Clustering with k-means and Gaussian mixture distributions

Machine Learning and Category Representation 2012-2013

Jakob Verbeek, November 23, 2012

Course website:

http://lear.inrialpes.fr/~verbeek/MLCR.12.13

Objectives of visual recognition

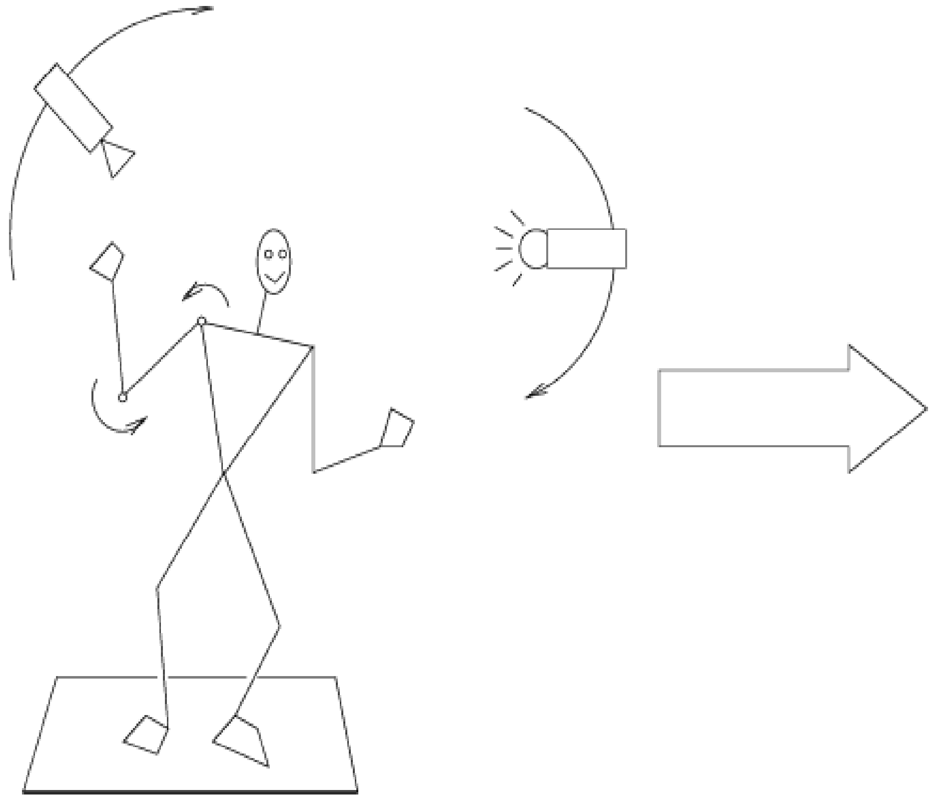
- **Image classification:** predict presence of objects in the image

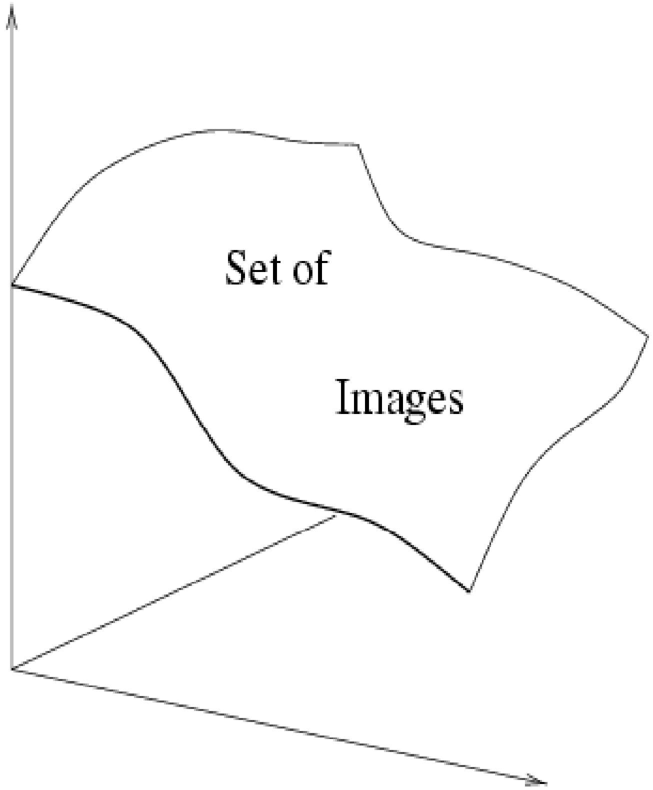
Car: present
Cow: present
Bike: not present
Horse: not present
...

- **Object localization:** define the location and the category

Category label
+ location

Difficulties: appearance variation of same object





- Variability in appearance of the same object:
  - Viewpoint and illumination,
  - occlusions,
  - articulation of deformable objects
  - ...

Difficulties: within-class variations

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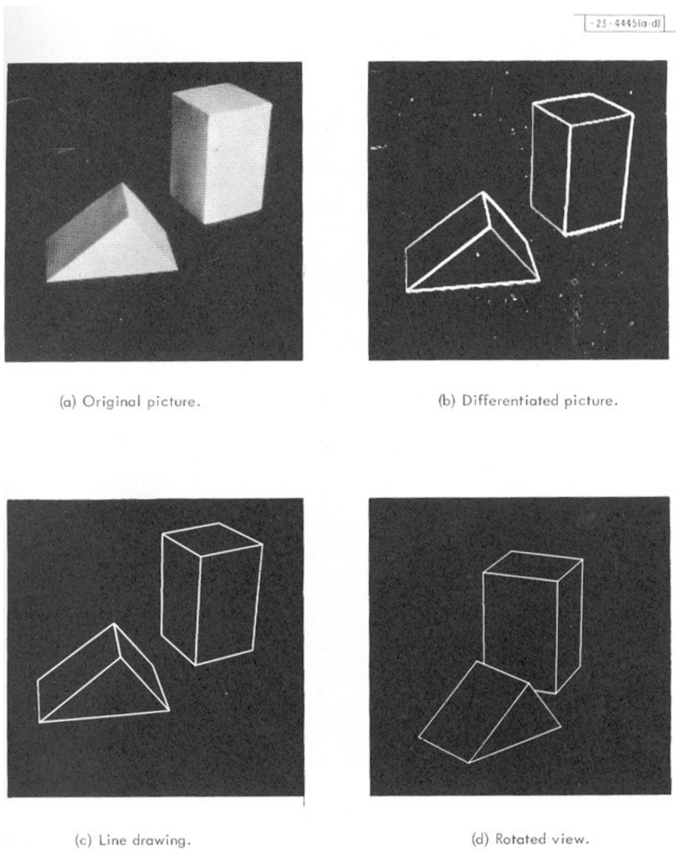
Visual category recognition

- Robust image description
  - Appropriate descriptors for objects and categories
  - Local descriptors to be robust against occlusions

- Machine learning techniques to learn models from examples
  - scene types (city, beach, mountains,...) : images
  - object categories (car, cat, person, ...) : cropped objects
  - human actions (run, sit-down, open-door, ...): video clips

Why machine learning?

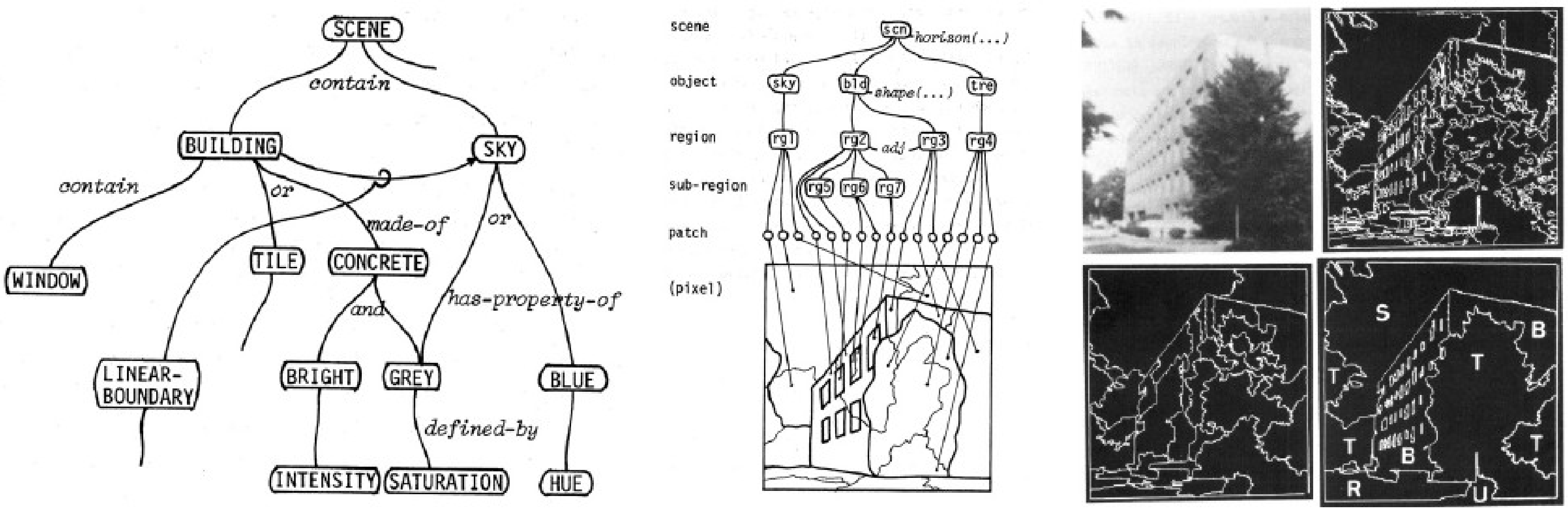
- Early approaches: simple features + handcrafted models
- Can handle only few images, simple tasks



L. G. Roberts, Ph.D. thesis
Machine Perception of Three Dimensional Solids,
MIT Department of Electrical Engineering, 1963.

Why machine learning?

- Early approaches: manual programming of rules
- Tedious, limited and does not take into account the data



(a) Bottom-up process (b) Top-down process (c) Result

Figure 3. A system developed in 1978 by Ohta, Kanade and Sakai [33, 32] for knowledge-based interpretation of outdoor natural scenes. The system is able to label an image (c) into semantic classes: S-sky, T-tree, R-road, B-building, U-unknown.

