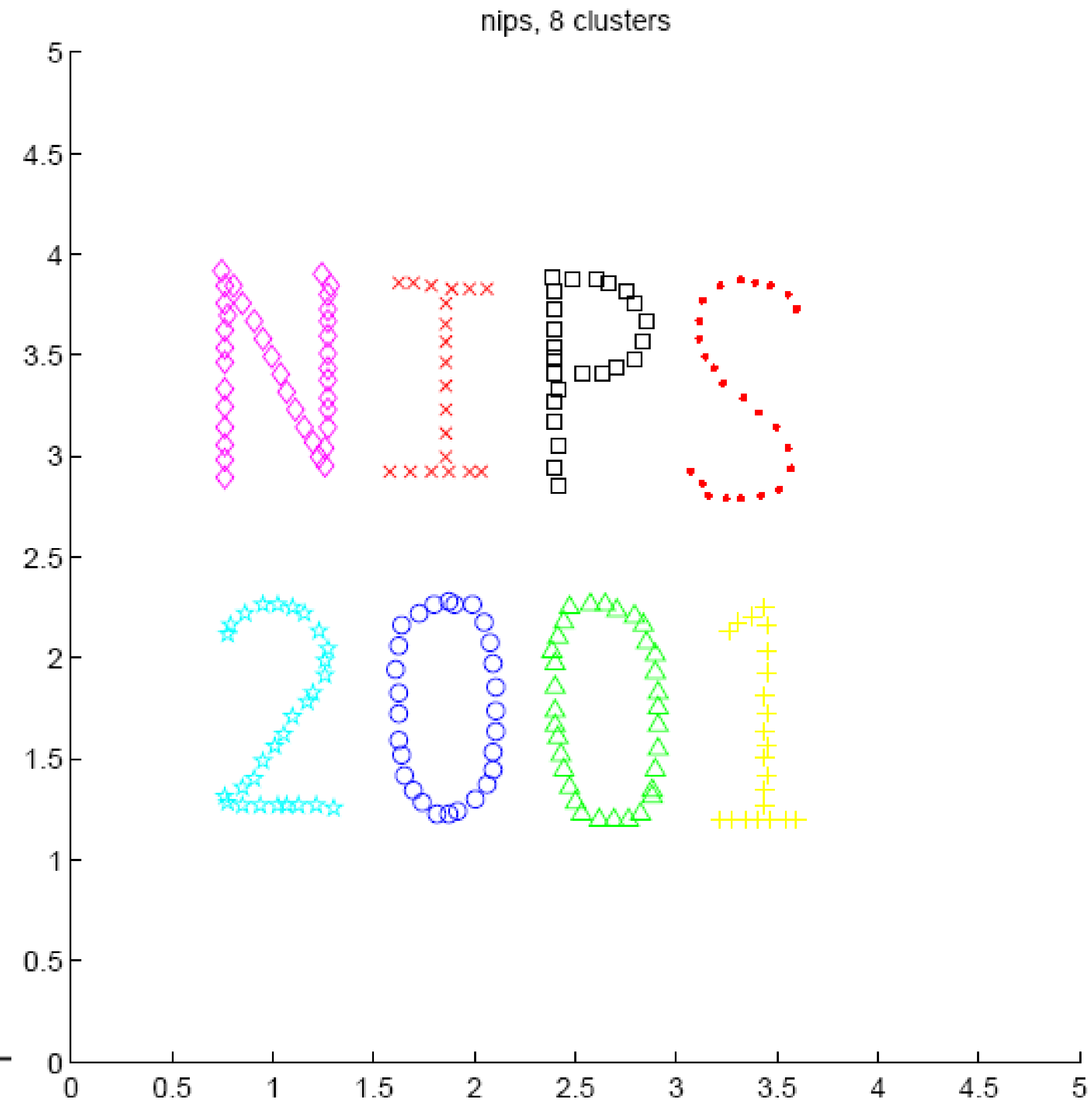
Examples





[Ng et al., 2001]

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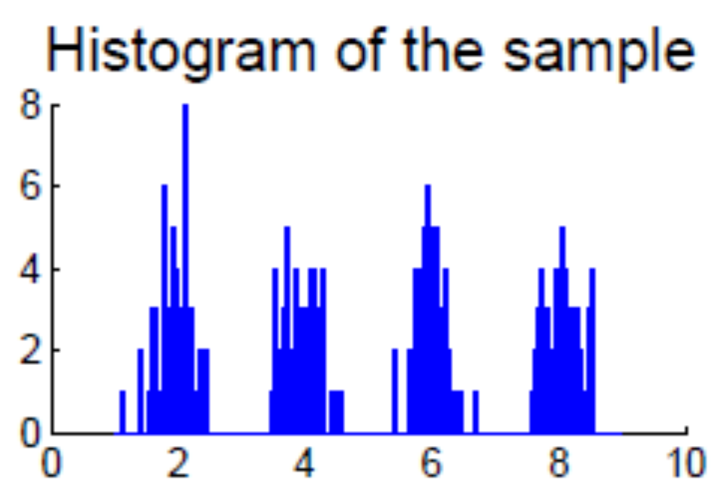
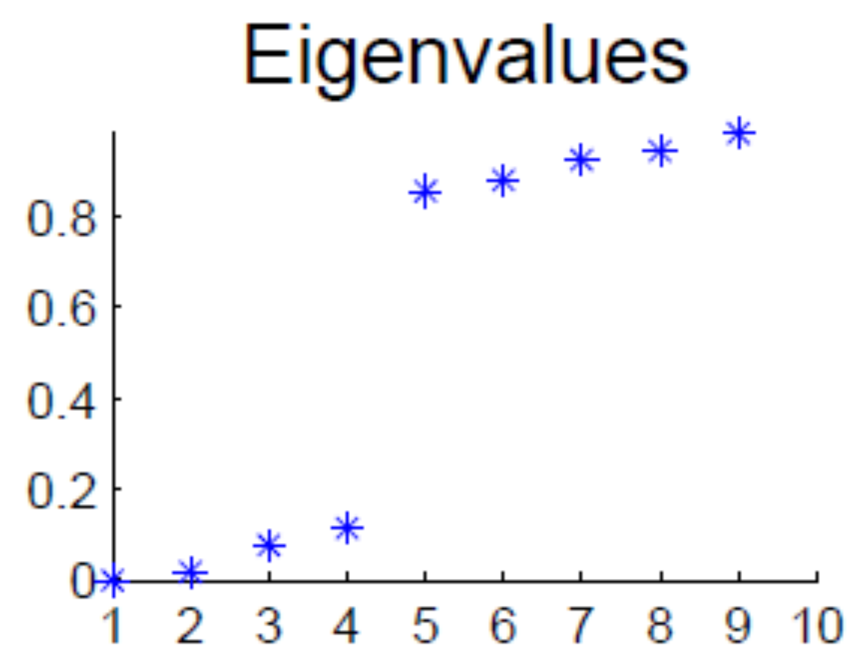
Some Issues

