Nonparametric Density Estimation (I)

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Outline

- Nonparametric Density Estimation
- Histogram Approach
- Parzen-window method
- K_n-Nearest-Neighbor Estimation
- Gaussian Mixture Models
- Expectation and Maximization

Nonparametric Density Estimation

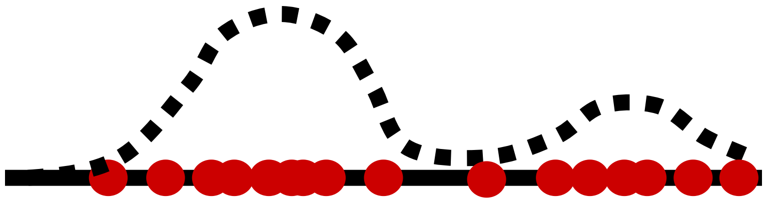
- The common parametric forms rarely fit the densities actually encountered in practice.
- Classical parametric densities are unimodal, whereas many practical problems involve multimodal densities.
- We examine nonparametric procedures that can be used with arbitrary distribution and without the assumption that the parametric forms of the underlying densities are known.

Nonparametric Density Estimation

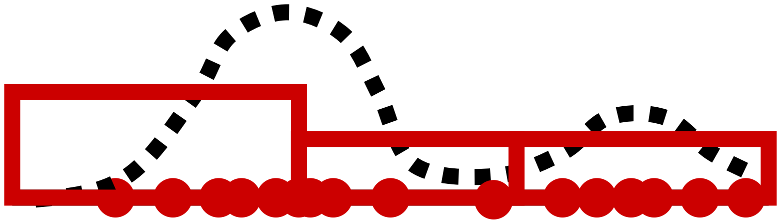
- There are several types of nonparametric methods:
  - Procedures for estimating the density functions $p(\mathbf{x}|\omega_j)$ from sample patterns (Likelihood estimation).
  - Procedures for directly estimating a posteriori probability $p(\omega_j|\mathbf{x})$
    - K-Nearest neighbor classifier which bypass probability estimation, and go directly to decision functions.

The Histogram Method: Example

- Assume (one dimensional) data
- Some points were sampled from a combination of two Gaussians:

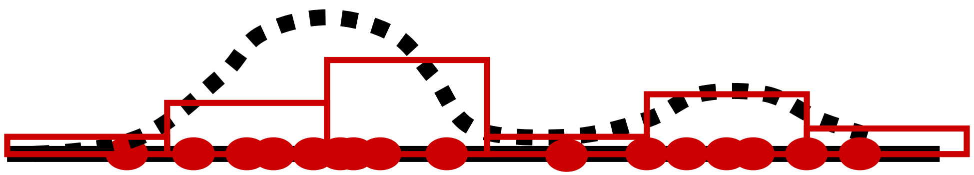


- 3 bins

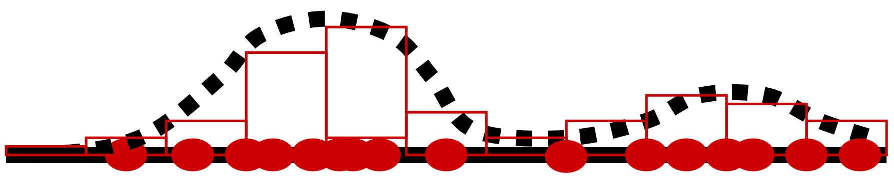


The Histogram Method: Example

- 7 bins



- 11 bins



Density Estimation

- The probability for $\boldsymbol{x}$ to fall into R is
$$p = \int_R p(\boldsymbol{x}')d\,\boldsymbol{x}'$$

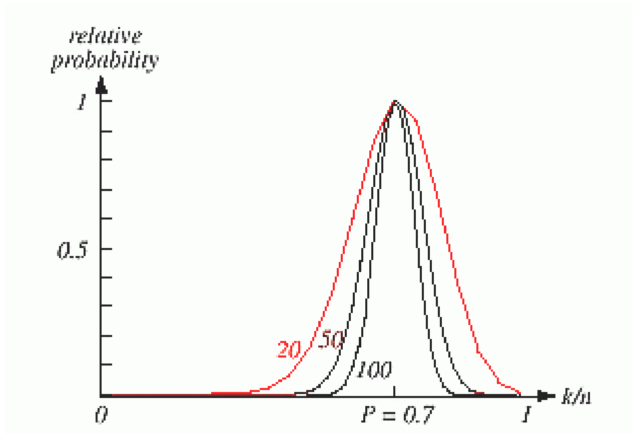
- Suppose we have n i. i.d. samples $\boldsymbol{x_1}, \ldots, \boldsymbol{x_n}$ drawn according to $p(\boldsymbol{x})$. The probability that k of them fall in R is
$$P_k = \binom{n}{k} p^k (1-p)^{n-k}$$

- The expected value for k is $E[k] = np$ and variance is $\mathrm{var}(k) = np(1-p)$.
- The relative part of samples which fall into R, (k/n), is also a random variable for which
$$E\left[\frac{k}{n}\right] = p, \qquad \mathrm{var}\left[\frac{k}{n}\right] = \frac{p(1-p)}{n}$$

- When n is growing up, the variance is making smaller and $\frac{k}{n}$ is becoming to be better estimator for p.

Density Estimation

- The distribution of k/n sharply peaks about the mean, so the k/n is a good estimate of p, *i.e.*,



$$p \approx k/n$$

- For small enough R

$$p = \int_R p(\mathbf{x}')d\,\mathbf{x}' \approx p(\mathbf{x})\,V \approx k/n,$$

where $\mathbf{x}$ is within R and $\boldsymbol{V}$ is a volume enclosed by R.

- Thus $p(\mathbf{x}) \approx \frac{k/n}{V}$ $\qquad (*)$

Histogram Approach

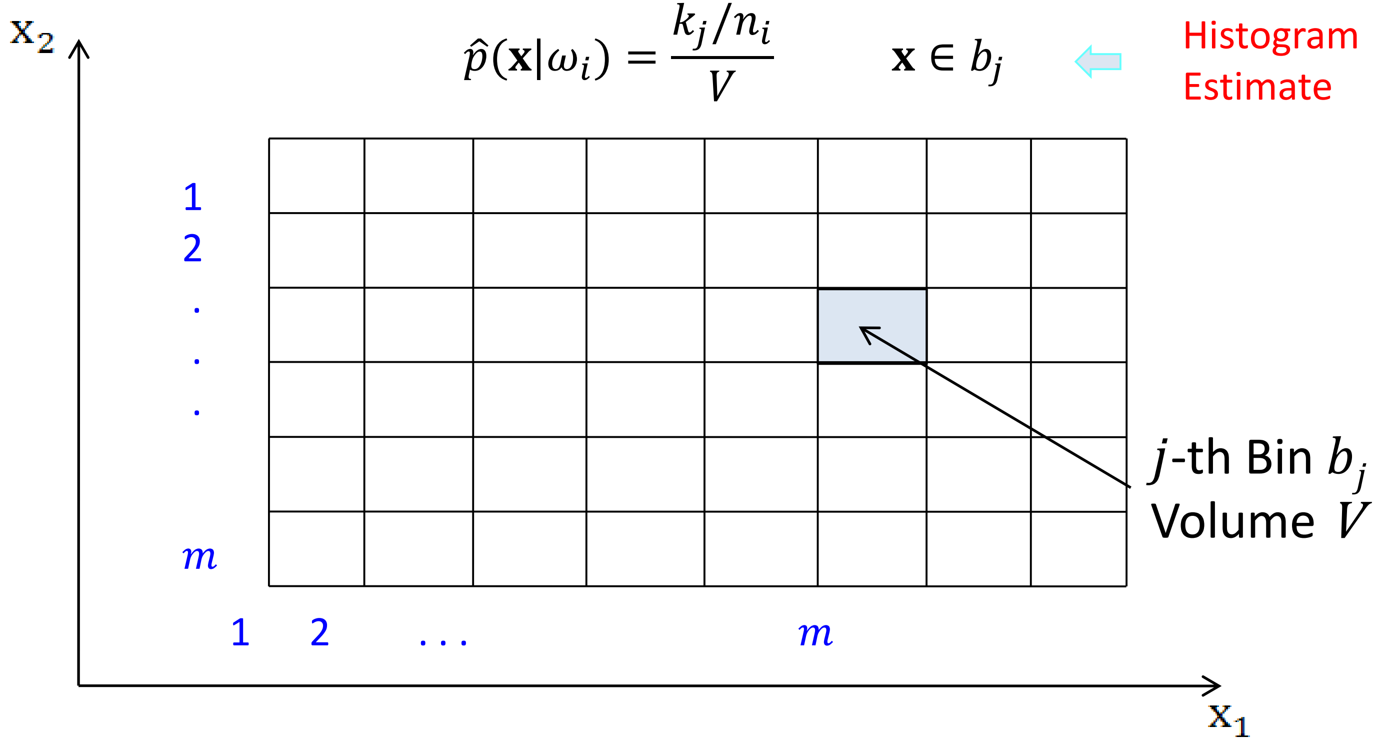
- Histogram is the simplest method of estimating a p.d.f.

  n_i samples in class ω_i , i.e., $\mathbf{x}_l \in \omega_i,\ l = 1, \ldots, n_i$

  The number of $\mathbf{x}_l \in \omega_i$ in b_j is k_j .

$$\hat{p}(\mathbf{x}|\omega_i) = \frac{k_j/n_i}{V} \qquad \mathbf{x} \in b_j$$

Histogram Estimate



Histogram Approach

- The $\hat{p}(\mathbf{x}|\omega_i)$ is constant over b_j
- Let us verify that $\hat{p}(\mathbf{x}|\omega_i)$ is a density function:

$$\int \hat{p}(\mathbf{x}|\omega_i)d\mathbf{x} = \sum_{j=1}^{m} \int_{b_j} \frac{k_j}{n_i V} d\mathbf{x} = \frac{1}{n_i} \sum_{j=1}^{m} k_j = 1$$