Y. Ohta, T. Kanade, and T. Sakai, "An Analysis System for Scenes Containing objects with Substructures," *International Joint Conference on Pattern Recognition*, 1978.

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Bag-of-features image classification

- Excellent results in the presence of
  - background clutter,
  - occlusion,
  - lighting variations,
  - viewpoint changes

bikes books building cars people phones trees

Bag-of-features image classification in a nutshell

1) Extract local image regions
   - For example using interest point detectors
2) Compute descriptors of these regions
   - For example SIFT descriptors

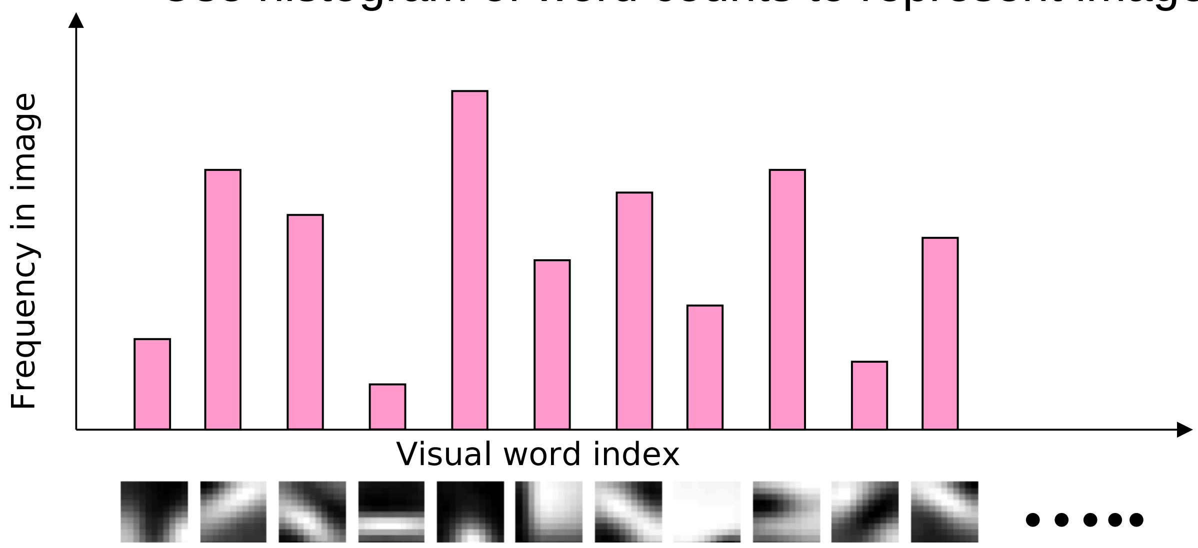
3) Aggregate the local descriptors into global image representation
   - **This is where clustering techniques come in**

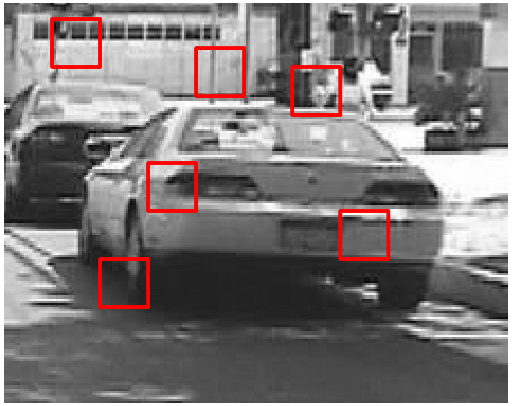
4) Classification of the image based on this representation
   - SVM or other classifier

Bag-of-features image classification in a nutshell

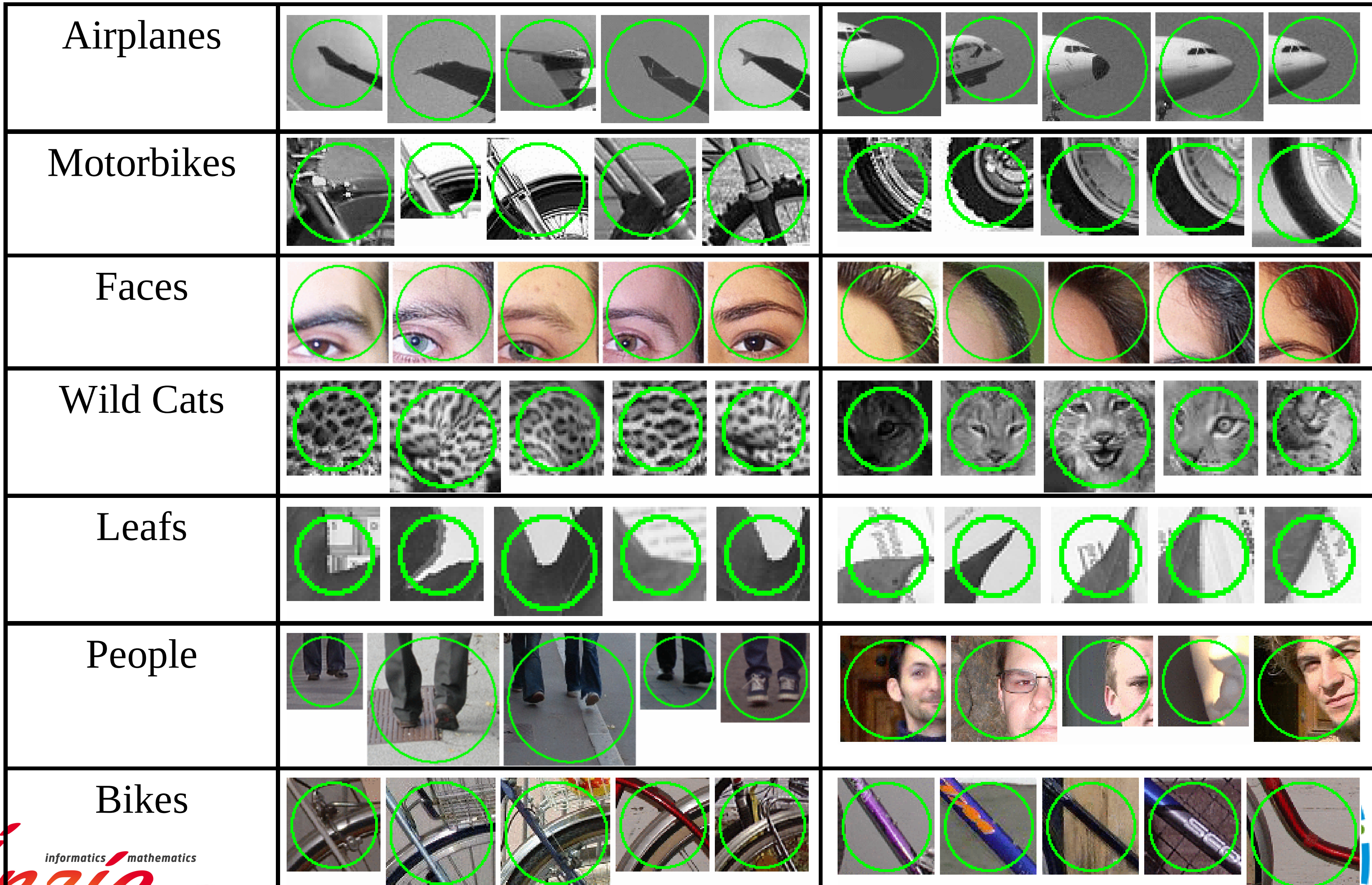
1) Extract local image regions
   - For example using interest point detectors
2) Compute descriptors of these regions
   - For example SIFT descriptors

3) Aggregate the local descriptors into bag-of-word histogram
   - Map each local descriptor to one of K clusters (a.k.a. “visual words”)
   - Use histogram of word counts to represent image





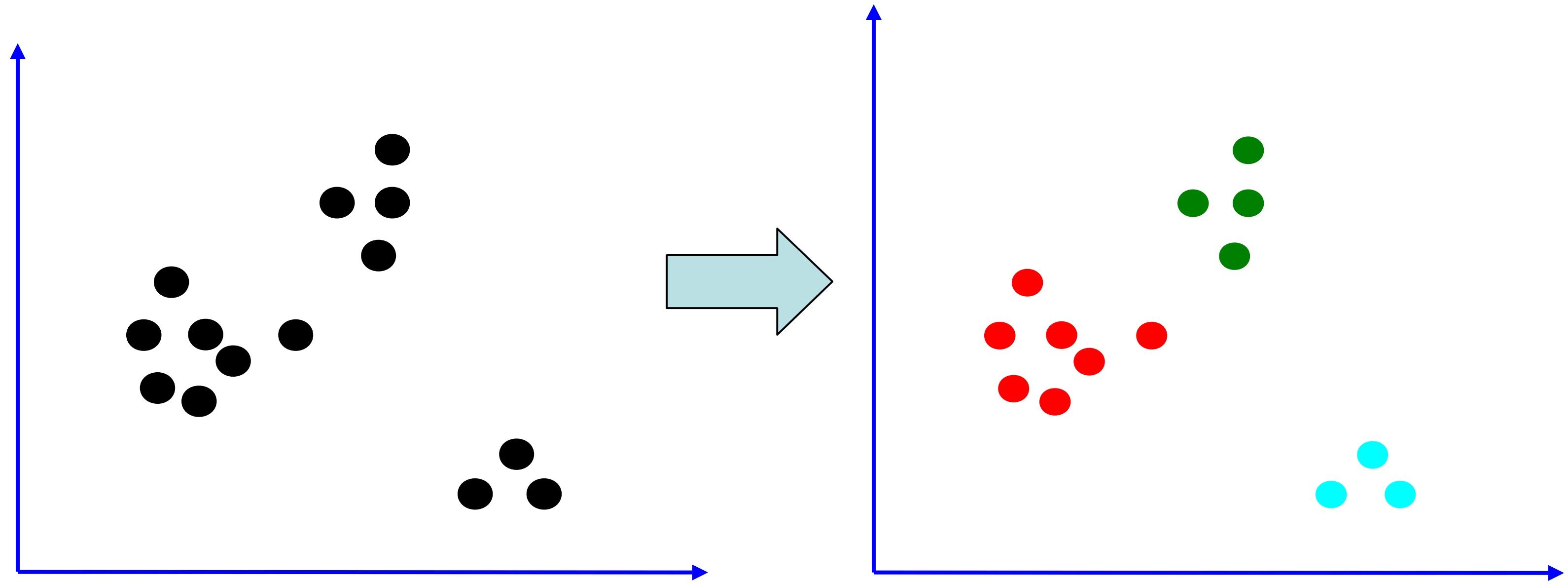
Example visual words found by clustering