- Choice of number of clusters k
  - Most stable clustering is usually given by the value of k that maximizes the eigengap (difference between consecutive eigenvalues)

$$\Delta_k = \left| \lambda - \lambda_{k-1} \right|$$





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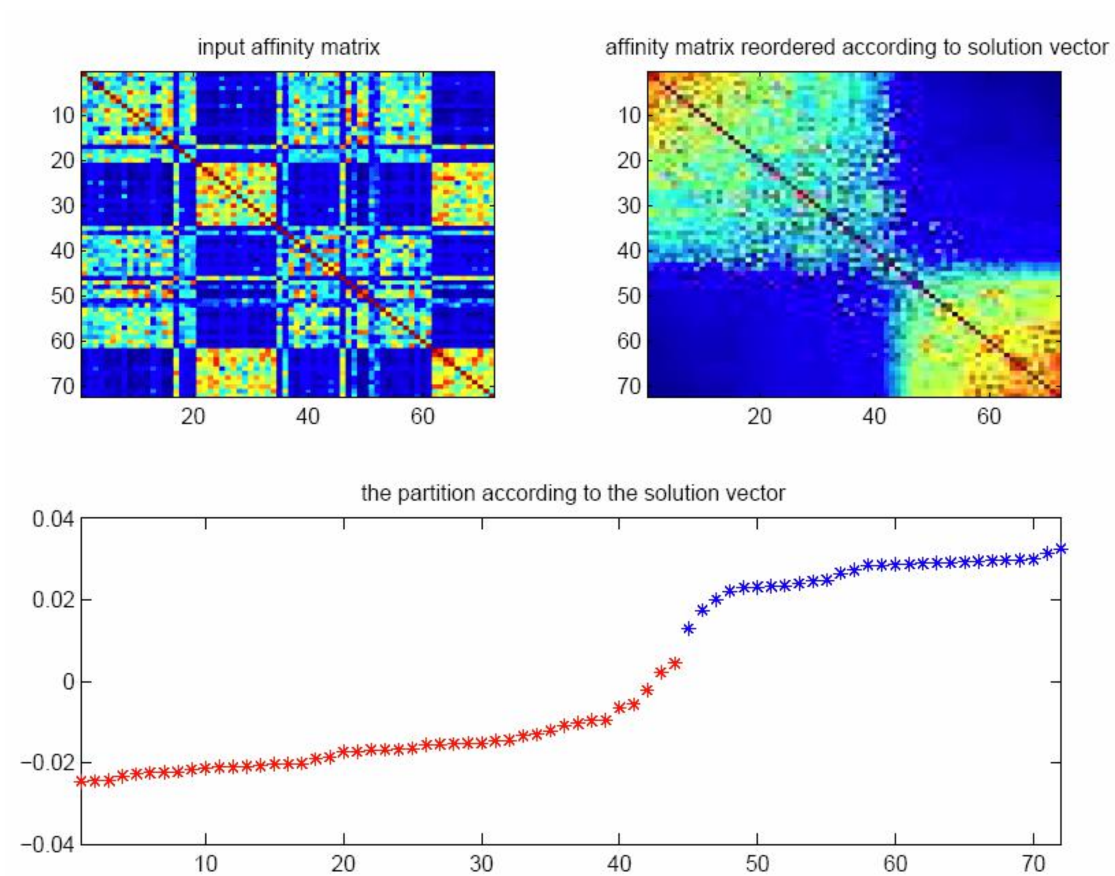
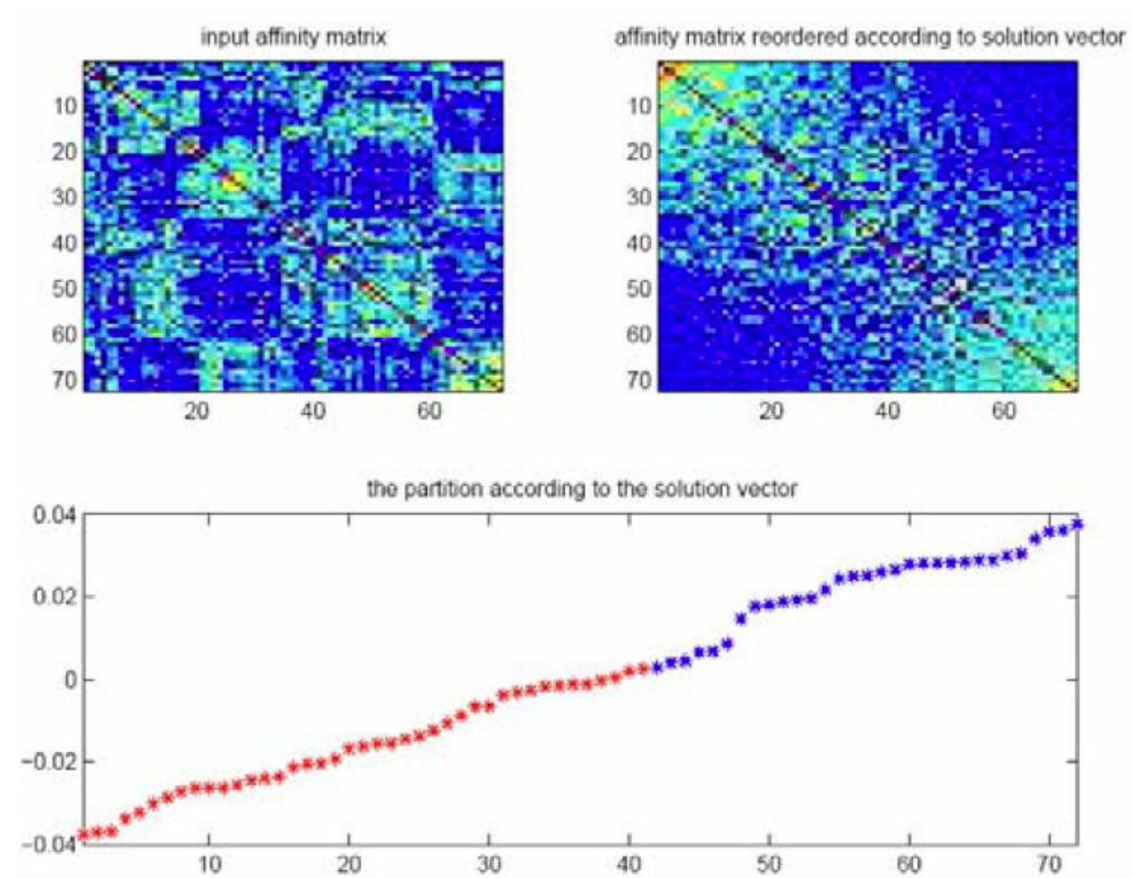
Some Issues