- We can choose the number of bins in each axis, m , and their starting points. Fixation of starting points is not critical, but m is important.
- It place a role of smoothing parameter. Too big m makes histogram spiky, for too little m we loose a true form of the density function

Histogram Approach

- The histogram p.d.f. estimator is very effective.
- We can do it *online* : all we should do is to update the counters k_j during the run time, so we do not need to keep all the data which could be huge.
- But its usefulness is limited only to low dimensional vectors $\boldsymbol{x}$, because the number of bins, N_b , grows exponentially with dimensionality d :
$$N_b = m^d.$$
- This is the so called "curse of dimensionality"

Three Conditions for Density Estimation

- Reducing the region by increasing the samples
- Let us take a growing sequence of samples $n = 1, 2, 3 \ldots$
- We take regions R_n with reduced volumes $V_1 > V_2 > V_3 > \cdots$
- Let k_n be the number of samples falling in R_n
- Let $p_n(x)$ be the n^{th} estimate for $p(x)$
- If $p_n(x)$ is to converge to $p(x)$, 3 conditions must be required:
  - $\lim_{n\to\infty} V_n = 0$, resolution as big as possible (for smoothing)
  - $\lim_{n\to\infty} k_n = \infty$, to preserve $\int p(x)dx = 1$
  - $\lim_{n\to\infty} {}^{k_n}/_{n} = 0$ to guarantee convergence of $p(\mathbf{x}) \approx \frac{k/n}{V} \quad (*)$

PARZEN WINDOW and KNN

- How to obtain the sequence $R_1, R_2, ..$?
- There are 2 common approaches of obtaining sequences of regions that satisfy the convergence conditions:
  - Shrink an initial region by specifying the volume V_n as some function of n , such as $V_n = 1/\sqrt{n}$ and show that k_n and k_n/n behave properly i.e. $p_n(x)$ converges to $p(x)$.
    $k_n = \sqrt{n}$.
  - **This is Parzen-window (or kernel) method .**
  - Specify k_n as some function of n, such as $k_n = \sqrt{n}$. Here the volume V_n is grown until it encloses k_n neighbors of x.
  - **This is k_n —nearest-neighbor method .**

$$\lim_{n\to\infty} V_n = 0$$
$$\lim_{n\to\infty} k_n = \infty$$
$$\lim_{n\to\infty} {}^{k_n}/_{n} = 0$$

PARZEN WINDOWS

- Assume that the region R_n is a d −dimensional hypercube.
- If h_n is the length of an edge of that hypercube, then its volume is given by $V_n = h_n^d$.
- Define the following window function:

$$\varphi(\mathbf{u}) = \begin{cases} 1 & |u_j| \leq 1/2\,; \;\; j = 1, \ldots, d \\ 0 & \text{otherwise.} \end{cases}$$

  which defines a unit hypercube centered at the origin.
- $\phi((\mathbf{x} - \mathbf{x}_i)/h_n) = 1$ if x_i falls within the hypercube of volume V_n centered at x, and is zero otherwise i.e. $\mathbf{x} - \frac{h_n}{2} \leq \mathbf{x}_i \leq \mathbf{x} + \frac{h_n}{2}$.
- The number of samples in this hypercube is given by:

$$k_n = \sum_{i=1}^{n} \phi\left(\frac{\mathbf{x} - \mathbf{x}_i}{h_n}\right)$$

PARZEN WINDOWS cont.

- Since $p_n(\mathbf{x}) = \frac{k_n/n}{V_n}$,

$$p_n(\mathbf{x}) = \frac{1}{n}\sum_{i=1}^{n}\frac{1}{V_n}\phi\left(\frac{\mathbf{x}-\mathbf{x}_i}{h_n}\right).$$

- Rather than limiting ourselves to the hypercube window, we can use a more general class of window functions such as Gaussian.
- The window function is being used for interpolation. Each sample contributing to the estimate in accordance with its distance from $\boldsymbol{x}$.
- $p_n(\boldsymbol{x})$ must:
  - be nonnegative
  - integrate to 1.

PARZEN WINDOWS cont.

- This can be assured by requiring the window function itself be a density function, i.e.,

$$\phi(\mathbf{x}) \geq 0 \quad \text{and} \quad \int \phi(\mathbf{u})\ d\mathbf{u} = 1\,.$$

- Effect of the window size h_n on $p(x)$
  - Define the function

$$\delta_n(\mathbf{x}) = \frac{1}{V_n}\phi(\frac{\mathbf{x}}{h_n})$$

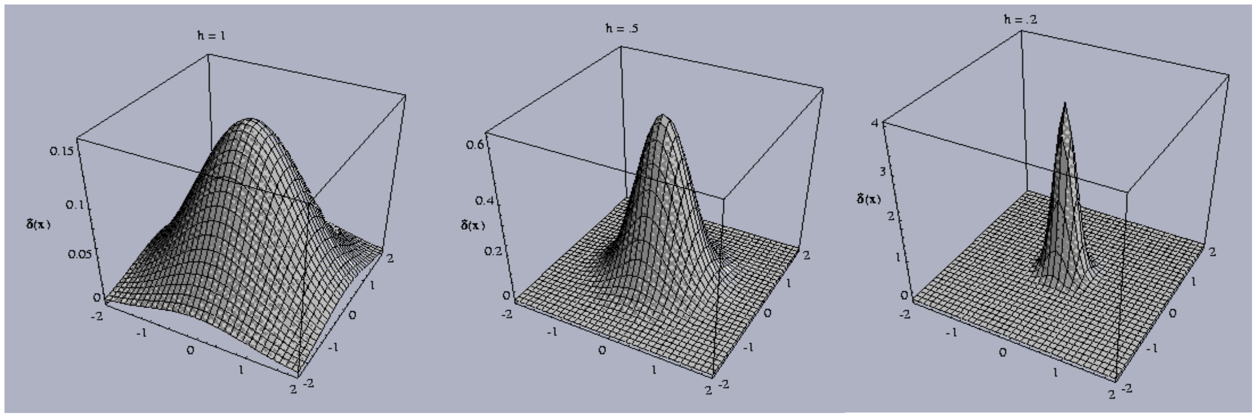
  - then, we write $p_n(\boldsymbol{x})$ as the average

$$p_n(\mathbf{x}) = \frac{1}{n}\sum_{i=1}^{n}\delta_n(\mathbf{x}-\mathbf{x}_i)$$

$$\boxed{p_n(\mathbf{x}) = \frac{1}{n}\sum_{i=1}^{n}\frac{1}{V_n}\phi\left(\frac{\mathbf{x}-\mathbf{x}_i}{h_n}\right)}$$

  - Since $V_n = h_n^d,\ h_n$ affects both the amplitude and the width of $\delta_n(\mathbf{x})$

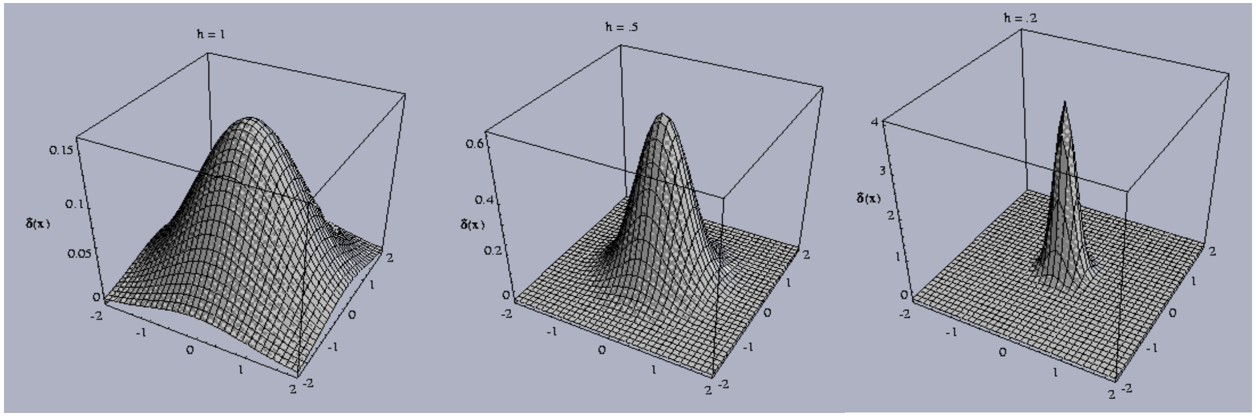
PARZEN WINDOWS cont.



- Examples of two-dimensional circularly symmetric normal Parzen windows for 3 different values of h_n.