Clustering

- Finding a group structure in the data
  - Data in one cluster similar to each other
  - Data in different clusters dissimilar

- Map each data point to a discrete cluster index
  - “flat” methods find K groups
  - “hierarchical” methods define a tree structure over the data

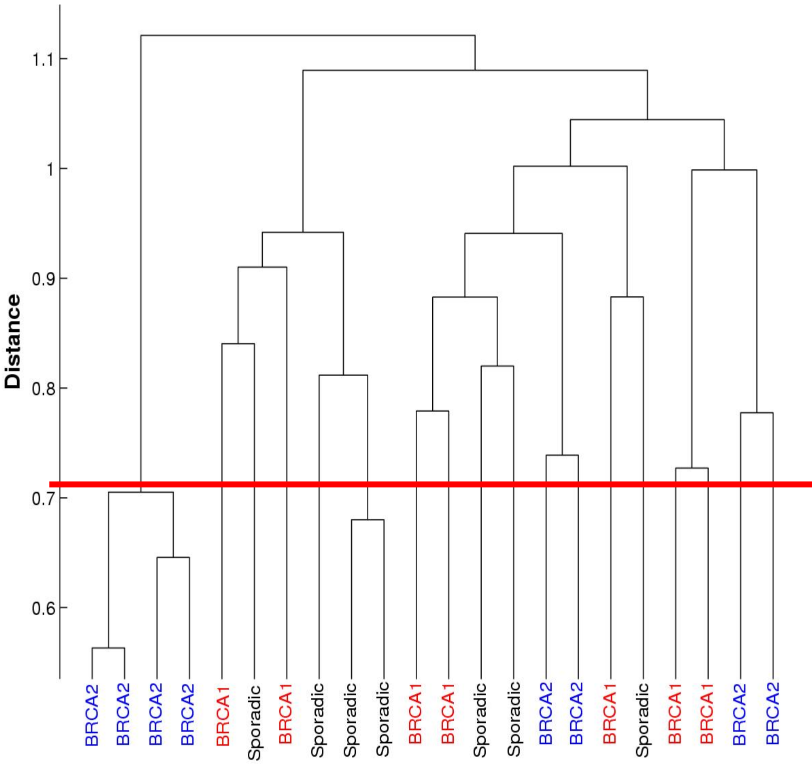


Hierarchical Clustering

- Data set is organized into a tree structure

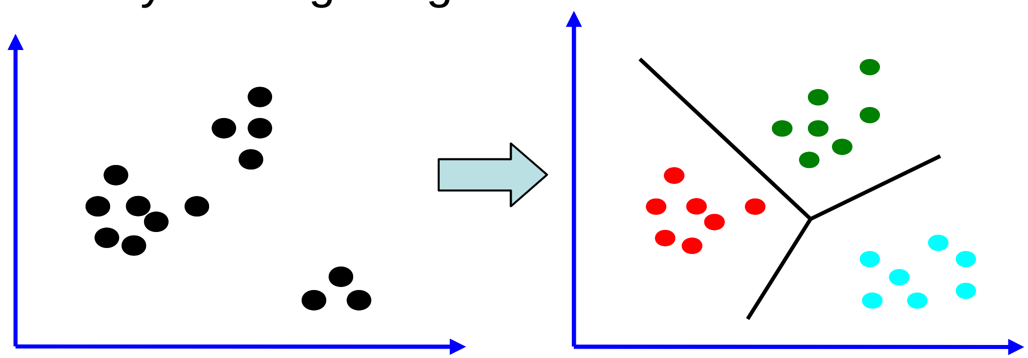
- Top-down construction
  - Start all data in one cluster: root node
  - Apply “flat” clustering into k groups
  - Recursively cluster the data in each group

- Bottom-up construction
  - Start with all points in separate cluster
  - Recursively merge “closest” clusters
  - Distance between clusters A and B
    - E.g. min, max, or mean distance between x in A, and y in B

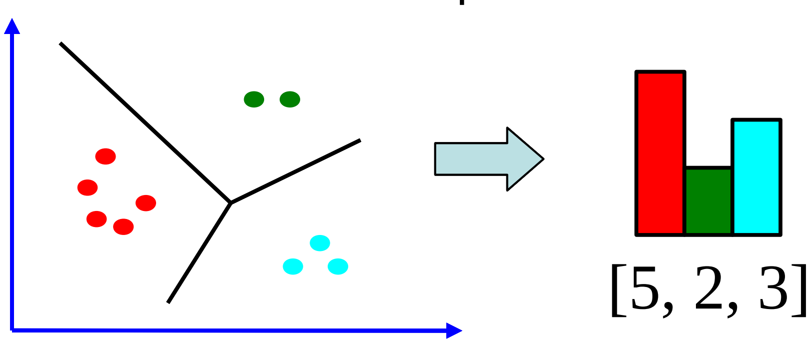


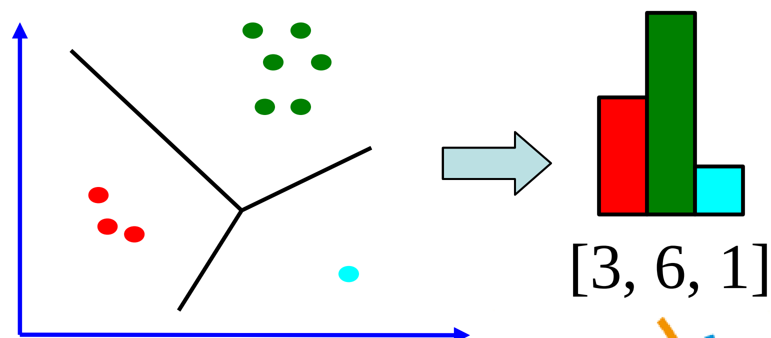
Clustering descriptors into visual words

- **Offline clustering**: Find groups of similar local descriptors
  - Using many descriptors from many training images



- **Encoding a new image:**
  - Detect local regions
  - Compute local descriptors
  - Count descriptors in each cluster





Definition of k-means clustering

- Given: data set of N points x_n, n=1,…,N
- Goal: find K cluster centers m_k, k=1,…,K

  that **minimize the squared distance to nearest cluster centers**

$$E\left(\{m_k\}_{k=1}^{K}\right)=\sum_{n=1}^{N} min_{k\in\{1,\ldots,K\}}\|x_n-m_k\|^2$$

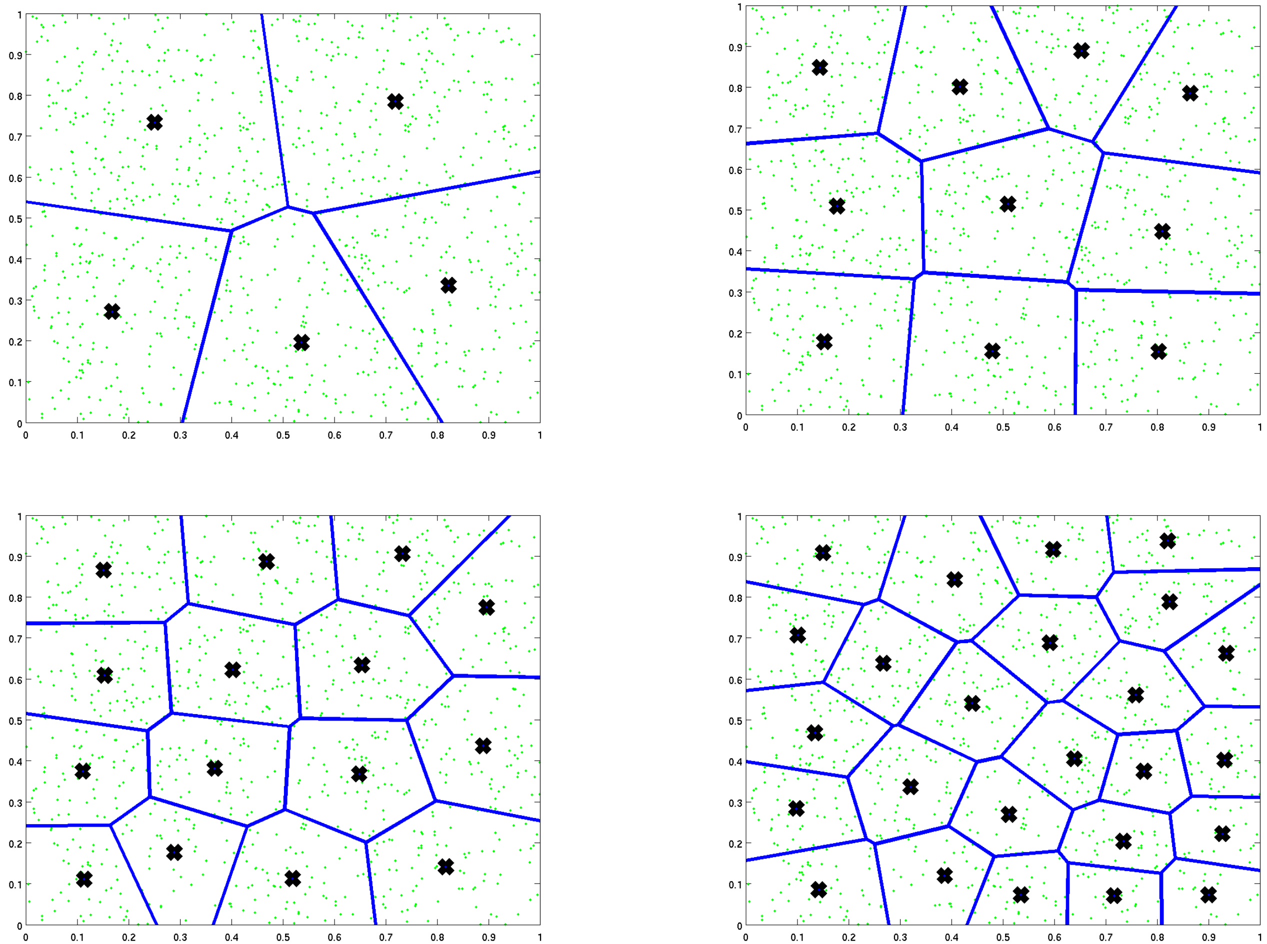
- **Clustering = assignment** of data points to nearest cluster center
  - Indicator variables r_{nk}=1 if x_n assgined to x_n, r_{nk}=0 otherwise