- Choice of number of clusters k
- Choice of similarity
  - Choice of kernel

  for Gaussian kernels, choice of σ



Good similarity measure



Poor similarity measure

slide by Aarti Singh

Some Issues

- Choice of number of clusters k
- Choice of similarity
  - Choice of kernel

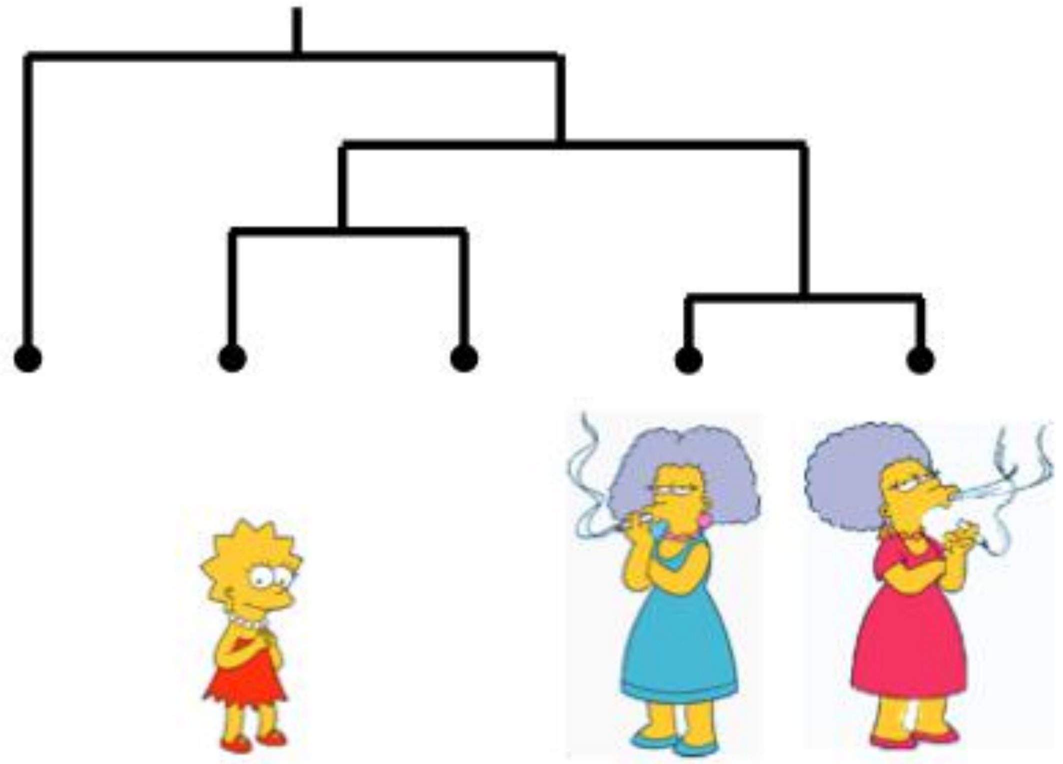
  for Gaussian kernels, choice of σ
- Choice of clustering method
  - k-way vs. recursive 2-way

slide by Aarti Singh

Hierarchical clustering

Hierarchical Clustering

- Bottom-Up (agglomerative): Starting with each item in its own cluster, find the best pair to merge into a new cluster. Repeat until all clusters are fused together.



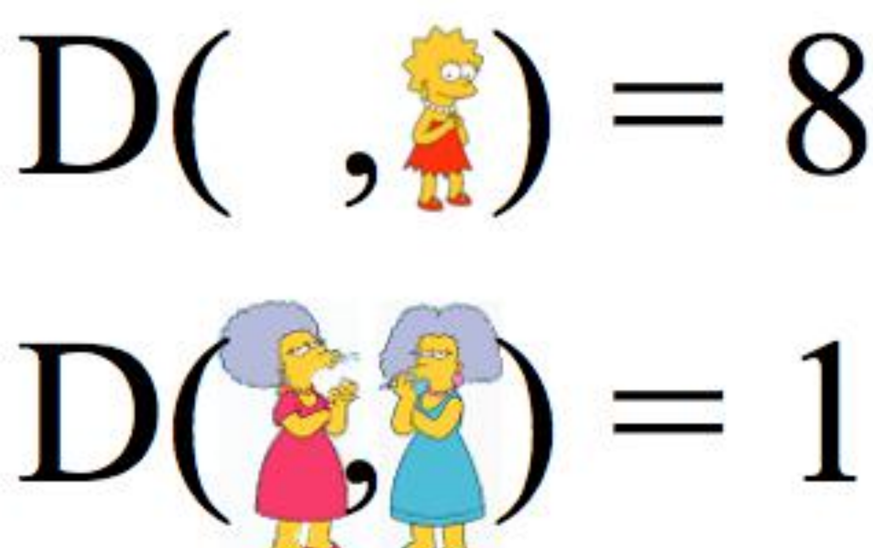
- The number of dendrograms with
  n leafs = (2n -3)!/[(2(n -2)) (n -2)!]

Number of leafs	Number of possible Dendrongrams
2	1
3	3
4	15
5	105
…	…
10	34,459,425

slide by Andrew Moore

We begin with a distance matrix which contains the distances between every pair of objects in our dataset

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



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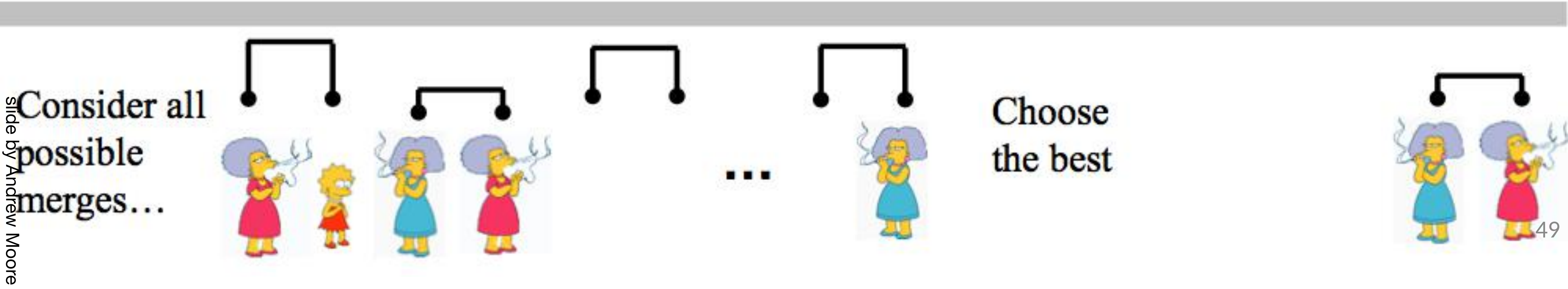
Bottom-Up (agglomerative):

Start with each item in its own cluster, find the best pair to merge into a new cluster. Repeat until all clusters are fused together.