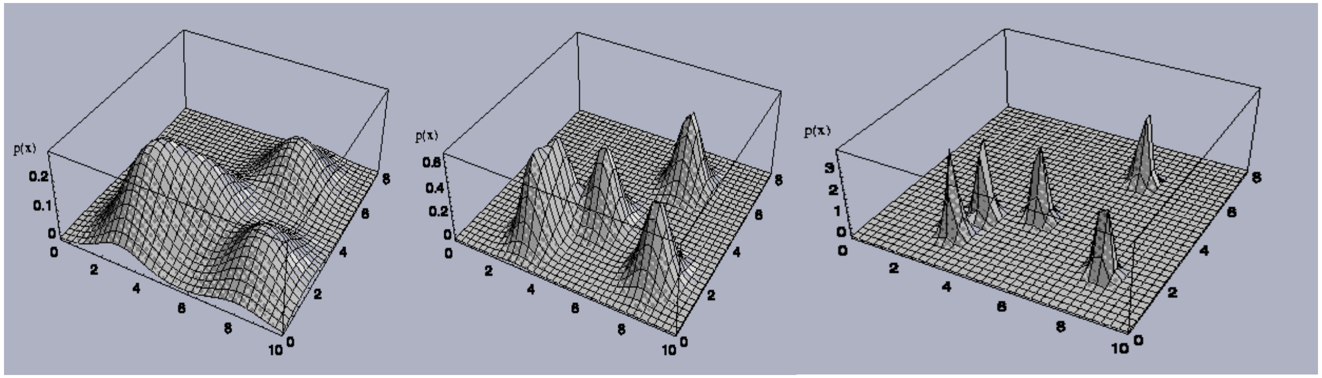
- If h_n is very large, the amplitude of $\delta_n(\mathbf{x})$ is small, and $\boldsymbol{x}$ must be far from $\boldsymbol{x_i}$ since $\delta_n(\mathbf{x}-\mathbf{x}_i)$ decreases slowly from $\delta_n(\mathbf{0})$
- In this case, $p_n(\boldsymbol{x})$ is the superposition of n broad, slowly varying functions, and is very smooth "out-of-focus" estimate for $p(\boldsymbol{x})$.

PARZEN WINDOWS cont.



- If h_n is very small, the peak value of $\delta_n(\mathbf{x} - \mathbf{x}_i)$ is large, and occurs near $\boldsymbol{x} = \boldsymbol{xi}$.
- In this case, $p_n(\boldsymbol{x})$ is the superposition of *n* sharp pulses centered at the samples: an erratic, "noisy" estimate.
- As h_n approaches zero, $\delta_n(\mathbf{x} - \mathbf{x}_i)$ approaches a Dirac delta function centered at $\boldsymbol{x_i}$, and $p_n(\boldsymbol{x})$ approaches a superposition of delta functions centered at the samples.

PARZEN WINDOWS cont.



- 3 Parzen-window density estimates using 5 samples,
  - The choice of h_n (or V_n) has an important effect on $p_n(\boldsymbol{x})$
  - If V_n is too large, the estimate will suffer from too little resolution
  - If V_n is too small the estimate will suffer from too much statistical variability.
  - If there is limited number of samples, then seek some acceptable compromise.
  - If we have unlimited number of samples, then let V_n approach zero as n increases, and have $p_n(\boldsymbol{x})$ converge to the unknown density $p(\boldsymbol{x})$.

PARZEN WINDOWS cont.

- Example 1: $p(\boldsymbol{x})$ is a zero-mean, unit variance, univariate normal density. Let the widow function be of the same form:

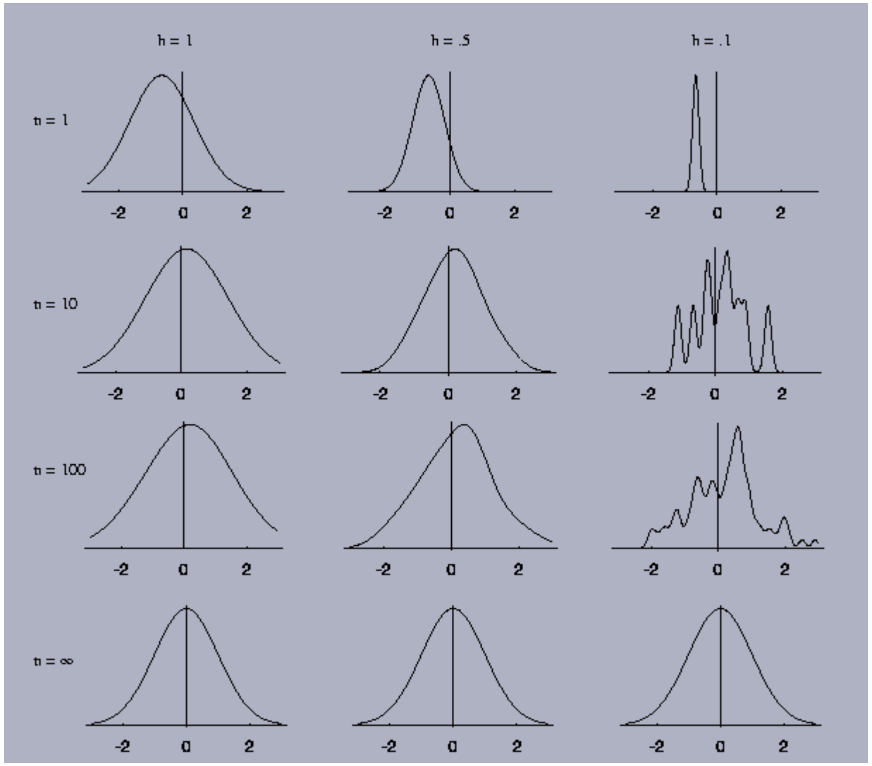
$$\phi(u) = \frac{1}{\sqrt[d]{2\pi}} e^{-u^T u/2}$$

  - Let $h_n = h_1/\sqrt{n}$ where h_1 is a parameter
  - $p_n(\boldsymbol{x})$ is an average of normal densities centered at the samples:

$$p_n(x) = \frac{1}{n}\sum_{i=1}^{n} \frac{1}{h_n^d} \phi(\frac{x - x_i}{h_n}) .$$

Examples cont.

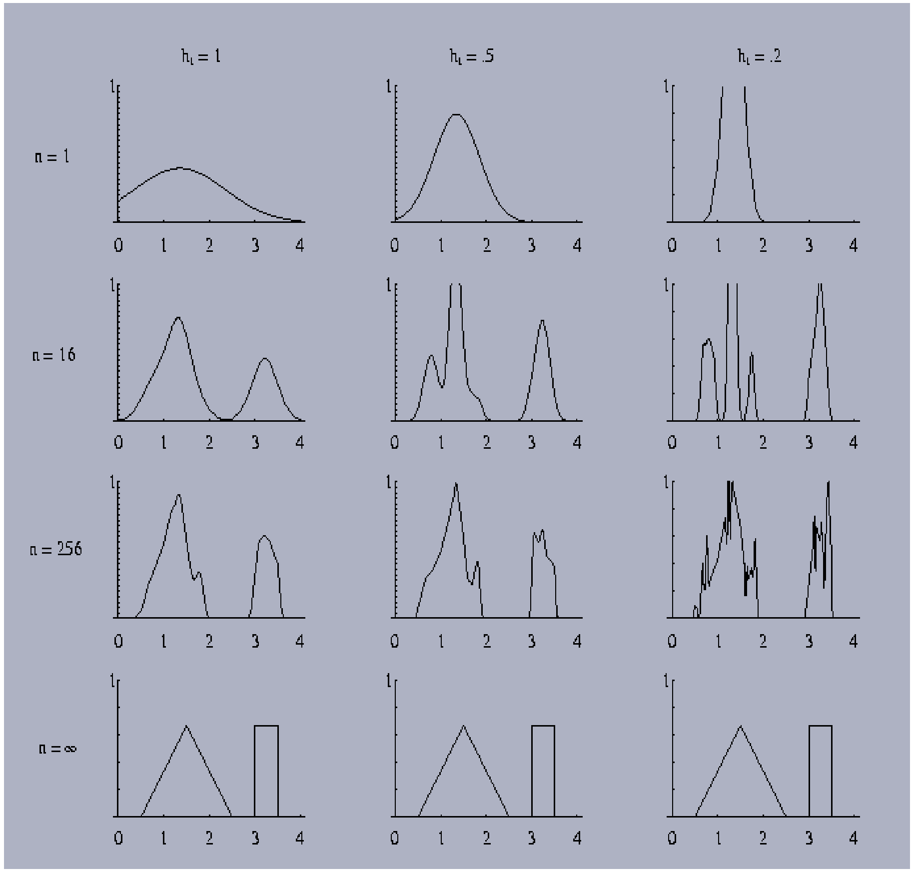
- Generate a set of normally distributed random samples.
- Vary n and h_1.



- ✓ The results depend both on n and h_1.
- ✓ For $n = 1, p_n(\boldsymbol{x})$ is merely a single Gaussian centered about the first sample, which has neither the mean nor the variance of the true distribution.
- ✓ For $n = 10$ and $h_1 = 0.1$, the contributions of the individual samples are discernible. This is not the case for $h_1 = 1$ and $h_1 = 0.5$.

Examples cont.

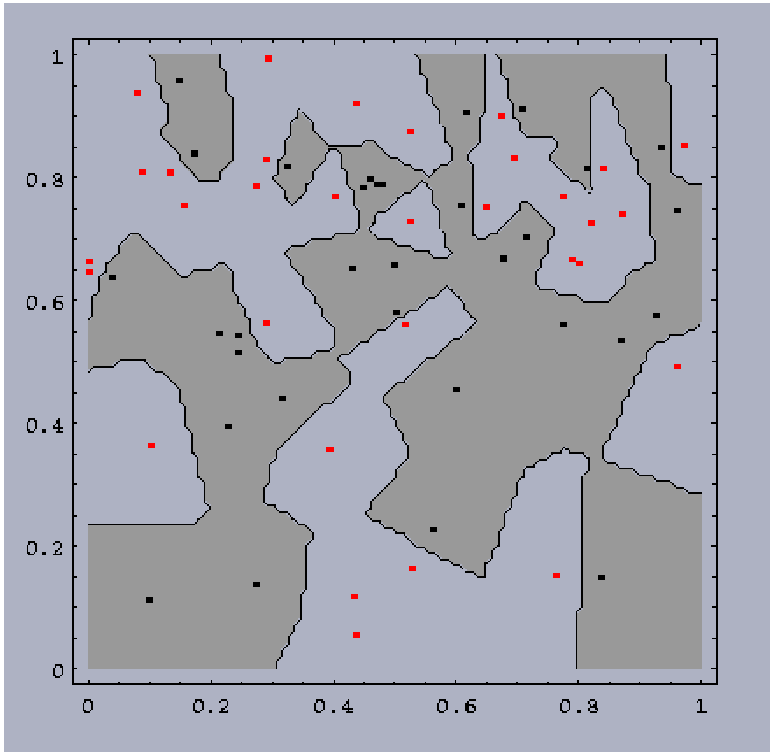
- Example 2:
- ✓ Let $\phi(u)$ and h_n be the same as in Example 1. but let the unknown density be a mixture of uniform and a triangle density.
- ✓ The case $n = 1$ tells more about the window function than it tells about the unknown density.
- ✓ For $n = 16$, none of the estimates is good.
- ✓ For $n = 256$, and $h_1 = 1$, the estimates are beginning to appear acceptable.