- **For fixed cluster centers**, error criterion equals sum of squared distances between each data point and assigned cluster center

$$E\left(\{m_k\}_{k=1}^{K}\right)=\sum_{n=1}^{N}\sum_{k=1}^{K} r_{nk}\|x_n-m_k\|^2$$

Examples of k-means clustering

- Data uniformly sampled in unit square
- k-means with 5, 10, 15, and 25 centers



Minimizing the error function

- Goal find centers m_k to minimize the error function

$$E\left(\{m_k\}_{k=1}^{K}\right)=\sum_{n=1}^{N} min_{k\in\{1,\dots,K\}} \|x_n-m_k\|^2$$

- **Any set of assignments**, not only the best assignment, **gives an upper-bound on the error:**

$$F\left(\{m_k\}_{k=1}^{K}\right)=\sum_{n=1}^{N}\sum_{k=1}^{K} r_{nk}\|x_n-m_k\|^2$$

- The iterative **k-means algorithm** minimizes this bound
  1) Initialize cluster centers, eg. on randomly selected data points
  2) **Update assignments** r_{nk} for fixed centers m_k
  3) **Update centers** m_k for fixed data assignments r_{nk}
  4) If cluster centers changed: return to step 2
  5) Return cluster centers

Minimizing the error bound

$$F\left(\{m_k\}_{k=1}^{K}\right) = \sum_{n=1}^{N} \sum_{k=1}^{K} r_{nk} \|x_n - m_k\|^2$$

- **Update assignments** r_{nk} for fixed centers m_k
  - Decouples over the data points
  - Constraint: exactly one r_{nk}=1, rest zero
  - Solution: assign to closest center

$$\sum_k r_{nk} \|x_n - m_k\|^2$$

- **Update centers** m_k for fixed assignments r_{nk}
  - Decouples over the centers
  - Set derivative to zero
  - Put center at mean of assigned data points

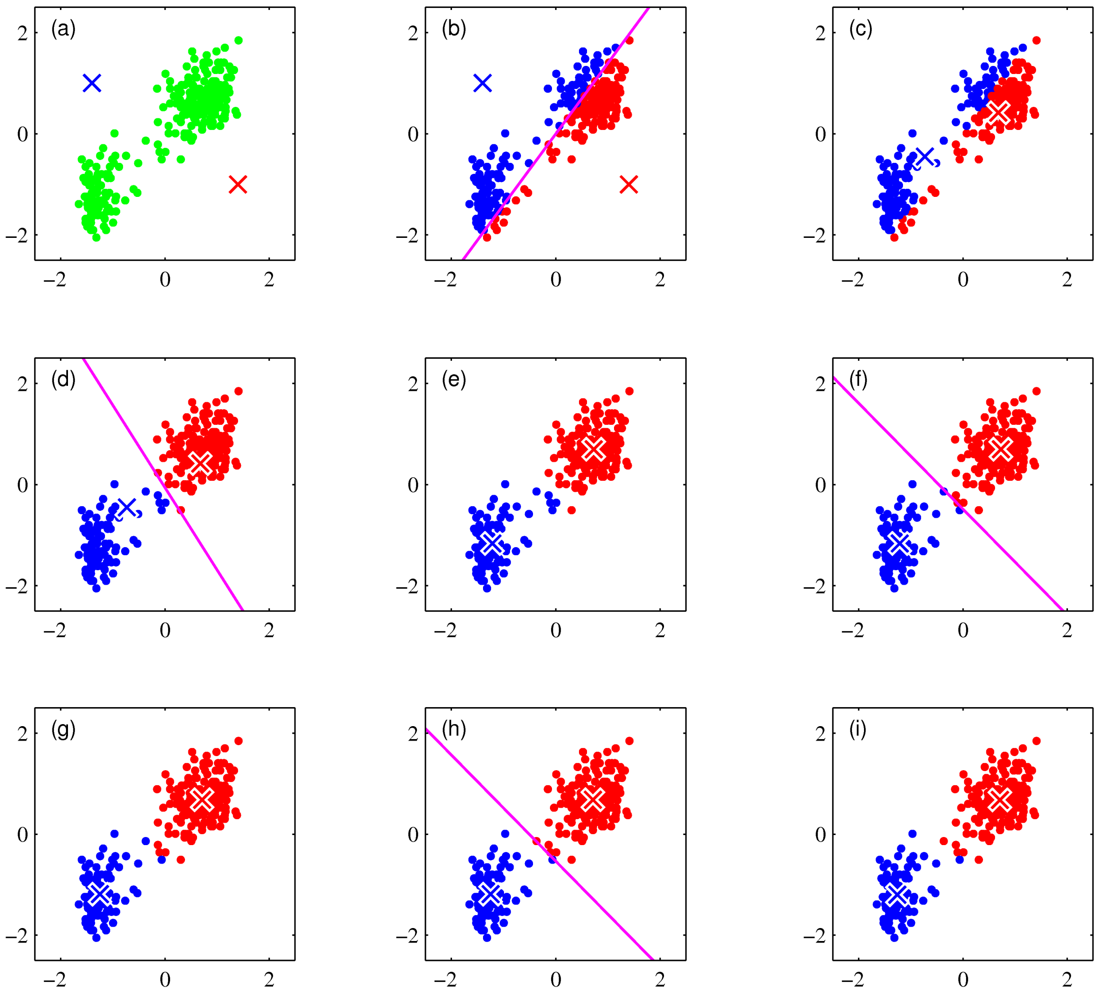
$$\sum_n r_{nk} \|x_n - m_k\|^2$$

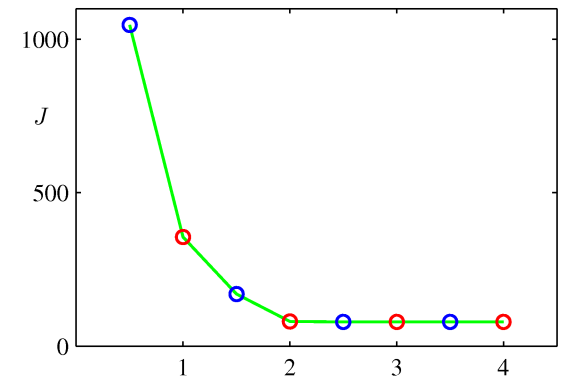
$$\frac{\partial F}{\partial m_k} = 2 \sum_n r_{nk} (x_n - m_k) = 0$$

$$m_k = \frac{\sum_n r_{nk} x_n}{\sum_n r_{nk}}$$

Examples of k-means clustering

- Several k-means iterations with two centers





Error function

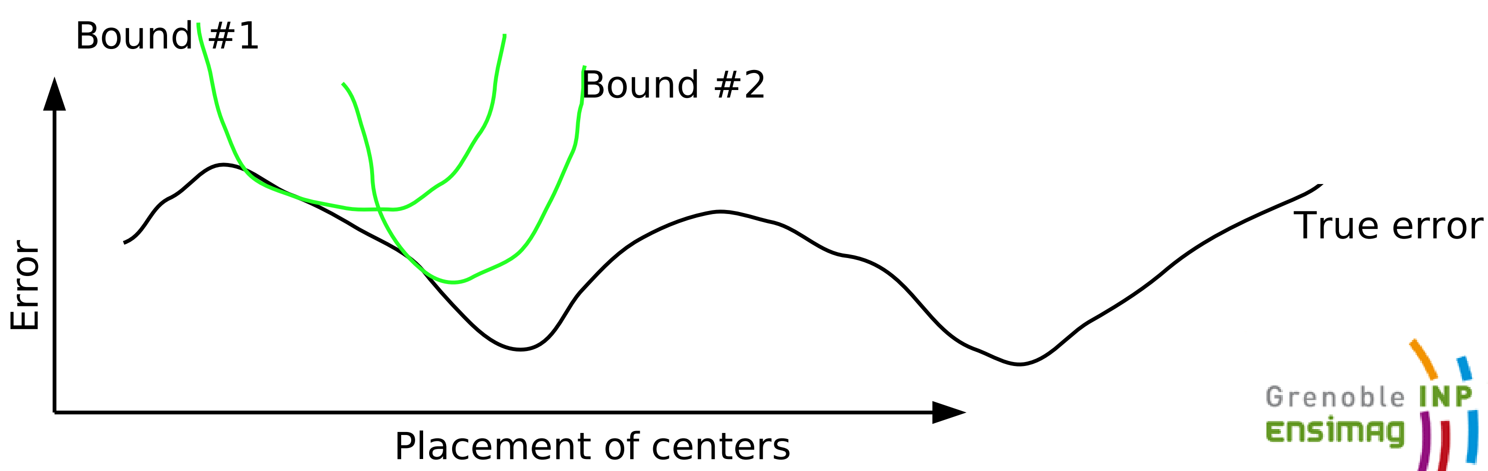
Minimizing the error function

$$E\left(\{m_k\}_{k=1}^{K}\right)=\sum_{n=1}^{N} min_{k\in\{1,\ldots,K\}} \|x_n-m_k\|^2$$

- Goal find centers m_k to minimize the error function
  - Proceeded by iteratively minimizing the error bound