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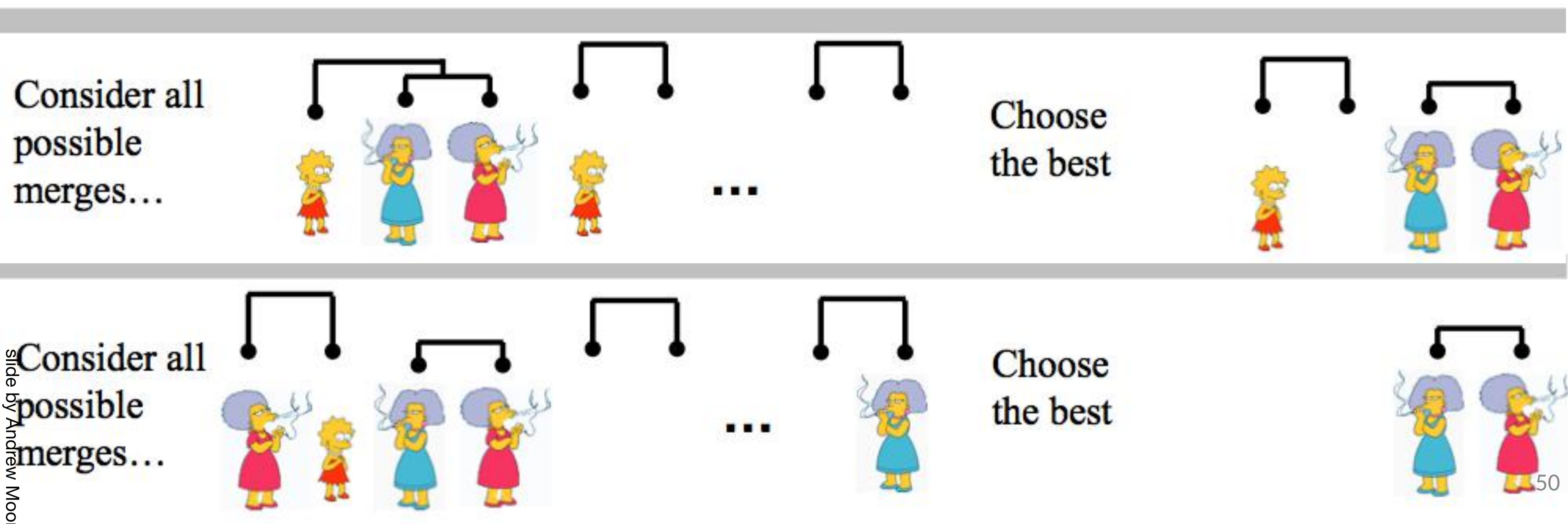

slide by Andrew Moore

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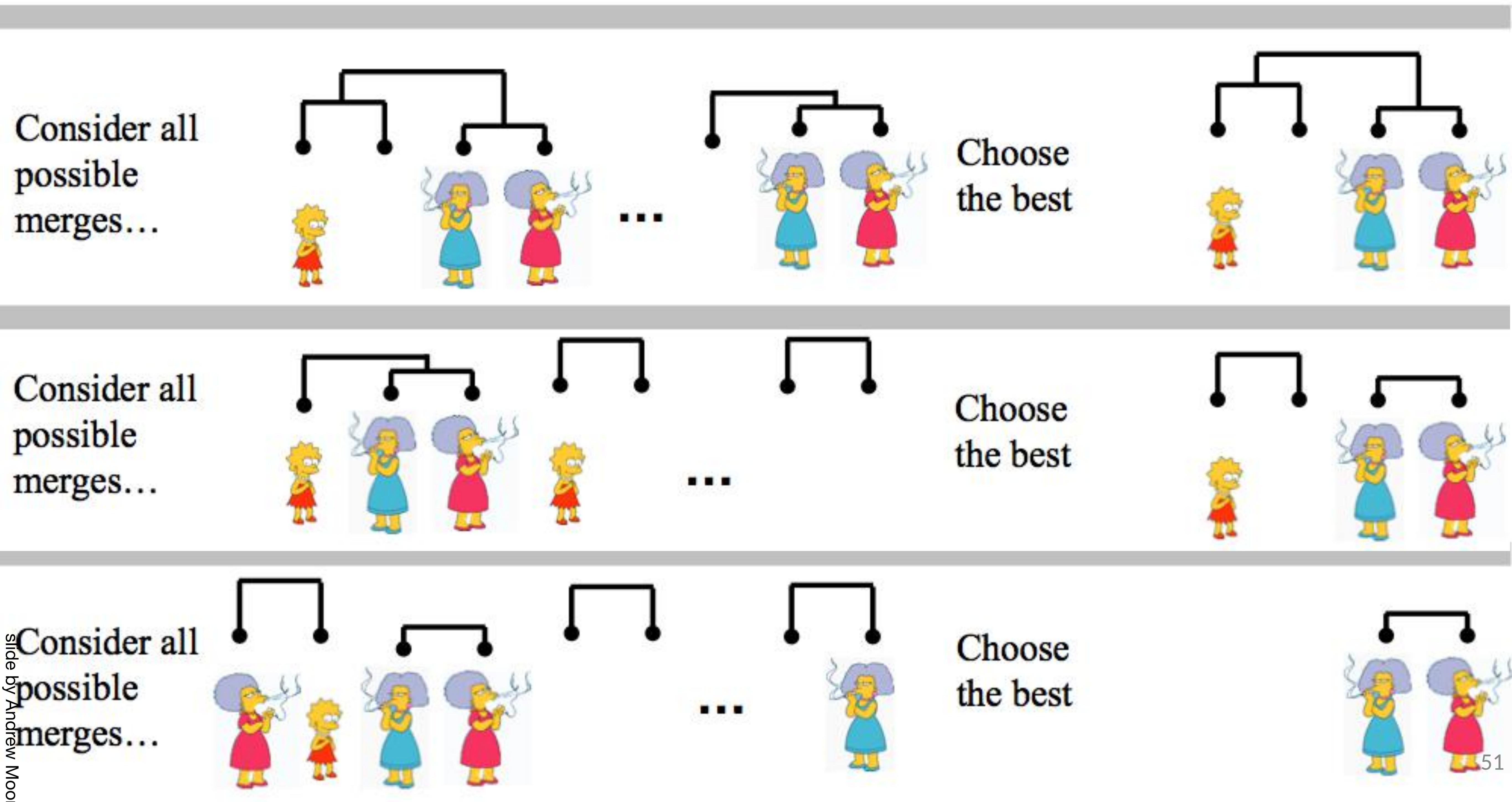