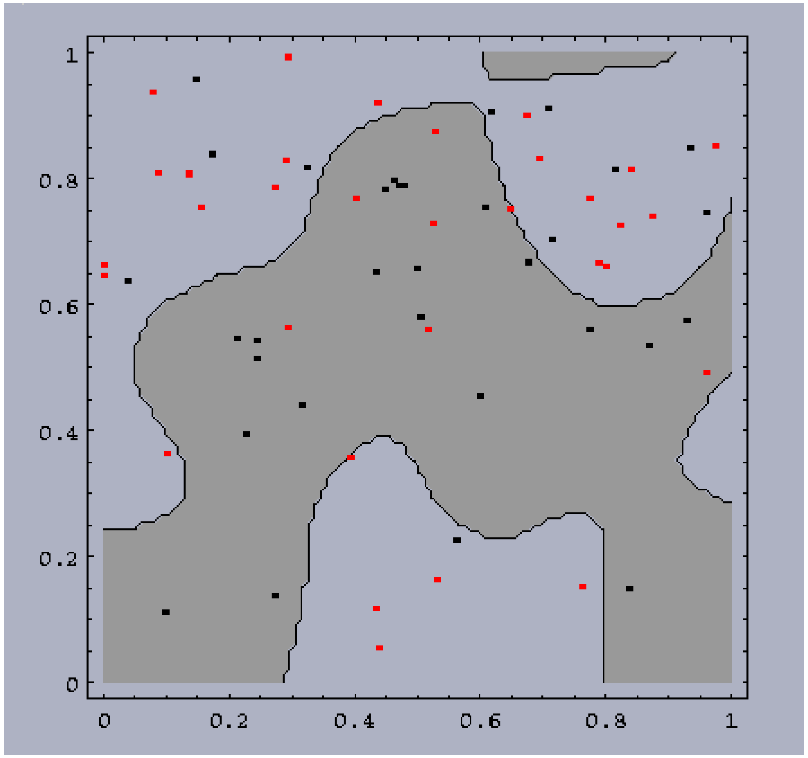


Examples cont.

- Classification
  - To make a classification we should:
    - ✓ Estimate the density for each category using Parzen-window method.
    - ✓ Classify a test point by the label corresponding to the maximum posterior.
  - The decision regions for a Parzen-window classifier depend upon the choice of window function.

Examples cont.





Small h: more complicated boundaries.   Large h: Less complicated boundaries.

Examples cont.

- A small h would be appropriate for the higher density region, while a large h for the lower density region.
- No single window width is ideal overall.
- In general, the training error can be made arbitrarily low by making the window width sufficiently small.
- Remember, the goal of creating a classifier is to classify novel patterns, and a low training error does not guarantee a small test error.

Advantages of Nonparametric Techniques

- Generality: same procedure can be used for unimodal normal and multimodal mixture.
- We do not need to make assumption about the distribution ahead of time.
- With enough samples, we are assured of convergence to an arbitrarily complicated target density

Disadvantages of Nonparametric Techniques

- Number of samples needed may be very large (much larger than would be required if we knew the form of the unknown density) .
- Severe requirements for computation time and storage.
- The large number of samples grows exponentially with the dimensionality of the feature space ("curse of dimensionality")
- Sensitivity to the choice of the window size:
  - Too small: most of the volume will be empty, and the estimate $p_n(\boldsymbol{x})$ will be very erratic.
  - Too large: important variations may be lost due to averaging.
- It may be the case that a cell volume appropriate for one region of the feature space might be entirely unsuitable in a different region.

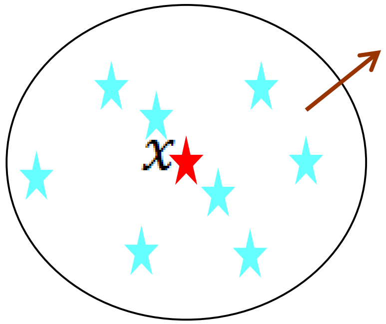
K_n-Nearest-Neighbor Estimation

- To estimate $p(x)$ from n training samples, we center a cell about x and let it grow until it captures k_n samples, where k_n is some specified function of n.
- These samples are the k_n ***nearest-neighbors*** of x.
- If the density is high near x, the cell will be relatively small

$\Longrightarrow$ good resolution.

$$p(\mathbf{x}) \approx \frac{k_n/n}{V} \qquad (*)$$

$$\lim_{n\to\infty} V_n = 0, \qquad \lim_{n\to\infty} k_n = \infty, \qquad \lim_{n\to\infty} \frac{k_n}{n} = 0$$



K_n-Nearest-Neighbor Estimation

- If we take $p_n(x) = \frac{k_n/n}{V_n}$, we determine $k_n\ for \lim_{n\to\infty} k_n = \infty$ for $p_n(x)$ to be a good estimate of probability density
- But k_n should grow sufficiently slow so that the volume of the cell captured k_n samples will shrink to zero.
- Thus $\lim_{n\to\infty} \frac{k_n}{n} = 0$ is necessary and sufficient for $p_n(x)$ to converge to $p(x)$.
- If $k_n = \sqrt{n}$ and assume that $p_n(x)$ is good approximation for $p(x)$, i.e., $V_n \approx 1/(\sqrt{n}p(x))$.
- Thus $V_n \approx V_1/\sqrt{n}$ but with $V_1 = 1/p(x)$ determined by the nature of the data

Comparison of Density Estimators

- Parzen window estimates
  - require the storage of all the observations
  - n evaluations of the kernel function for each estimate
  - Computational complexity: $O(dn)$, parallel circuit
- Nearest neighbor estimates
  - also require the storage of all the observations
  - Computational complexity: $O(dn)$, parallel circuit, 3 algorithms
- Histogram estimates
  - do not require storage for all the observations,
  - Just require storage for description of the bins.
  - But the number of the bins grows exponentially with dimension.

Interim Summary

Histogram
From histogram to density estimation
Convergence conditions
Parzen window
Parzen window Function (Kernel)
Cube kernel, Gaussian kernel
Window size and performance
Classification
K_n – Nearest Neighbor

$$p(\mathbf{x}) \approx \frac{k_n/n}{V} \qquad (*)$$

$$\lim_{n\to\infty} V_n = 0\,, \qquad \lim_{n\to\infty} k_n = \infty\,, \qquad \lim_{n\to\infty} \frac{k_n}{n} = 0$$

$$\lim_{n\to\infty} p_n(x) = p(x).$$

K_n – Nearest Neighbor	Parzen window
$k_n = \sqrt{n}$	$V_n = 1/\sqrt{n}$
$V_n \approx 1/(\sqrt{n}p(x))$	$k_n = \sum_{i=1}^{n} \phi\left(\frac{\mathbf{x}-\mathbf{x}_i}{h_n}\right)$
⬇	⬇
$p_n(x) = \frac{k_n/n}{V_n}$	$p_n(\mathbf{x}) = \frac{1}{n}\sum_{i=1}^{n}\frac{1}{V_n}\phi\left(\frac{\mathbf{x}-\mathbf{x}_i}{h_n}\right).$
Adaptive window size	Same window size

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Interim Summary

Histogram

From histogram to density estimation

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Parzen window Function (Kernel)

Cube kernel, Gaussian kernel

Window size and performance

Classification

K_n – Nearest Neighbor

$$p(\mathbf{x}) \approx \frac{k/n}{V} \qquad (*)$$

$$\lim_{n\to\infty} V_n = 0, \qquad \lim_{n\to\infty} k_n = \infty, \qquad \lim_{n\to\infty} \frac{k_n}{n} = 0$$

$$\lim_{n\to\infty} p_n(x) = p(x).$$

$\boxed{k_n = \sqrt{n}}$

$\boxed{V_n \approx 1/(\sqrt{n}\, p(x))}$

$\boxed{p_n(x) = \frac{k_n/n}{V_n}}$

Adaptive window size

K_n – Nearest Neighbor

$\boxed{V_n = 1/\sqrt{n}}$

$\boxed{k_n = \sum_{i=1}^{n} \varphi\left(\frac{\mathbf{x}-\mathbf{x}_i}{h_n}\right)}$

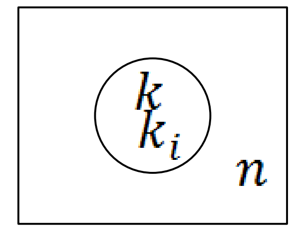
$\boxed{p_n(\mathbf{x}) = \frac{1}{n}\sum_{i=1}^{n} \frac{1}{V_n} \varphi\left(\frac{\mathbf{x}-\mathbf{x}_i}{h_n}\right).}$

Same window size

Parzen window

Classification with K-NN and Parzen window: Estimation of a posteriori probabilities

- The k-NN (and Parzen window) techniques can be used to estimate the a posteriori probabilities $p(\omega_i|\mathbf{x})$ from a set of n labeled samples.
- Suppose that we place a cell of volume V around x and capture k samples:
  - k_i are labeled ω_i
  - $k - k_i$ have other labels.