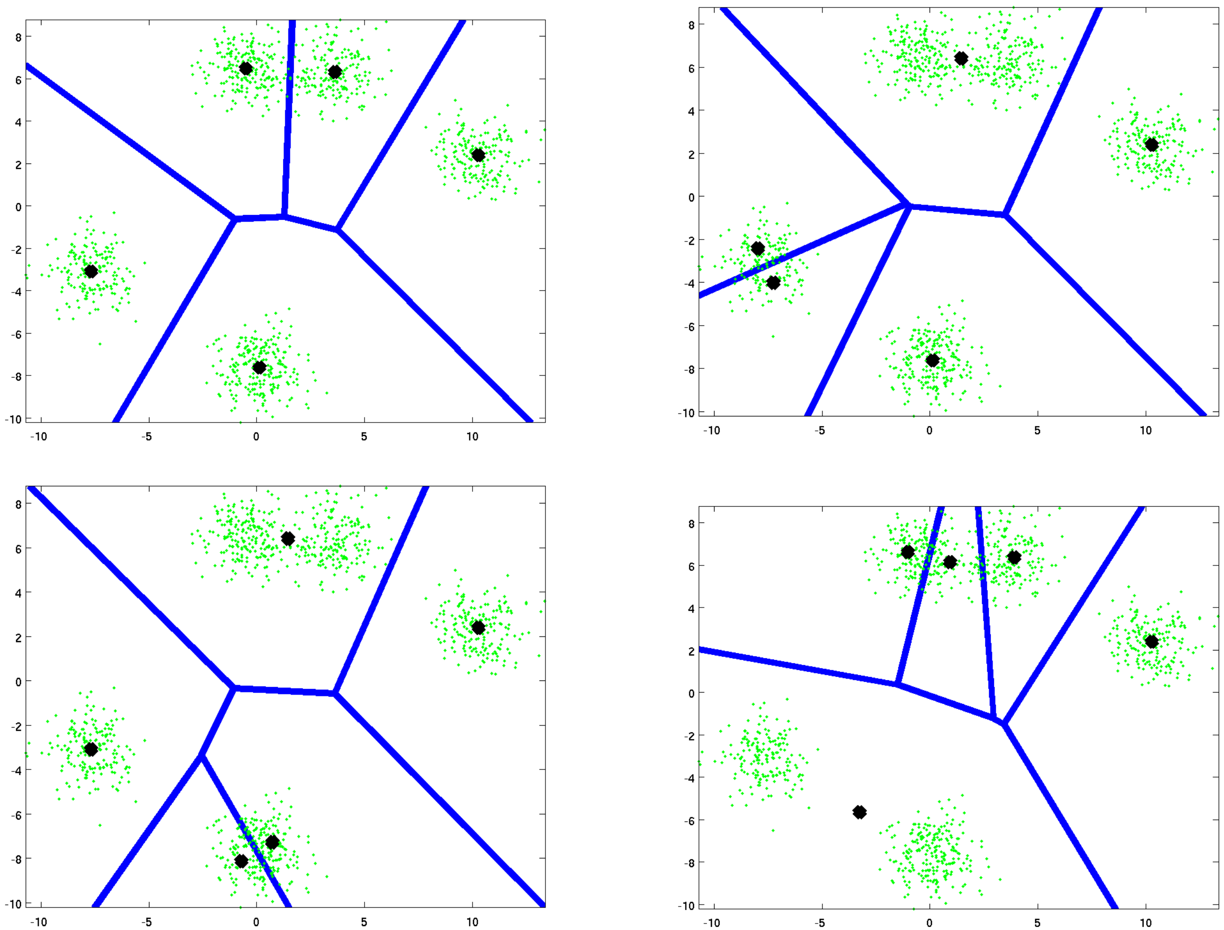
$$F\left(\{m_k\}_{k=1}^{K}\right)=\sum_{n=1}^{N}\sum_{k=1}^{K} r_{nk}\|x_n-m_k\|^2$$

- **K-means iterations monotonically decrease error function since**
  - Both steps reduce the error bound
  - Error bound matches true error after update of the assignments



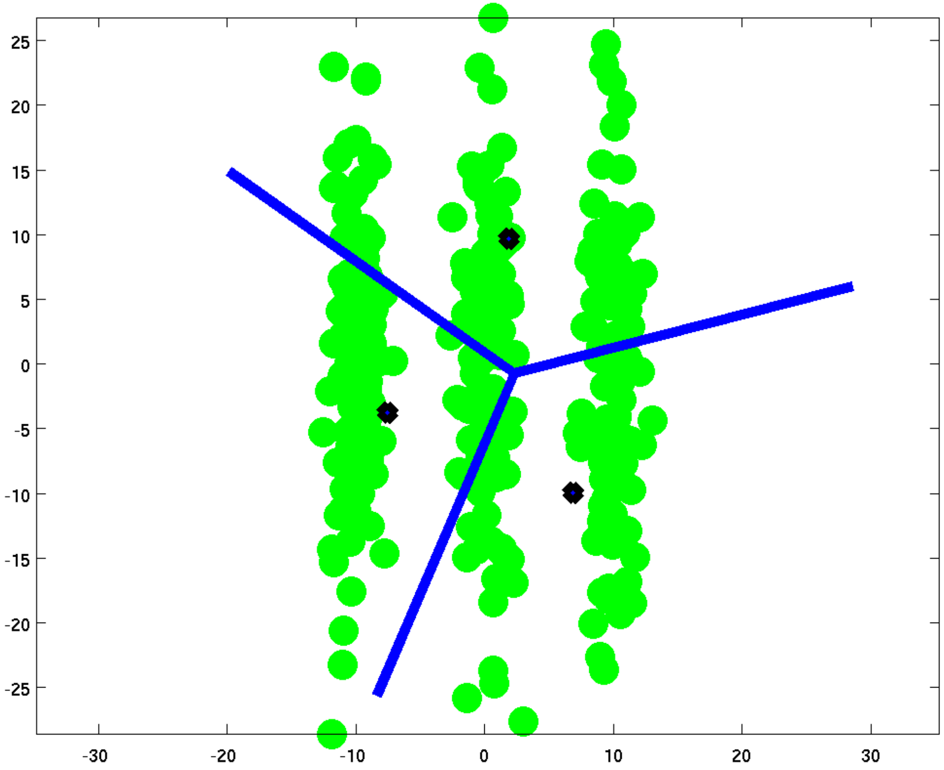
Problems with k-means clustering

- Solution depends heavily on initialization
  - Several runs from different initializations



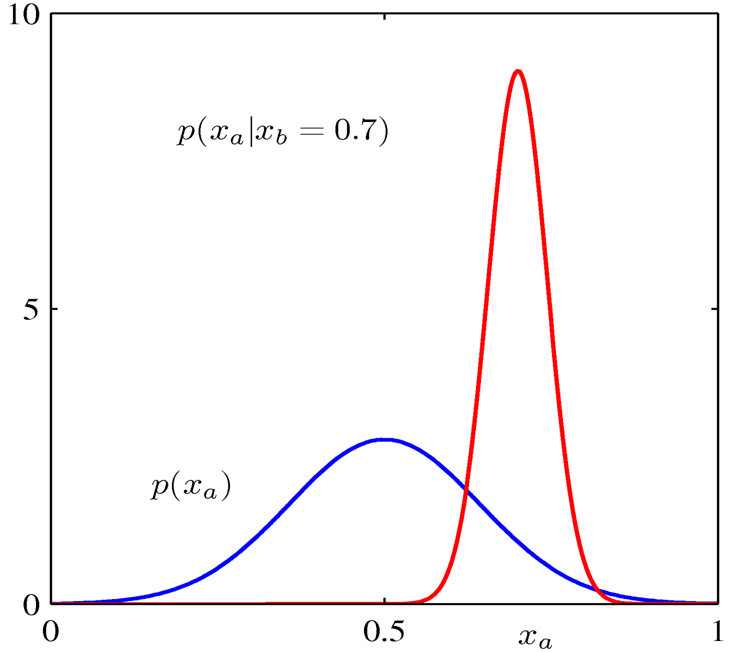
Problems with k-means clustering

- Assignment of data to clusters is only based on the distance to center
  - No representation of the shape of the cluster
  - Implicitly assumes spherical shape of clusters

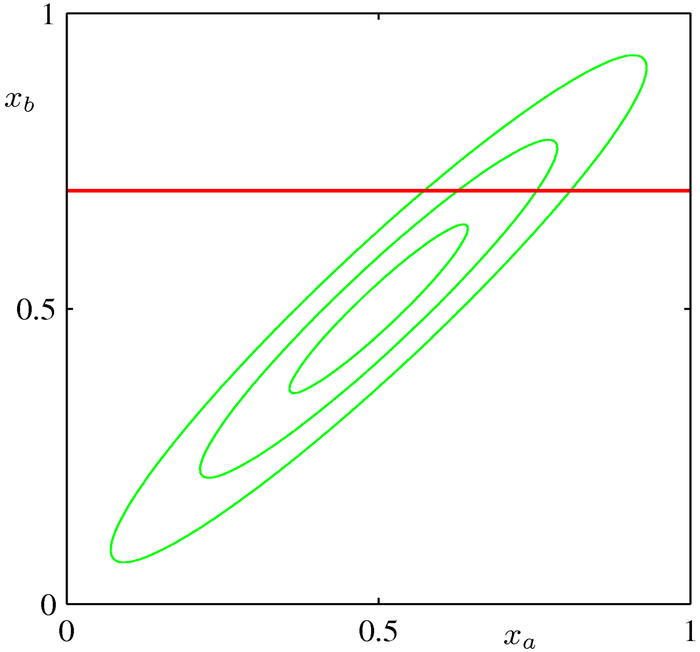


Clustering with Gaussian mixture density

- Each cluster represented by Gaussian density
  - Parameters: center m, covariance matrix C
  - Covariance matrix encodes spread around center,
    can be interpreted as defining a non-isotropic distance around center



Two Gaussians in 1 dimension



A Gaussian in 2 dimensions

Clustering with Gaussian mixture density

- Each cluster represented by Gaussian density
  - Parameters: center m, covariance matrix C
  - Covariance matrix encodes spread around center,
    can be interpreted as defining a non-isotropic distance around center

- Definition of Gaussian density in d dimensions

$$N(x|m,C) = (2\pi)^{-d/2} |C|^{-1/2} \exp\left(-\frac{1}{2}(x-m)^T C^{-1} (x-m)\right)$$