slide by Andrew Moore

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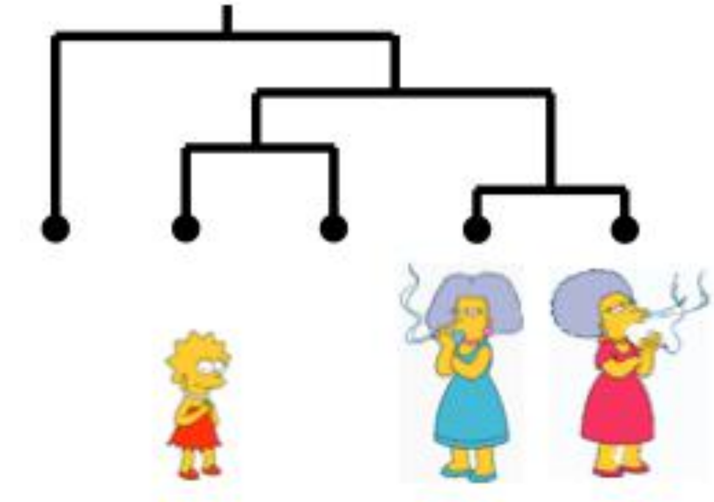
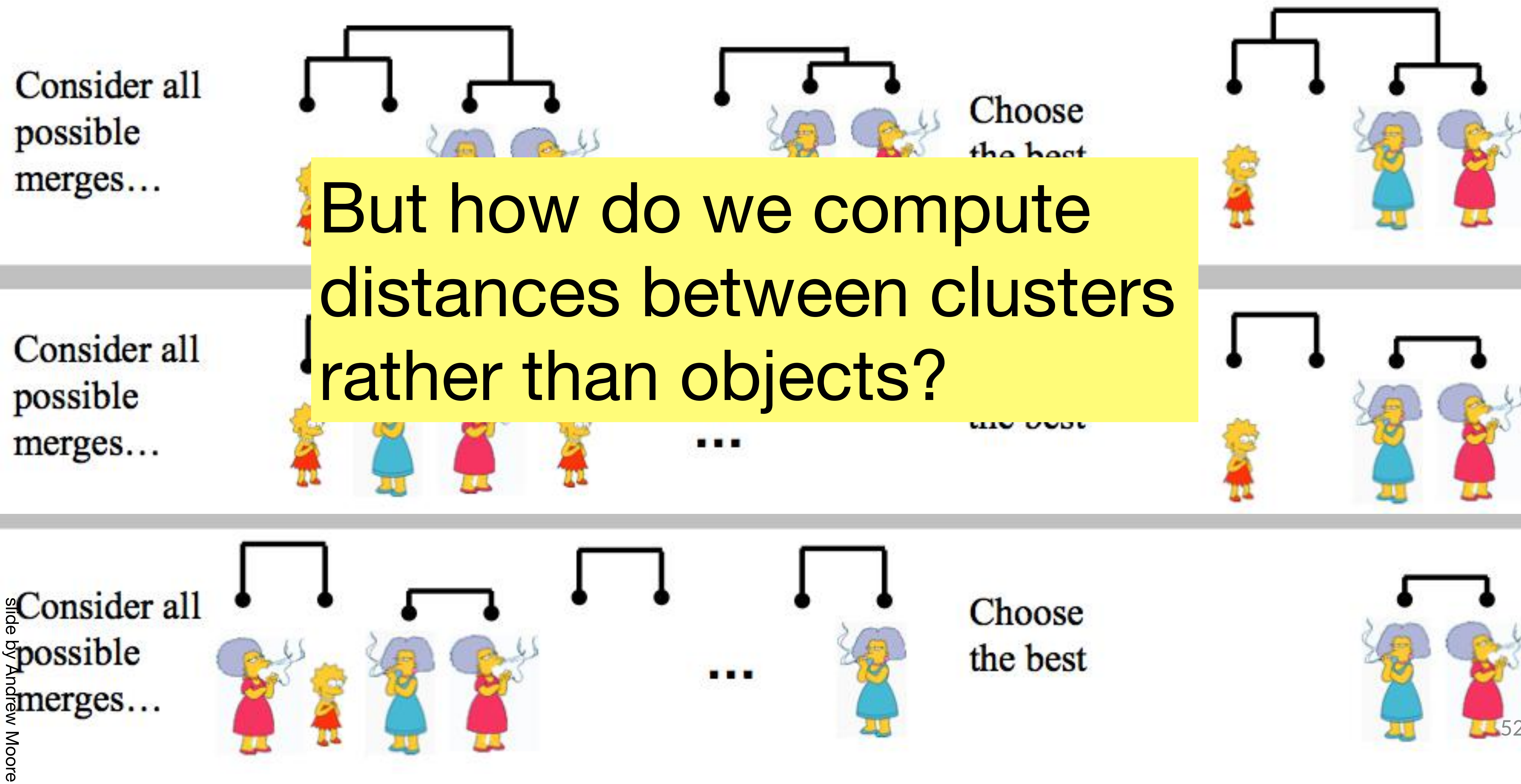
Start with each item in its own cluster, find the best pair to merge into a new cluster. Repeat until all clusters are fused together.