- A simple estimate for the joint probability density $p(\mathbf{x}, \omega_i)$ is

$$p_n(\mathbf{x}, \omega_i) = \frac{k_i/n}{V}$$

- A reasonable estimate for $p(\omega_i|\mathbf{x})$ is

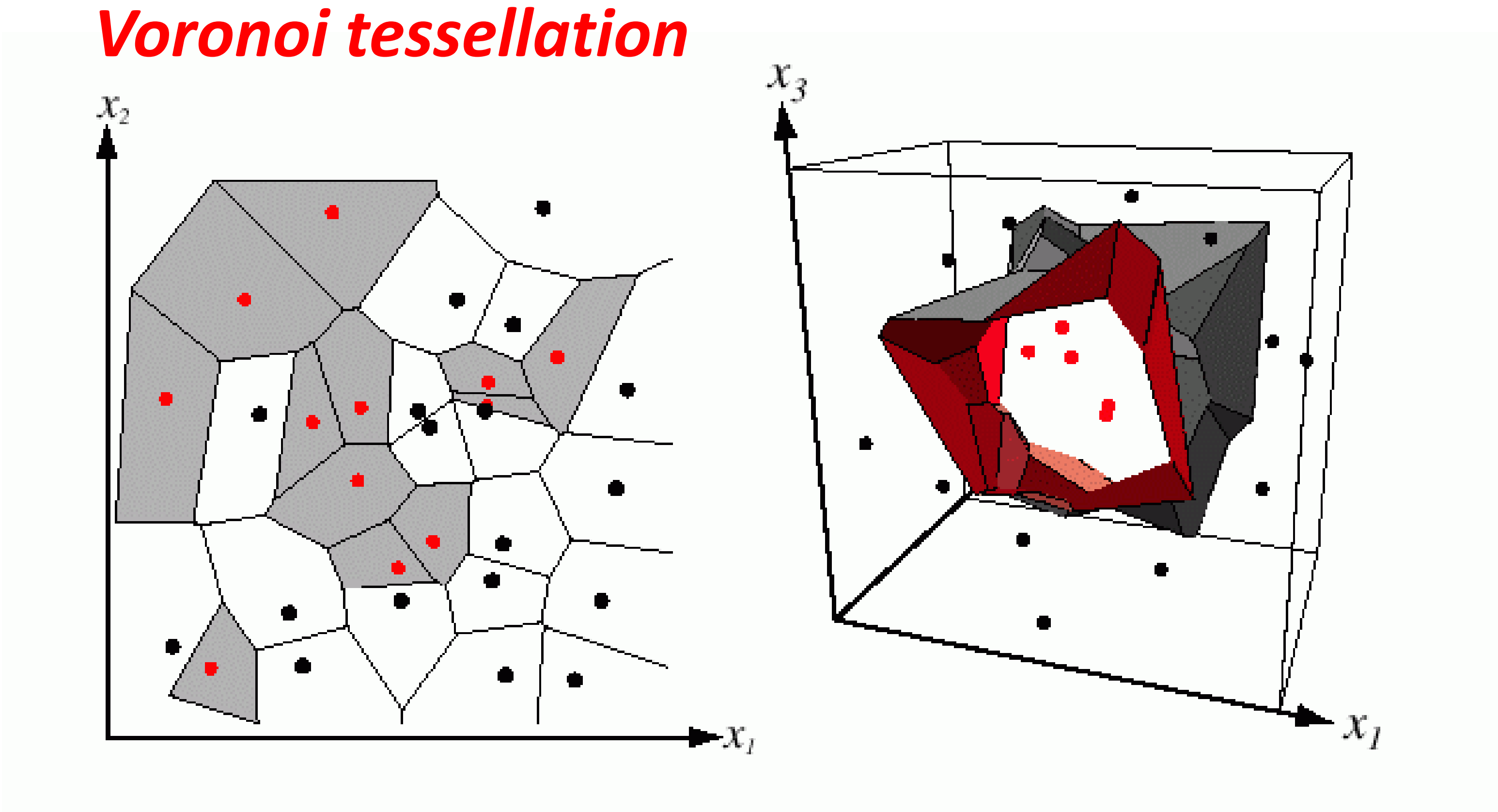
$$p_n(\omega_i|\mathbf{x}) = \frac{p_n(\mathbf{x},\omega_i)}{\sum_{j=1}^{C} p_n(\mathbf{x},\omega_j)} = \frac{k_i}{k}$$

Instance-Based Learning Classifier
Approximated Minimum error classifier

Classification With Nearest Neighbor Rule

- Let $D^n = \{\mathbf{x}_1, \ldots, \mathbf{x}_n\}$ denote a set of n labeled prototypes and let $\mathbf{x}' \in D^n$ be the prototype nearest to a test point $\mathbf{x}$.
- Then the Nearest Neighbor Rule: assign the label of $\mathbf{x}'$ to $\mathbf{x}$.
- This rule is suboptimal, but when the number of prototypes is large, its error is never worse than twice the Bayes rate.

Classification With Nearest Neighbor Rule

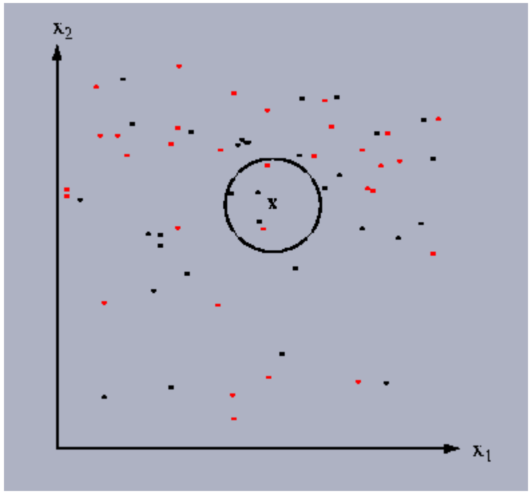


Voronoi cells

Classification With the k-Nearest Neighbor Rule

- The k-NN query starts at the test point and grows a spherical region until it encloses k training samples, and it labels by a majority vote of these samples.
- **Algorithm**:
  - For each sample point Compute Distance (sample point, test point)
  - Sort the distances
  - Inspect the k smallest distances
  - Label test point by a majority vote.

$$p_n(\omega_i|\mathbf{x}) = \frac{p_n(\mathbf{x},\omega_i)}{\sum_{j=1}^{C} p_n(\mathbf{x},\omega_j)} = \frac{k_i}{k}$$



Classification With the k-Nearest Neighbor Rule

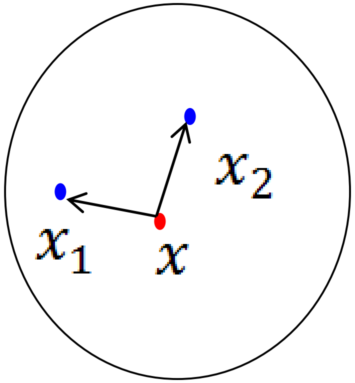
- Question.
  - If a *posteriori* probabilities $p(\omega_i|\boldsymbol{x}), i = 1, 2$ for two classes are known, for example

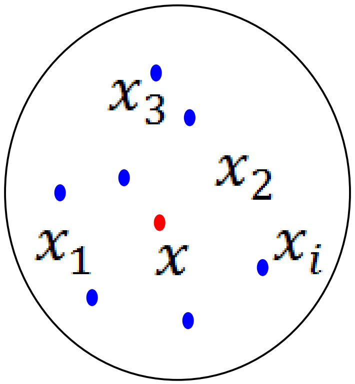
$$p(\omega_1|\mathbf{x}) > p(\omega_2|\mathbf{x})$$

  - What is a probability of choosing a class ω_1 for x with the Bayes, the nearest neighbor, the k-NN classifiers?

Classification With the k-Nearest Neighbor Rule.

- **Answer**
  - Bayes: always w_1
  - NN: $p(w_1|x)$
  - K-NN: $\sum_{i=(k+1)/2}^{k} \binom{k}{i} p(\omega_1|\mathbf{x})^i (1 - p(\omega_1|\mathbf{x}))^{k-i}$





Exercise

한 해안가에서 연어가 잡힐 확률은 0.6 이고 농어가 잡힐 확률은 0.4 이다.

잡힌 연어 중 40 cm 이하의 크기일 확률은 20%이고,

농어 중 40cm 이하일 확률은 3%이다.

잡은 고기가 40cm 이하 일 때 연어로 분류할 확률을 각각

Bayes, NN, K-NN(K=9) Classifier 에서 구하여라.

답안

P(연어) = 0.6, P(농어) = 0.4

P(40cm이하|연어) = 0.2, P(40cm이하|농어) = 0.03

Posteriori probability P(연어|40cm이하) 와 P(농어|40cm이하) 를 구하면 다음과 같다.

P(연어|40cm이하) = $\frac{\text{P(40cm이하|연어)P(연어)}}{\text{P(40cm이하)}} = \frac{0.2*0.6}{0.6*0.2+0.4*0.03}$ =90.9%

P(농어|40cm이하) = $\frac{\text{P(40cm아하|농어)P(농어)}}{\text{P(40cm이하)}} = \frac{0.03*0.4}{0.6*0.2+0.4*0.03}$ =9.09%

이 posteriori probability를 이용하여 연어로 판정할 확률을 구하면 다음과 같다.

(1) Baye Classifier 의 경우 항상 연어로 분류한다. (100%)

(2) NN의 경우 P(연어|40cm이하) = 90.9% 확률로 연어로 분류한다.