Determinant of
covariance matrix C

Quadratic function of
point x and mean m
Mahanalobis distance

Mixture of Gaussian (MoG) density

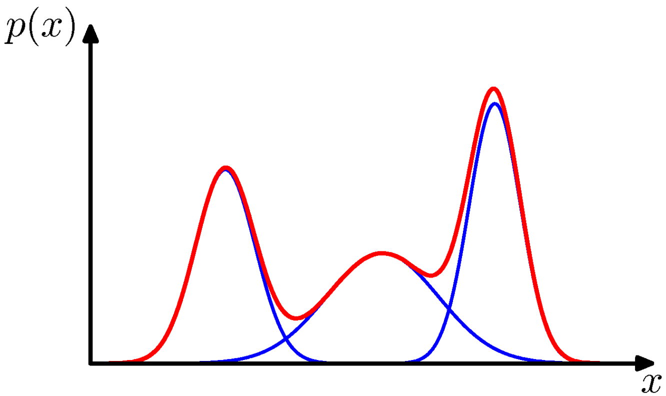
- Mixture density is weighted sum of Gaussian densities
  - Mixing weight: importance of each cluster

$$p(x) = \sum_{k=1}^{K} \pi_k N(x|m_k, C_k)$$

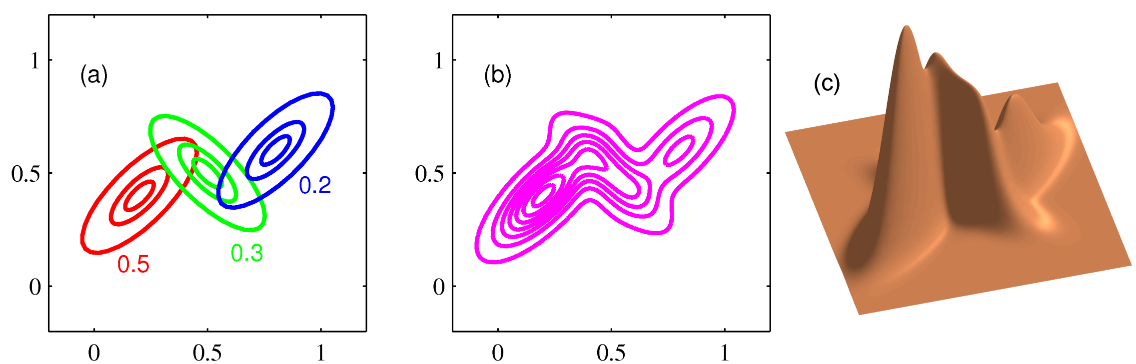
- Density has to integrate to 1, so we require

$$\pi_k \geq 0$$

$$\sum_{k=1}^{K} \pi_k = 1$$



Mixture in 1 dimension



Mixture in 2 dimensions

Clustering with Gaussian mixture density

- Given: data set of N points x_n, n=1,…,N
- Find mixture of Gaussians (MoG) that best explains data
  - Maximize log-likelihood of fixed data set w.r.t. parameters of MoG
  - Assume data points are drawn independently from MoG

$$L(\theta) = \sum_{n=1}^{N} \log p(x_n) = \sum_{n=1}^{N} \log \sum_{k=1}^{K} \pi_k N(x_n | m_k, C_k)$$

$$\theta = \{\pi_k, m_k, C_k\}_{k=1}^{K}$$

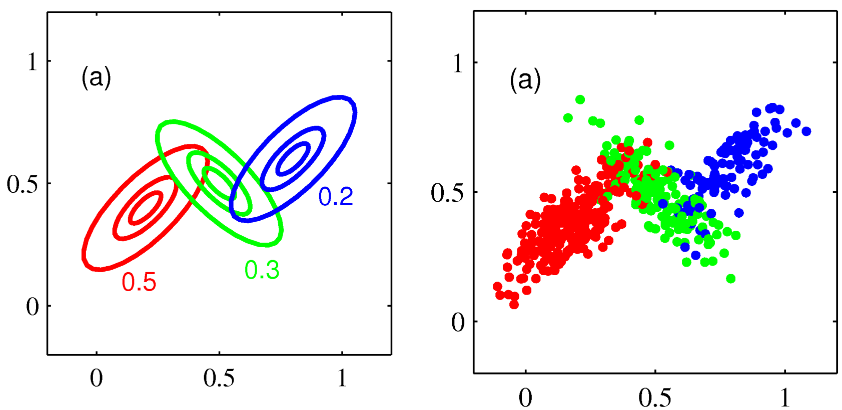
- MoG learning very similar to k-means clustering
  - Also an iterative algorithm to find parameters
  - Also sensitive to initialization of paramters

Assignment of data points to clusters

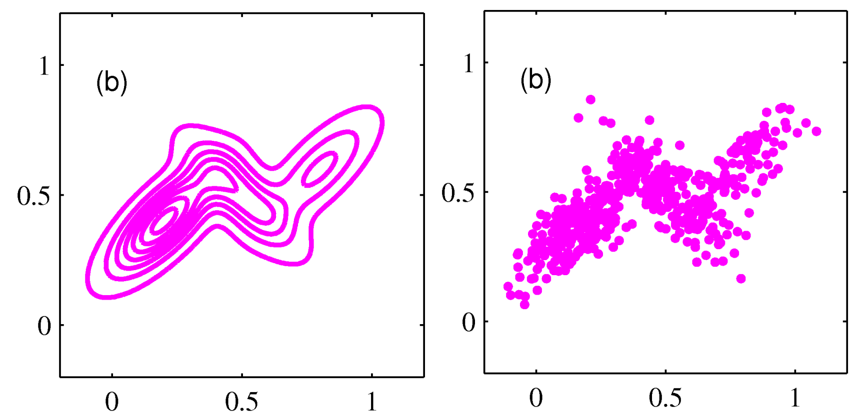
- As with k-means z_n indicates cluster index for x_n
- To sample data point from MoG
  - Select cluster with probability given by mixing weight $p(z=k)=\pi_k$
  - Sample point from the k-th Gaussian $p(x|z=k)=N(x|m_k, C_k)$
  - MoG recovered if we marginalize over the unknown cluster index

$$p(x)=\sum_k p(z=k)\,p(x|z=k)=\sum_k \pi_k N(x|m_k, C_k)$$

Color coded model and data of each cluster



Mixture model and data from it



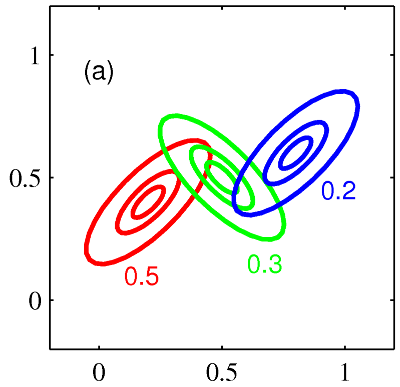
Soft assignment of data points to clusters

- Given data point x, infer cluster index z

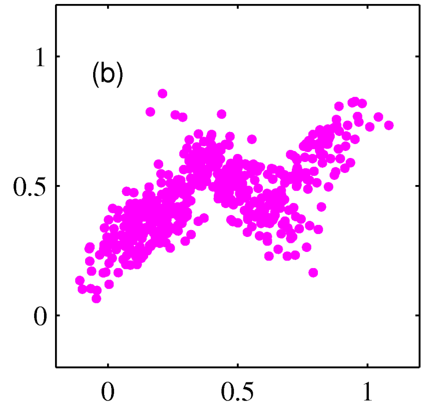
$$p(z=k|x)=\frac{p(z=k,x)}{p(x)}$$

$$=\frac{p(z=k)\,p(x|z=k)}{\sum_k p(z=k)\,p(x|z=k)}=\frac{\pi_k N(x|m_k,C_k)}{\sum_k \pi_k N(x|m_k,C_k)}$$

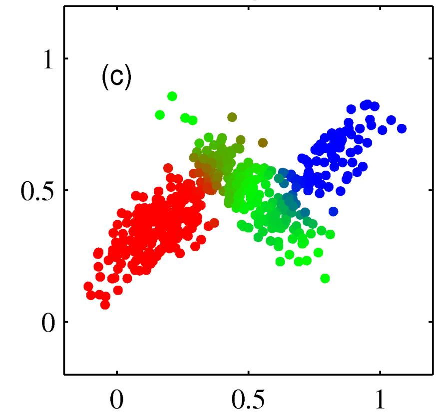
MoG model



Data



Color-coded soft-assignments



Maximum likelihood estimation of single Gaussian

- Given data points x_n, n=1,…,N
- Find **single Gaussian** that maximizes data log-likelihood

$$L(\theta)=\sum_{n=1}^{N}\log p(x_n)=\sum_{n=1}^{N}\log N(x_n|m,C)=\sum_{n=1}^{N}\left(-\frac{d}{2}\log\pi-\frac{1}{2}\log|C|-\frac{1}{2}(x_n-m)^T C^{-1}(x_n-m)\right)$$

- Set derivative of data log-likelihood w.r.t. parameters to zero

$$\frac{\partial L(\theta)}{\partial m}=C^{-1}\sum_{n=1}^{N}(x_n-m)=0$$

$$m=\frac{1}{N}\sum_{n=1}^{N}x_n$$

$$\frac{\partial L(\theta)}{\partial C^{-1}}=\sum_{n=1}^{N}\left(\frac{1}{2}C-\frac{1}{2}(x_n-m)(x_n-m)^T\right)=0$$

$$C=\frac{1}{N}\sum_{n=1}^{N}(x_n-m)(x_n-m)^T$$

- Parameters set as **data covariance and mean**

Maximum likelihood estimation of MoG

- No simple equation as in the case of a single Gaussian
- Use **EM algorithm**
  - Initialize MoG: parameters or soft-assign
  - E-step: soft assign of data points to clusters
  - M-step: update the mixture parameters
  - Repeat EM steps, terminate if converged
    - Convergence of parameters or assignments