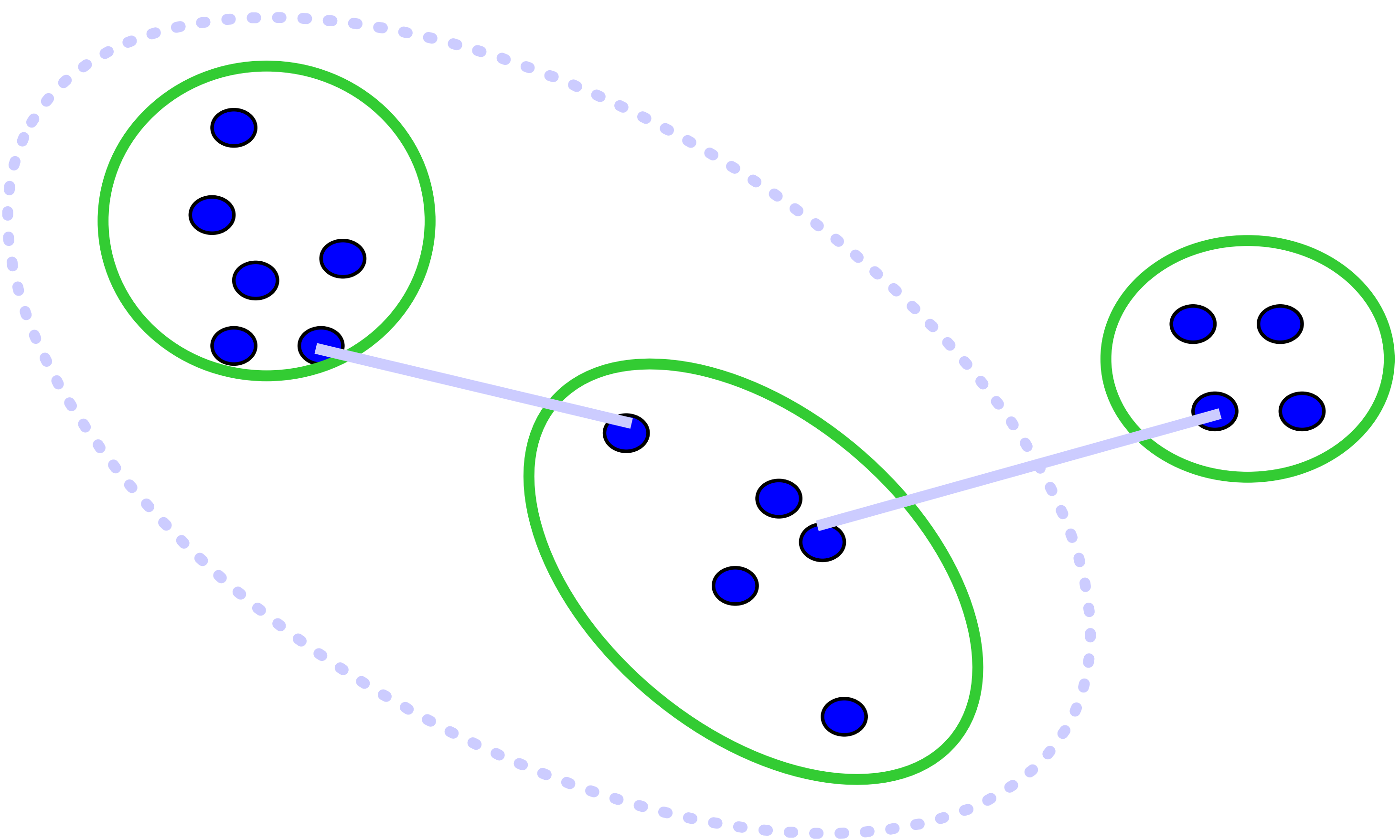
But how do we compute distances between clusters rather than objects?