(3) K= 9일 때, $\sum_{i=5}^{9}\binom{9}{5}P(\text{연어}|\text{40cm이하})^{i}(1-P\left(\text{연어}\middle|\text{40cm이하}\right))^{k-i}$ 를 구한다. 따라서

$$14*(0.909)^5*(0.0909)^4+84*(0.909)^6*(0.0909)^3+36*(0.909)^7*(0.0909)^2+9*(0.909)^8*(0.0909)^1+(0.909)^9*(0.0909)^0 = 0.9937837$$

약 99.4%의 확률로 연어로 분류한다.

Gaussian Mixture Estimation

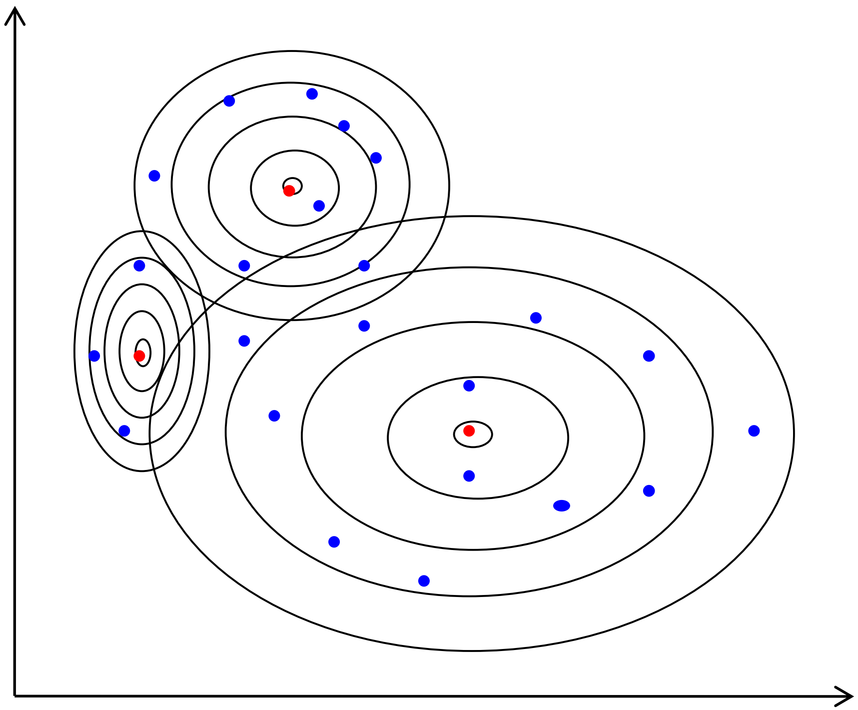
- Parzen Window

$$p_n(\mathbf{x}) = \frac{1}{n}\sum_{i=1}^{n}\frac{1}{V_n}\phi\left(\frac{\mathbf{x}-\mathbf{x}_i}{h_n}\right).$$

- Gaussian Mixture

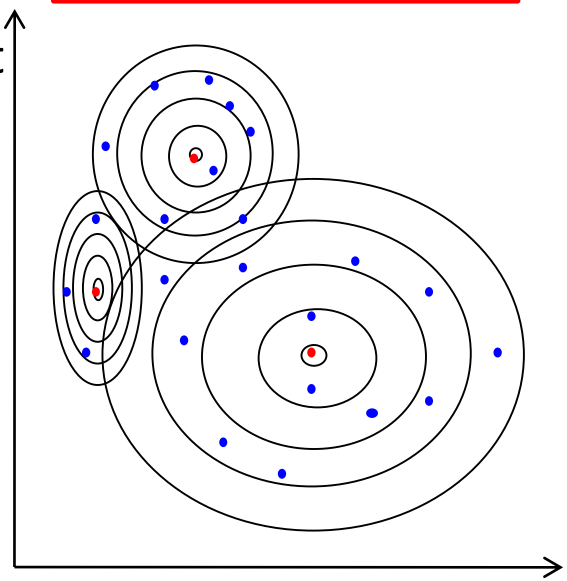
$$p(\mathbf{x}) = \sum_{k1}^{K} w_k\varphi\left(\frac{\mathbf{x}-\mu_k}{\sigma_k}\right).$$

$$p(\mathbf{x}) = \sum_{k=1}^{K} p(\mathbf{x}|\theta_k)p(\theta_k).$$



Gaussian Mixture Estimation

$$p(\mathbf{x}) = \sum_{k=1}^{K} p(\mathbf{x}|\theta_k)p(\theta_k)\,.$$



- Gaussian Mixture Model

  where , $p(x|\theta_k)$ are Gaussian density functions.
- $K, \theta_k, and\ p(\theta_k)$ can be estimated from a data set using Expectation-Maximization (EM)algorithm
- Example of EM: $\theta_k = [\mu_k, \Sigma_k]$, fixed K

$$p(\mathbf{x}) = \sum_{k1}^{K} w_k \varphi\left(\frac{\mathbf{x}-\mu_k}{\sigma_k}\right).$$

- Class conditional PDF
- $p(\mathrm{x}|\theta) = \sum_k p(\mathrm{x}|\theta_k)p(\theta_k|\theta)$

  $= \sum_Z p(\mathrm{x}, Z|\theta) = \sum_{Z=k} p(\mathrm{x}|Z=k,\theta)p(Z=k|\theta)$
- $p(\mathrm{x}|\theta) = \int_Z p(\mathrm{x}, Z, |\theta)d_Z$

Expectation-Maximization (EM)

- EM aims to find parameter values that maximize likelihood,

$$L(\theta\,;X) = p(X|\theta) = \textstyle\sum_Z p(X,Z|\theta) = \sum_Z L(\theta\,;X\,,Z)\,,$$

$$L(\theta\,;X) = p(X|\theta) = \textstyle\int_Z p(X,Z|\theta)dz = \int_Z L(\theta\,;X\,,Z)dz$$

$$p(\mathbf{x}|\theta) = \sum_{k=1}^{K} p(\mathbf{x}|\theta_k)p(\theta_k)$$

$$p(\mathbf{x}|\theta) = \sum_{k1}^{K} w_k\varphi\left(\frac{\mathbf{x}-\mu_k}{\sigma_k}\right)$$

where Z is latent variable.

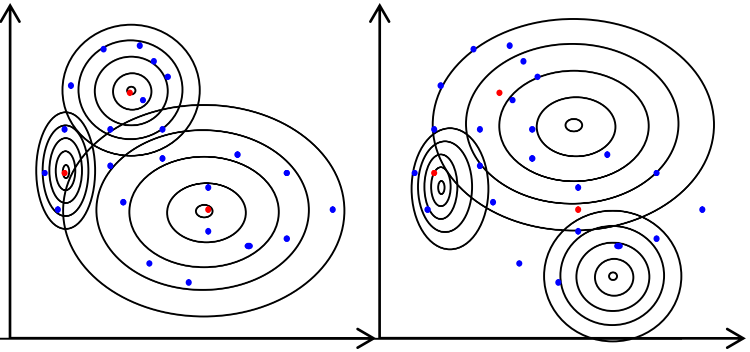
- **E-step:** For given θ^t, X, find expectation of the likelihood on the conditional distribution of Z given $X\ and\ \theta^t$.

$$Q(\theta|\theta^t) = E_{Z|X,\theta^t}[\log L\,(\theta\,;X\,,Z)] = \textstyle\sum_Z p(Z|\,X,\theta^t)\log L\,(\theta\,;X\,,Z)$$

- **M-step:** Find θ^{t+1} maximizing Q.

$$\theta^{t+1} = \underset{\theta}{\operatorname{argmax}} Q(\theta|\theta^t)$$

- Repeat E-step and M-step.



$$Q(\theta|\theta^t) = E_{Z|X,\theta^t}[\log L\,(\theta\,;X\,,Z)] = \sum_Z p(Z|\,X,\theta^t)\log L\,(\theta\,;X\,,Z)$$

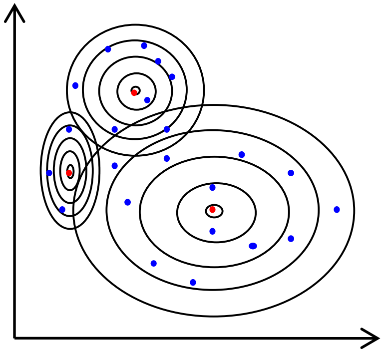
Expectation-Maximization (EM)

- Likelihood of GMM

$$L(\theta\,;X) = p(X|\theta) = \sum_Z p(X,Z|\theta)\left(:=\sum_Z L(\theta\,;X\,,Z)\right)$$
$$= \sum_Z p(X|Z,\theta)p(Z|\theta) = \sum_{Z=k} p(X|Z=k,\theta)p(Z=k|\theta)$$
$$= \sum_{k=1}^{K} \prod_{m=1}^{M} p(x_m|\theta_k)p(\theta_k) = \sum_{k=1}^{K} \quad \prod_{m=1}^{M} p(x_m\,;\mu_k,\Sigma_k)p(Z=k)$$

- $L(\theta\,;X=x_m,Z=k) = p(x_m\,;\mu_k,\Sigma_k)\tau_k$

$$= \exp\left(\log\tau_k - \frac{1}{2}\log|\Sigma_k| - \frac{1}{2}(x_m-\mu_k)^T\Sigma_k^{-1}(x_m-\mu_k)\right)$$



- **E-step**

$$\log L\,(\theta\,;X\,,Z=k) = \log\prod_m \quad L(\theta\,;X=x_m,Z=k)$$
$$= \sum_m \log L\,(\theta\,;X=x_m,Z=k)$$

$$Q(\theta|\theta^t) = \sum_m \sum_{Z=k} p(Z=k|X=x_m,\theta^t)\log L\,(\theta\,;X=x_m,Z=k)$$