- E-step: compute **soft-assignments**: $q_{nk} = p(z=k|x_n)$
- M-step: **update Gaussians** from weighted data points

$$\pi_k = \frac{1}{N} \sum_{n=1}^{N} q_{nk}$$

$$m_k = \frac{1}{N \pi_k} \sum_{n=1}^{N} q_{nk} x_n$$

$$C_k = \frac{1}{N \pi_k} \sum_{n=1}^{N} q_{nk} (x_n - m_k)(x_n - m_k)^T$$

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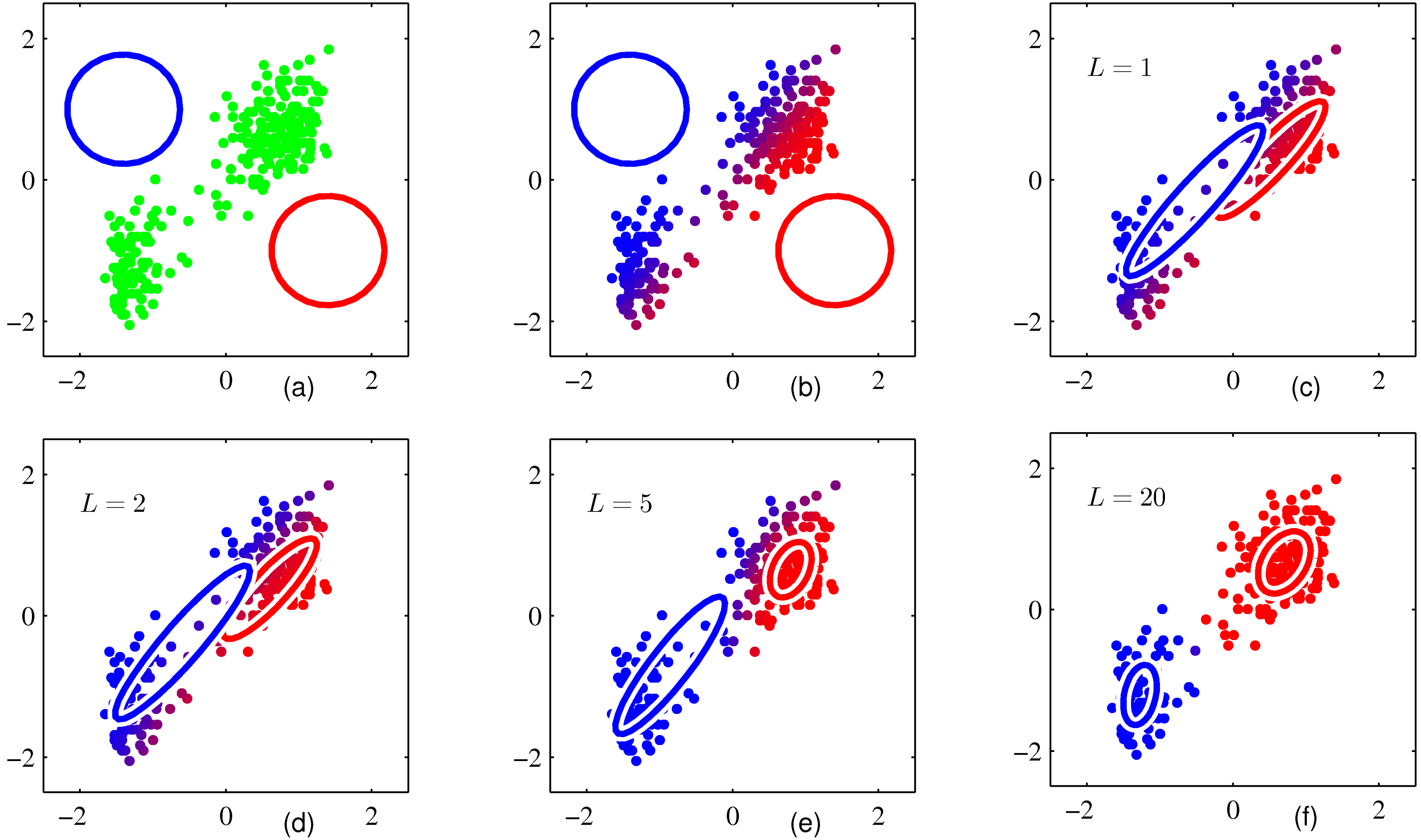
Maximum likelihood estimation of MoG

- Example of several EM iterations



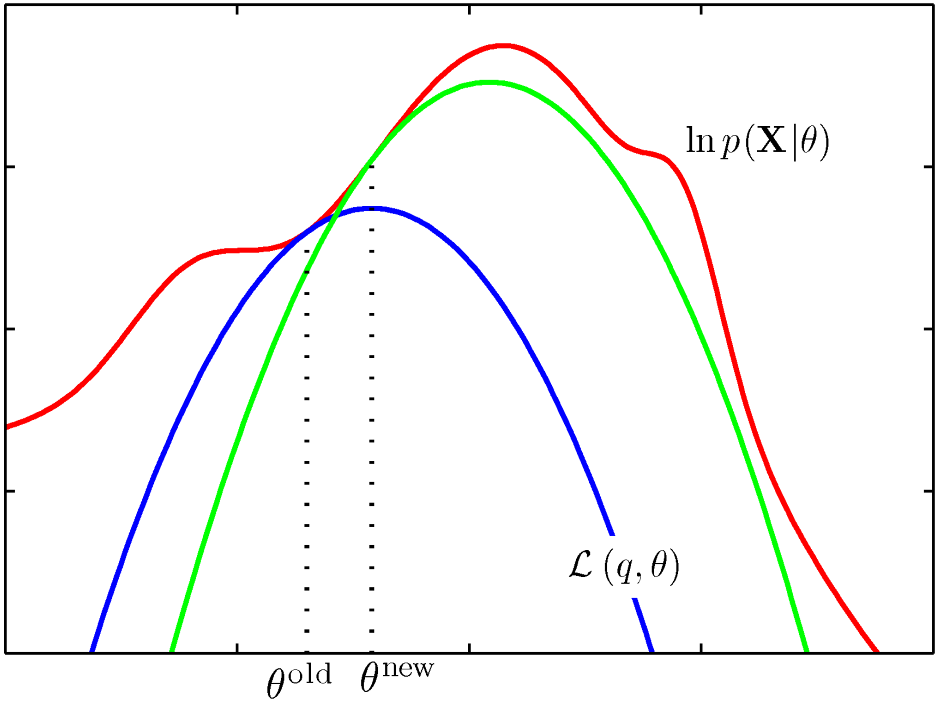
EM algorithm as iterative bound optimization

- Just like k-means, EM algorithm is an iterative bound optimization algorithm
  - Goal: Maximize data log-likelihood, can not be done in closed form

$$L(\theta)=\sum_{n=1}^{N}\log p(x_n)=\sum_{n=1}^{N}\log\sum_{k=1}^{K}\pi_k N(x_n|m_k,C_k)$$

  - Solution: iteratively maximize (easier) bound on the log-likelihood

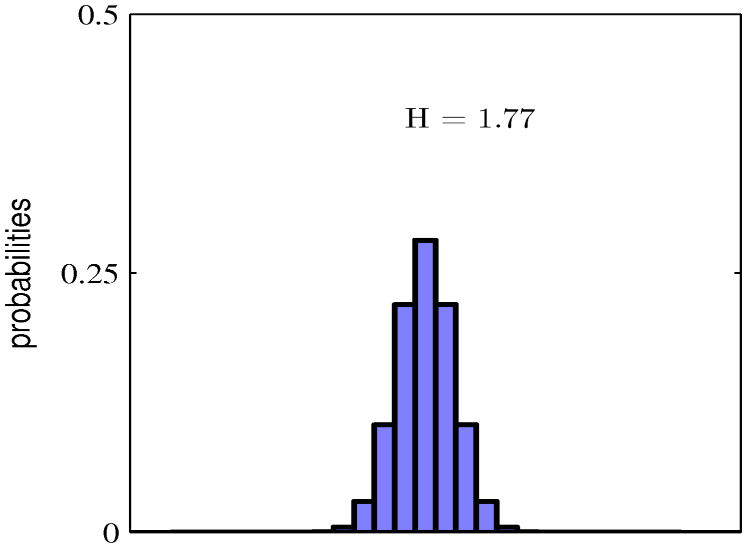
- Bound uses two information theoretic quantities
  - Entropy
  - Kullback-Leibler divergence



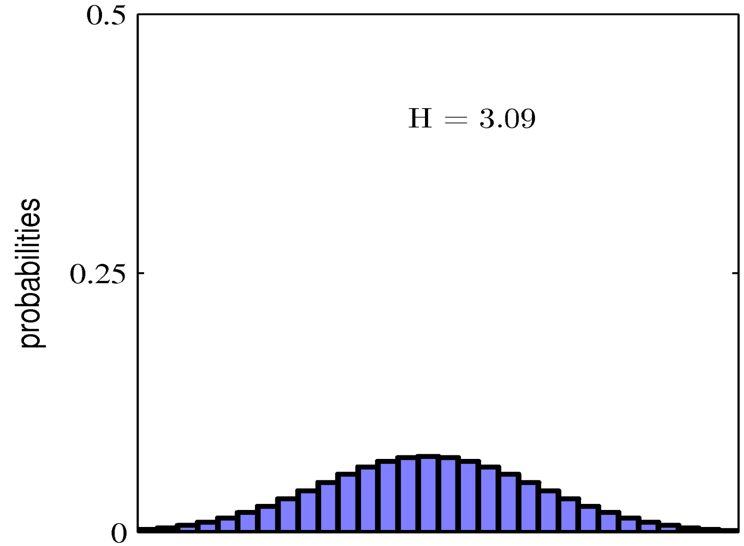
Entropy of a distribution

- Entropy captures uncertainty in a distribution
  - Maximum for uniform distribution
  - Minimum, zero, for delta peak on single value

$$H(q) = -\sum_{k=1}^{K} q(z=k) \log q(z=k)$$



Low entropy distribution



High entropy distribution

Entropy of a distribution

$$H(q) = -\sum_{k=1}^{K} q(z=k) \log q(z=k)$$

- Connection to information coding (Noiseless coding theorem, Shannon 1948)
  - Frequent messages short code, rare messages long code
  - optimal code length is (at least) -log p bits
  - Entropy: expected (optimal) code length per message

- Suppose uniform distribution over 8 outcomes: 3 bit code words
- Suppose distribution: 1/2,1/4, 1/8, 1/16, 1/64, 1/64, 1/64, 1/64, entropy 2 bits!
  - Code words: 0, 10, 110, 1110, 111100, 111101,111110,111111
- Codewords are “self-delimiting”:
  - Do not need a “space” symbol to separate codewords in a string
  - If first zero is encountered after 4 symbols or less, then stop. Otherwise, code is of length 6.