slide by Andrew Moore

Computing distance between clusters: **Single Link**

- Cluster distance = distance of two closest members in each class

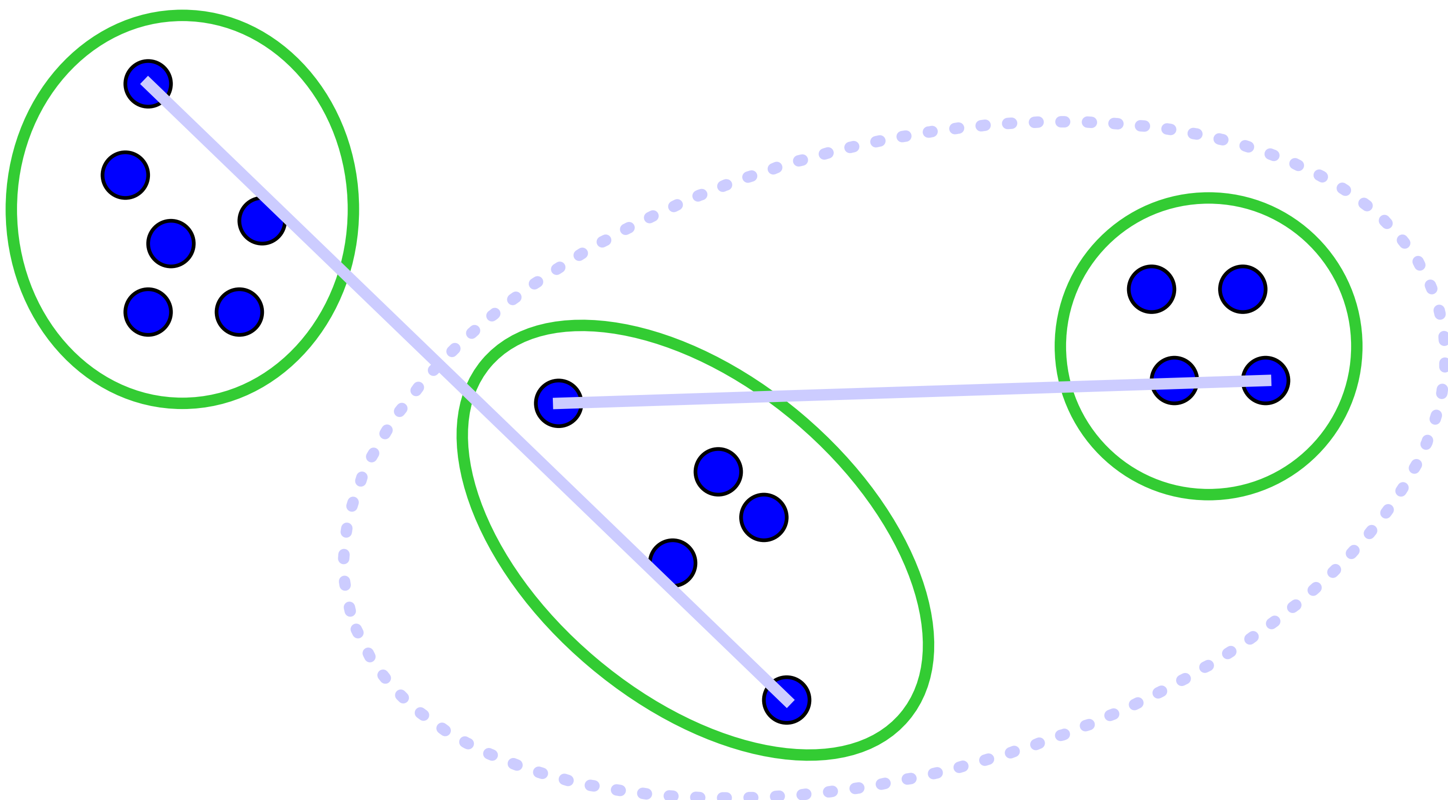
- Potentially long and skinny clusters



Computing distance between clusters: **Complete Link**

- Cluster distance = distance of two farthest members in each class

- Tight clusters



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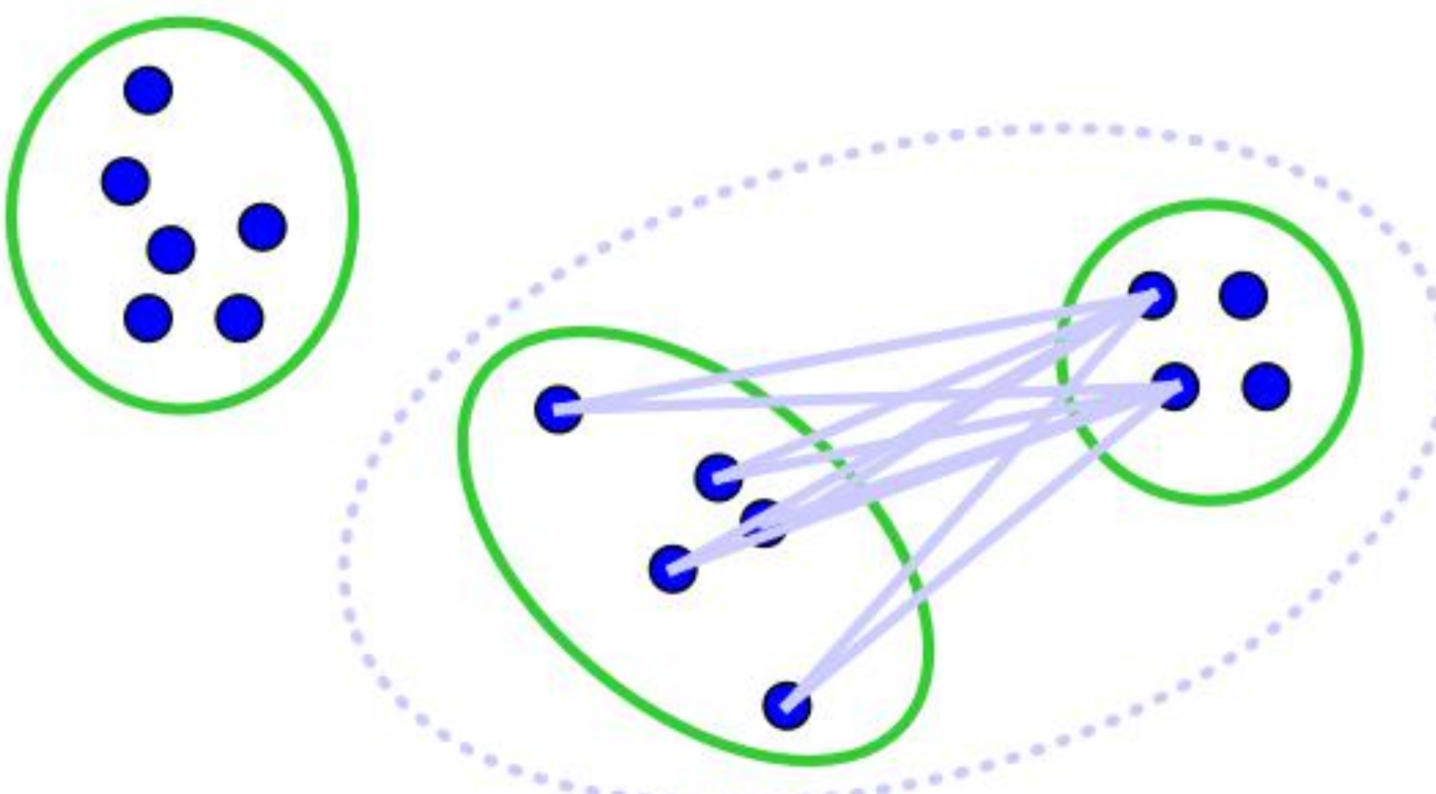
Computing distance between clusters: **Average Link**

- Cluster distance = average distance of all pairs



- The most widely used measure
- Robust against noise

slide by Andrew Moore

Agglomerative Clustering

Good

- Simple to implement, widespread application
- Clusters have adaptive shapes
- Provides a hierarchy of clusters

Bad

- May have imbalanced clusters
- Still have to choose number of clusters or threshold
  — **silhouette coefficient**
- Need to use an “ultrametric” to get a meaningful hierarchy

slide by Derek Hoiem

What is a good clustering?

What is a good clustering?

- Internal criterion: A good clustering will produce high quality clusters in which:
  - the intra-class (that is, intra-cluster) similarity is high
  - the inter-class similarity is low
  - The measured quality of a clustering depends on both the obj. representation and the similarity measure used
- External criteria for clustering quality
  - Quality measured by its ability to discover some or all of the hidden patterns or latent classes in gold standard data
  - Assesses a clustering with respect to ground truth
  - Example:
    - Purity
    - Entropy of classes in clusters (or Mutual Information between classes and clusters)