Expectation-Maximization (EM)

- **E-step**

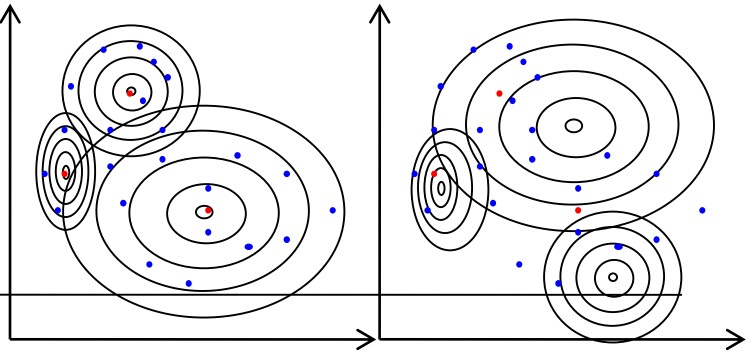
$$Q(\theta|\theta^t) = \sum_m \sum_k p(Z = k|\, X = x_m, \theta^t)\, \log L\, (\theta\, ; X = x_m, Z = k)$$

$$\log L\, (\theta\, ; X = x_m, Z = k)$$

$$= \left(\log\tau_k - \frac{1}{2}\log|\Sigma_k| - \frac{1}{2}(x_m - \mu_k)^T \Sigma_k^{-1}(x_m - \mu_k)\right)$$

$$T_{k,m}^t := p(Z = k|X = x_m, \theta^t) = \frac{p(X=x_m,\theta^t|Z=k)p(Z=k)}{\sum_k p(X=x_m,\theta^t|Z=k)p(Z=k)} = \frac{p(x_m\, ;\mu_k^t,\Sigma_k^t)\tau_k^t}{\sum_k p(x_m\, ;\mu_k^t,\Sigma_k^t)\tau_k^t}$$

$$\rightarrow\ Q(\theta|\theta^t) = \sum_m \sum_k T_{k,m}^t \left(\log\tau_k - \frac{1}{2}\log|\Sigma_k| - \frac{1}{2}(x_m - \mu_k)^T \Sigma_k^{-1}(x_m - \mu_k)\right)$$



Expectation-Maximization (EM)

- **M-step**

$$Q(\theta|\theta^t) = \sum_m \sum_k T_{k,m}^t \left(\log\tau_k - \frac{1}{2}\log|\Sigma_k| - \frac{1}{2}(x_m - \mu_k)^T \Sigma_k^{-1}(x_m - \mu_k)\right)$$

$$\tau^{t+1} = \underset{\tau}{\operatorname{argmax}} \sum_m \sum_k T_{k,m}^t \log\tau_k\,, \quad \text{Subject to } \sum \tau_k = 1$$

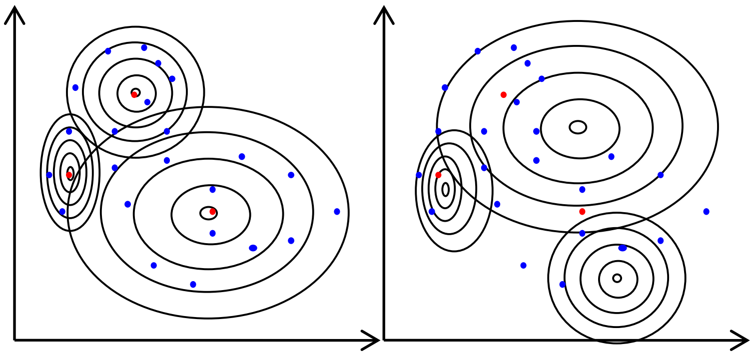
$$\left(\mu_k^{t+1}, \Sigma_k^{t+1}\right) = \underset{(\mu_k,\Sigma_k)}{\operatorname{argmax}} \sum_m T_{k,m}^t \left(-\frac{1}{2}\log|\Sigma_k| - \frac{1}{2}(x_m - \mu_k)^T \Sigma_k^{-1}(x_m - \mu_k)\right)$$

- Results

$$\boxed{\tau_k^{t+1} = \frac{\sum_m T_{k,m}^t}{\sum_k \sum_m T_{k,m}^t}}$$

$$\boxed{\mu_k^{t+1} = \frac{\sum_m T_{k,m}^t x_m}{\sum_k \sum_m T_{k,m}^t}}$$

$$\boxed{\Sigma_k^{t+1} = \frac{\sum_m T_{k,m}^t (x_m - \mu_k^{t+1})(x_m - \mu_k^{t+1})^T}{\sum_k \sum_m T_{k,m}^t}}$$



Expectation-Maximization (EM)

- EM Summary
  - Initialization
  - E-step

$$T_{k,m}^{t} := p(k|\mathbf{x} = x_m, \theta^t) = \frac{p(x_m\,; \mu_k^t, \Sigma_k^t)\tau_k^t}{\sum_k p(x_m\,; \mu_k^t, \Sigma_k^t)\tau_k^t},$$

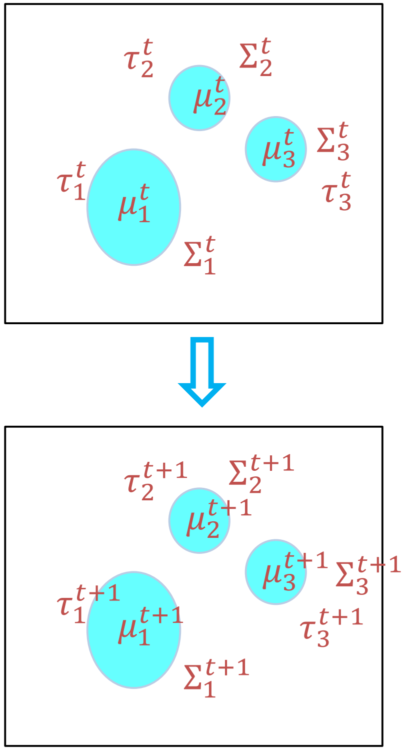
$$p(x_m\,; \mu_k^t, \Sigma_k^t) = \frac{1}{2\pi^{d}\sqrt{|\Sigma_k^t|}} \exp\left(-\frac{(x_m-\mu_k^t)^T {\Sigma_k^t}^{-1}(x_m-\mu_k^t)}{2}\right)$$

  - M-step

$$\tau_k^{t+1} = \frac{\sum_m T_{k,m}^t}{\sum_k \sum_m T_{k,m}^t},$$

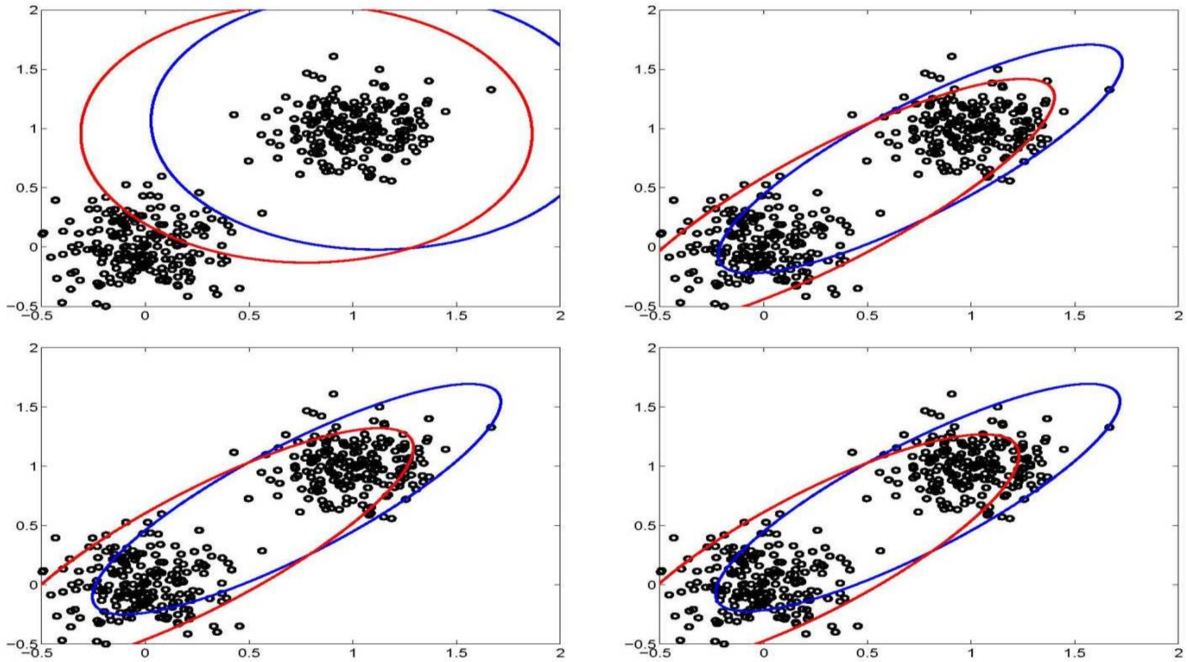
$$\mu_k^{t+1} = \frac{\sum_m T_{k,m}^t x_m}{\sum_k \sum_m T_{k,m}^t},$$

$$\Sigma_k^{t+1} = \frac{\sum_m T_{k,m}^t (x_m-\mu_k^{t+1})(x_m-\mu_k^{t+1})^T}{\sum_k \sum_m T_{k,m}^t}$$