Kullback-Leibler divergence

- Asymmetric dissimilarity between distributions
  - Minimum, zero, if distributions are equal
  - Maximum, infinity, if p has a zero where q is non-zero

$$D(q\|p)=\sum_{k=1}^{K} q(z=k)\log\frac{q(z=k)}{p(z=k)}$$

- Interpretation in coding theory
  - Sub-optimality when messages distributed according to q, but coding with codeword lengths derived from p
  - Difference of expected code lengths

$$D(q\|p)=-\sum_{k=1}^{K} q(z=k)\log p(z=k)-H(q)\geq 0$$

  - Suppose distribution q: 1/2,1/4, 1/8, 1/16, 1/64, 1/64, 1/64, 1/64
  - Coding with p: uniform over the 8 outcomes
  - Expected code length using p: 3 bits
  - Optimal expected code length, entropy H(q) = 2 bits
  - KL divergence D(q|p) = 1 bit

EM bound on MoG log-likelihood

- We want to bound the log-likelihood of a Gaussian mixture p(x)

$$p(x)=\sum_{k=1}^{K} \pi_k N(x; m_k, C_k)$$

- Using "true" posterior distribution on cluster assignment

$$p(z=k|x)=\frac{p(z=k)\,p(x|z=k)}{p(x)}$$

- And any arbitrary distribution q(z) over cluster assignment

- Bound log-likelihood by subtracting KL divergence D(q(z) || p(z|x))
  - Inequality follows immediately from non-negativity of KL

$$F(q,\theta)=\log p(x;\theta)-D\big(q(z)\,\|\,p(z|x,\theta)\big)\leq \log p(x;\theta)$$

Maximizing the EM bound on log-likelihood

- **E-step:**
  - fix model parameters,
  - update distributions q_n to maximize the bound

$$F(\theta, \{q_n\}) = \sum_{n=1}^{N} \left[\log p(x_n) - D(q_n(z_n) \| p(z_n | x_n)) \right]$$

  - KL divergence zero if distributions are equal
  - Thus set $q_n(z_n) = p(z_n|x_n)$
  - **After updating the q_n the bound equals the true log-likelihood**

Maximizing the EM bound on log-likelihood

- M-step:
  - fix the soft-assignments q_n,
  - update model parameters

$$F(\theta,\{q_n\}) = \sum_{n=1}^{N} \left[\log p(x_n) - D(q_n(z_n) \| p(z_n|x_n))\right]$$

$$= \sum_{n=1}^{N} \left[\log p(x_n) - \sum_k q_{nk} \left(\log q_{nk} - \log p(z_n = k|x_n)\right)\right]$$

$$= \sum_{n=1}^{N} \left[H(q_n) + \sum_k q_{nk} \log p(z_n = k, x_n)\right]$$

$$= \sum_{n=1}^{N} \left[H(q_n) + \sum_k q_{nk} \left(\log \pi_k + \log N(x_n; m_k, C_k)\right)\right]$$

- Terms for each Gaussian decoupled from rest !

Maximizing the EM bound on log-likelihood

- Derive the optimal values for the mixing weights
  - Maximize $\sum_{n=1}^{N} \sum_{k=1}^{K} q_{nk} \log \pi_k$
  - Take into account that weights sum to one, define $\pi_1 = 1 - \sum_{k=2}^{K} \pi_k$
  - Set derivative for mixing weight j >1 to zero

$$\frac{\partial}{\partial \pi_j} \sum_{n=1}^{N} \sum_{k=1}^{K} q_{nk} \log \pi_k = \frac{\sum_{n=1}^{N} q_{nj}}{\pi_j} - \frac{\sum_{n=1}^{N} q_{n1}}{\pi_1} = 0$$

$$\frac{\sum_{n=1}^{N} q_{nj}}{\pi_j} = \frac{\sum_{n=1}^{N} q_{n1}}{\pi_1}$$

$$\pi_1 \sum_{n=1}^{N} q_{nj} = \pi_j \sum_{n=1}^{N} q_{n1}$$

$$\pi_1 \sum_{n=1}^{N} \sum_{j=1}^{K} q_{nj} = \sum_{j=1}^{K} \pi_j \sum_{n} q_{n1}$$

$$\pi_1 N = \sum_{n=1}^{N} q_{n1}$$

$$\pi_j = \frac{1}{N} \sum_{n=1}^{N} q_{nj}$$

Maximizing the EM bound on log-likelihood

- Derive the optimal values for the MoG parameters
  - For each Gaussian maximize $\sum_n q_{nk} \log N(x_n; m_k, C_k)$
  - Compute gradients and set to zero to find optimal parameters

$$\log N(x; m, C) = \frac{d}{2}\log(2\pi) - \frac{1}{2}\log|C| - \frac{1}{2}(x_n - m)^T C^{-1}(x_n - m)$$

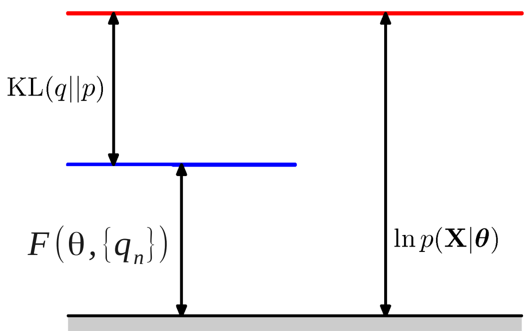
$$\frac{\partial}{\partial m}\log N(x; m, C) = C^{-1}(x - m)$$

$$\frac{\partial}{\partial C^{-1}}\log N(x; m, C) = \frac{1}{2}C - \frac{1}{2}(x - m)(x - m)^T$$

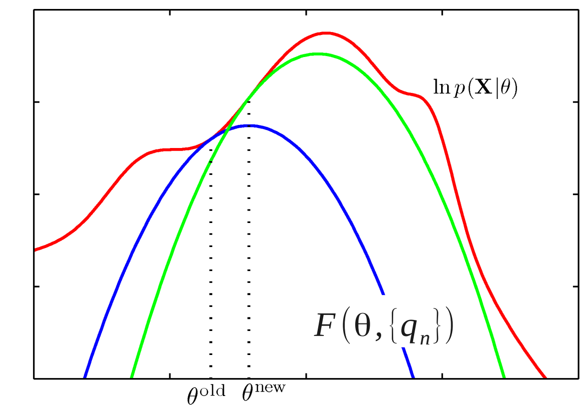
$$m_k = \frac{\sum_n q_{nk} x_n}{\sum_n q_{nk}} \qquad C_k = \frac{\sum_n q_{nk}(x_n - m)(x_n - m)^T}{\sum_n q_{nk}}$$

EM bound on log-likelihood

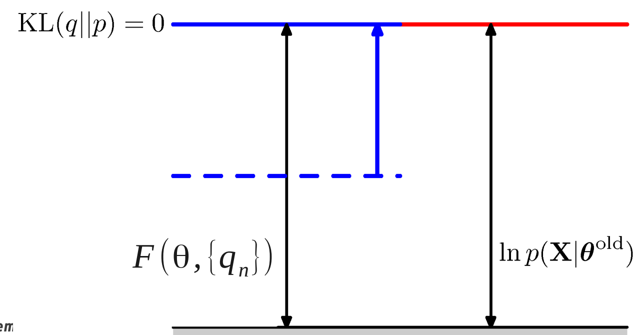
- L is bound on data log-likelihood for any distribution q

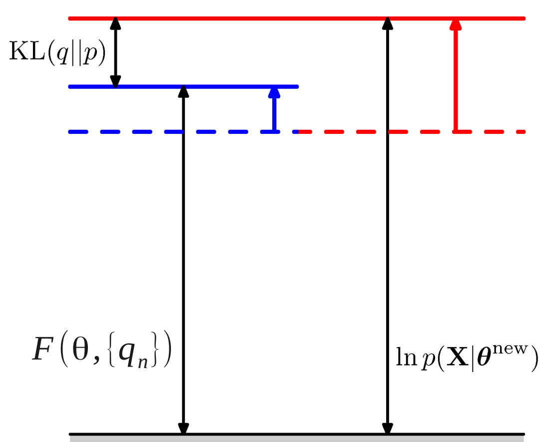


$$F(\theta,\{q_n\}) = \sum_{n=1}^{N} \left[\log p(x_n) - D(q_n(z_n)||p(z_n|x_n))\right]$$

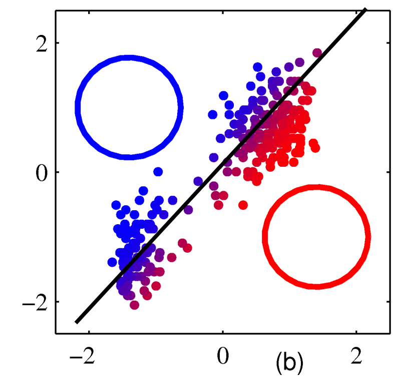


- Iterative coordinate ascent on F
  - E-step optimize q, makes bound tight
  - M-step optimize parameters





Clustering with k-means and MoG



- Assignment:
  - K-means: hard assignment, discontinuity at cluster border
  - MoG: soft assignment, 50/50 assignment at midpoint

- Cluster representation
  - K-means: center only
  - MoG: center, covariance matrix, mixing weight

- If mixing weights are equal and
  all covariance matrices are constrained to be $C_k = \epsilon I$ and $\epsilon \rightarrow 0$
  then EM algorithm = k-means algorithm

- For both k-means and MoG clustering
  - Number of clusters needs to be fixed in advance
  - Results depend on initialization, no optimal learning algorithms
  - Can be generalized to other types of distances or densities

informatics mathematics

Grenoble INP Ensimag

Reading material

- For more details on k-means and mixture of Gaussian learning with EM see the following book chapter: **highly recommended !**

    - Pattern Recognition and Machine Learning,
      Chapter 9
      Chris Bishop, 2006, Springer