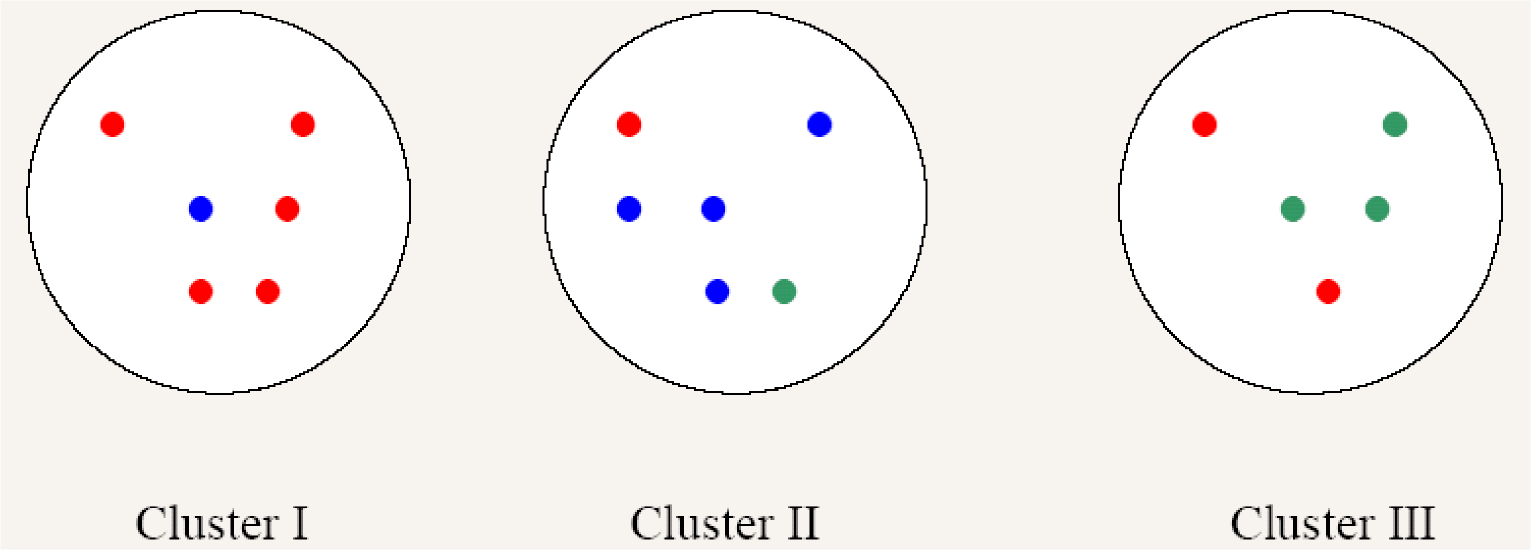
slide by Eric P. Xing

External Evaluation of Cluster Quality

- Simple measure: purity, the ratio between the dominant class in the cluster and the size of cluster
  - Assume documents with C gold standard classes, while our clustering algorithms produce K clusters, $\omega_1, \omega_2, ..., \omega_K$ with n_i members.

$$\text{purity}(\Omega, C) = \frac{1}{N} \sum_k \max_j |\omega_k \cap c_j|$$

  - Example:



purity = 1/17* (max(5, 1, 0)+max(1, 4, 1)+max(2, 0, 3))
= 1/17*(5+4+3) ≈ 0.71

slide by Eric P. Xing

External Evaluation of Cluster Quality

- Let:

  $$TC = TC_1 \cup TC_2 \cup \ldots \cup TC_n$$

  $$CC = CC_1 \cup CC_2 \cup \ldots \cup CC_m$$

  be the target and computed clusterings, respectively.

- $TC = CC =$ original set of data

- Define the following:
  - a: number of pairs of items that belong to the same cluster in both CC and TC
  - b: number of pairs of items that belong to different clusters in both CC and TC
  - c: number of pairs of items that belong to the same cluster in CC but different clusters in TC
  - d: number of pairs of items that belong to the same cluster in TC but different clusters in CC

slide by Christophe Giraud-Carrier

External Evaluation of Cluster Quality

$$P = \frac{a}{a + c}$$

$$R = \frac{a}{a + d}$$

$$F = \frac{2 \times P \times R}{P + R}$$

F-measure

$$\frac{a+b}{a+b+c+d}$$

Rand Index

Measure of clustering agreement: how similar are these two ways of partitioning the data?

slide by Christophe Giraud-Carrier

External Evaluation of Cluster Quality

$$\frac{a+b}{a+b+c+d}$$

Rand Index

$$\frac{2(ab-cd)}{(a+c)(c+b)+(a+d)(d+b)}$$

Adjusted Rand Index

Extension of the Rand index that attempts to account for items that may have been clustered by chance

slide by Christophe Giraud-Carrier

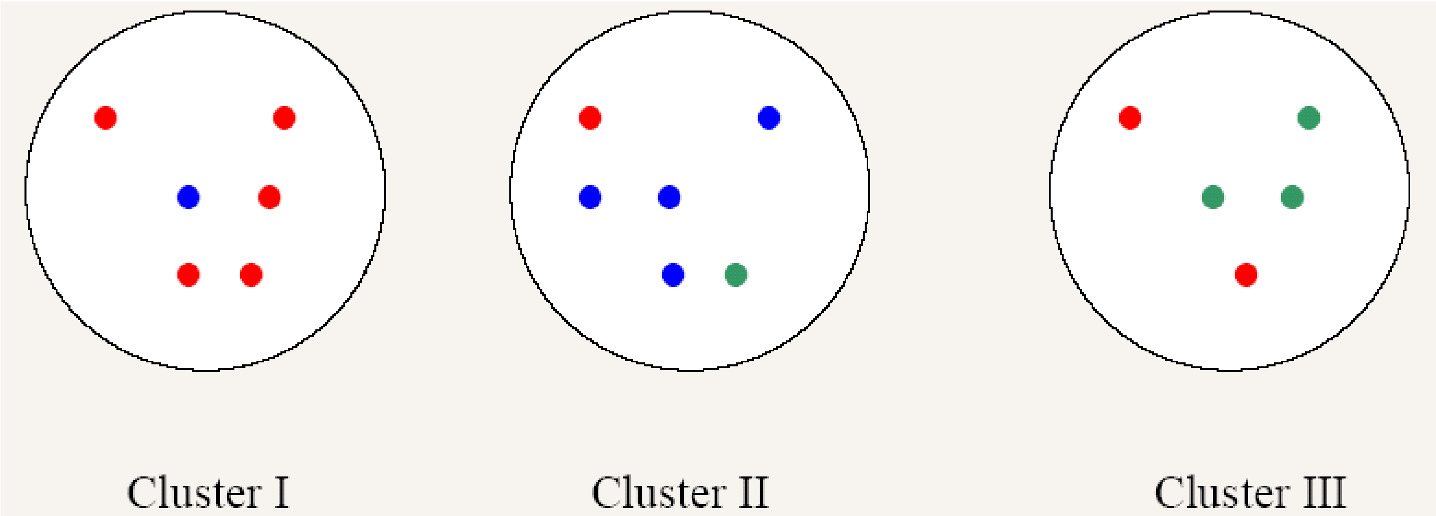
External Evaluation of Cluster Quality

$$Entropy(CC_i) = \sum_{TC_j \in TC} -p(TC_j \mid CC_i)\log p(TC_j \mid CC_i)$$

$$AvgEntropy(CC) = \sum_{i=1}^{m} \frac{|CC_i|}{|CC|} Entropy(CC_i)$$

Measure of purity wrt the target clustering

- Example:



$Entropy(CC_1)$ = (5/6)log(5/6) + (1/6)log(1/6) + (0/6)log(0/6) = -.650
$Entropy(CC_2)$ = (1/6)log(1/6) + (4/6)log(4/6) + (1/6)log(1/6) = -1.252
$Entropy(CC_3)$ = (2/5)log(2/5) + (0/5)log(0/5) + (3/5)log(3/5) = -.971

AvgEntropy(CC) = (-.650 * 6/17) + (-1.252 * 6/17) + (-.971 * 5/17)
AvgEntropy(CC) = -.956

Next Lecture:

Dimensionality Reduction