Example

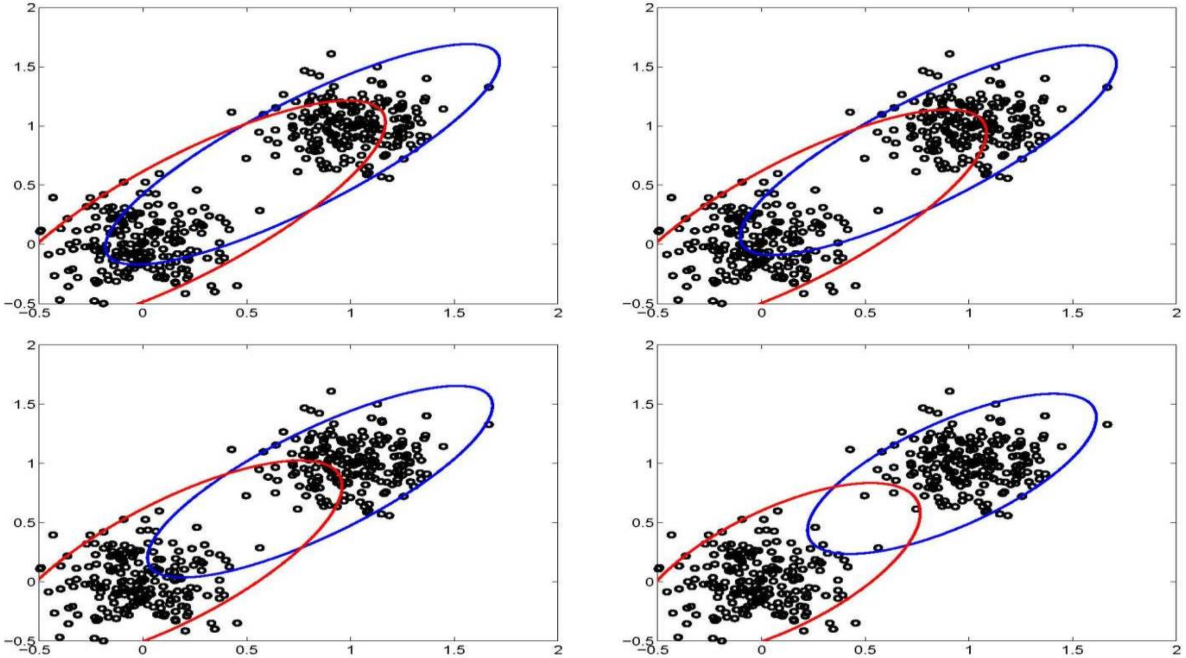
Mixture density estimation: example



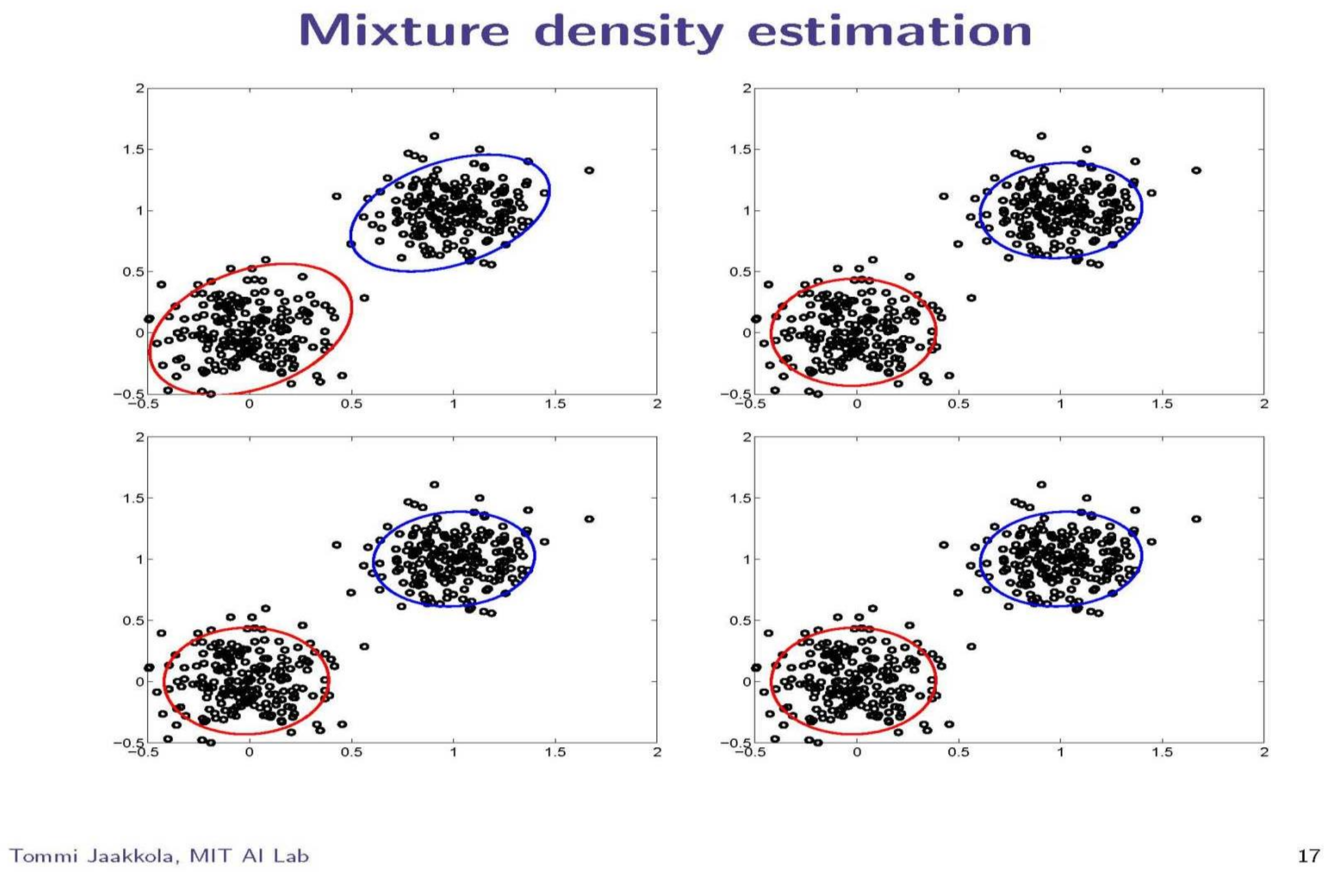
Tommi Jaakkola, MIT AI Lab

Example

Mixture density estimation



Example

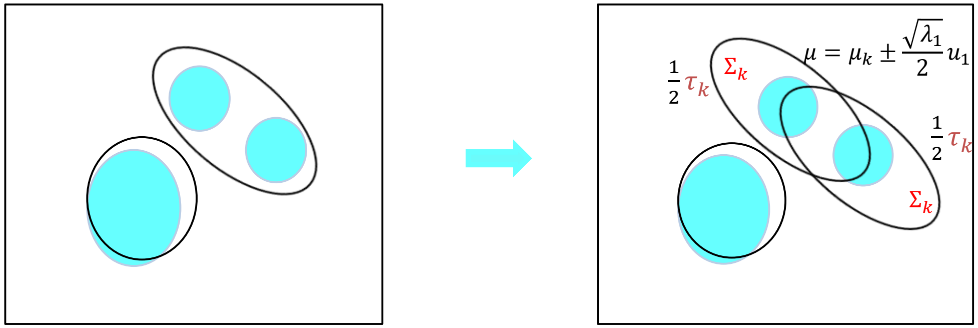


Automatic Model Order Selection

- For each component k, define a total responsibility $r(k)$ as

$$r(k) = \sum_{m=1}^{M} p(k|\mathbf{x} = x_m, \theta) = \sum_{m=1}^{M} \frac{p\left(x_m; \mu_k, \Sigma_k\right)\tau_k}{\sum_k p\left(x_m; \mu_k, \Sigma_k\right)\tau_k}$$

- The cluster with the lowest $r(k)$ is splitted.
- Covariance matrices equal to Σ_k
- New cluster center is set to $\mu = \mu_k \pm \frac{\sqrt{\lambda_1}}{2} u_1$, where λ_1 is the largest eigenvalue of Σ_k and u_1 is the corresponding eigenvector.



Automatic Model Order Selection

- Prior probabilities for the new components are set to $\frac{1}{2}p(\theta_k) = \frac{1}{2}\tau_k$
- K_i denotes the number of components in a model after i-th iteration
- L_i be the likelihood of the validation set given the model
  1. Apply EM for model with K_i components.
  2. Compute L_i for validation set
  3. If $(L_i - L_{i-1} \leq \varepsilon)$, STOP.
  4. Split the cluster k with the lowest total responsibility $r(k)$
  5. Set $K_{i+1} = K_i + 1$ and $i = i + 1$
  6. Go to 1.

Adaptive EM for Non-stationary Distributions

- In the context of dynamic vision, data are often sampled from non-stationary distributions.
- For example, the color of the object often changes gradually over time
- An algorithm for adaptively estimating such a mixture.
  - At each frame, t, a new set of data, $X^{(t)}$ can be used to update the mixture model.
  - Let $r_x^{(t)}$ for $x \in X^{(t)}$ denote the posterior probability for each k, as

$$r_x^{(t)} = p(\theta^{(t-1)}|x)$$

  - The parameters are first estimated by

$$\mu^{(t)} = \frac{\sum_{x \in X^{(t)}} r_x^{(t)} x}{\sum_{x \in X^{(t)}} r_x^{(t)}},$$

$$C^{(t)} = \frac{\sum_{x \in X^{(t)}} r_x^{(t)} (x - \mu^{(t-1)})(x - \mu^{(t-1)})^T}{\sum_{x \in X^{(t)}} r_x^{(t)}}$$

Interim Summary

- K_n-Nearest Neighbor Method
- Nearest Neighbor Method
- k -Nearest Neighbor Method
- k -Nearest Neighbor Classifier
- Bayes, the nearest neighbor, the k-NN classifiers
- Gaussian Mixture Model
- EM Algorithm
- Automatic GMM selection
- Adaptive GMM