Machine Learning – Lecture 3

Probability Density Estimation II

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Many slides adapted from B. Schiele

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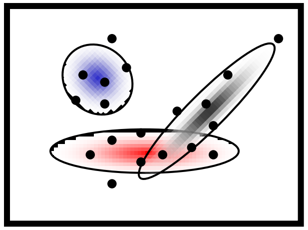
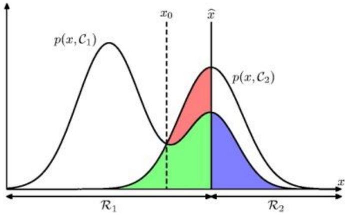
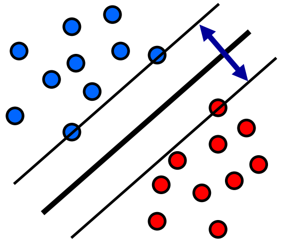
Course Outline

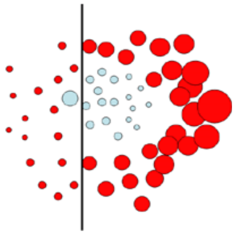
- Fundamentals (2 weeks)
  - Bayes Decision Theory
  - Probability Density Estimation



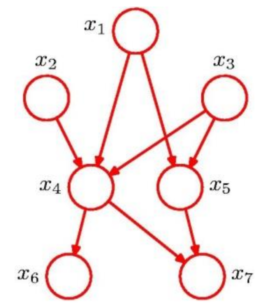


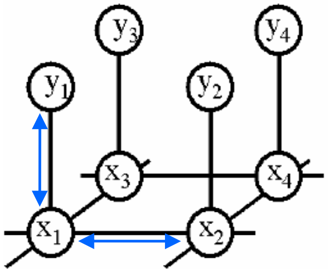
- Discriminative Approaches (5 weeks)
  - Linear Discriminant Functions
  - Support Vector Machines
  - Ensemble Methods & Boosting
  - Randomized Trees, Forests & Ferns





- Generative Models (4 weeks)
  - Bayesian Networks
  - Markov Random Fields





Topics of This Lecture

- Recap: Bayes Decision Theory
- Parametric Methods
  - Recap: Maximum Likelihood approach
  - Bayesian Learning
- Non-Parametric Methods
  - Histograms
  - Kernel density estimation
  - K-Nearest Neighbors
  - k-NN for Classification
  - Bias-Variance tradeoff

Recap: Bayes Decision Theory

- **Optimal decision rule**
  - **Decide for C_1 if**

$$p(\mathcal{C}_1|x) > p(\mathcal{C}_2|x)$$

  - **This is equivalent to**

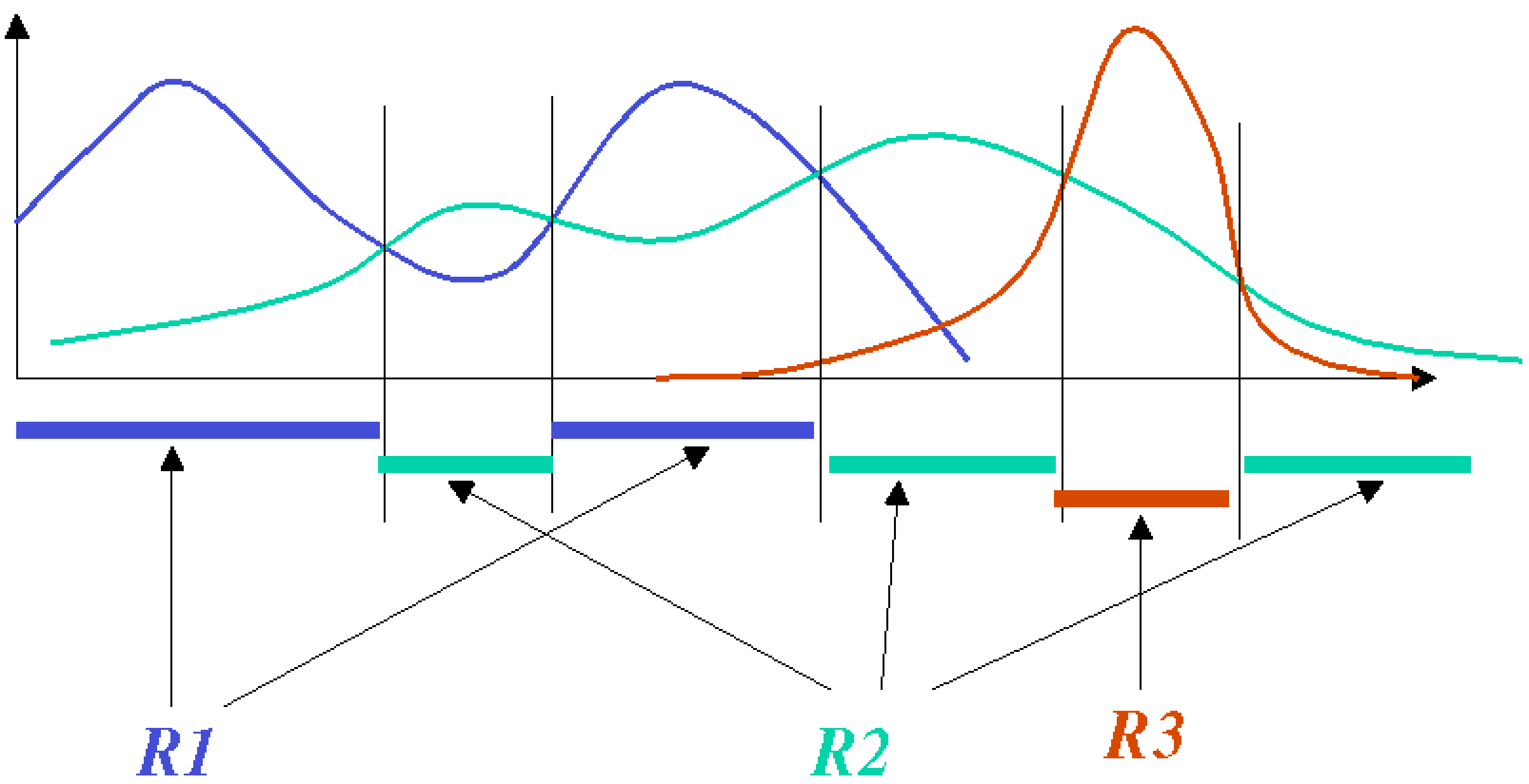
$$p(x|\mathcal{C}_1)p(\mathcal{C}_1) > p(x|\mathcal{C}_2)p(\mathcal{C}_2)$$

  - **Which is again equivalent to (Likelihood-Ratio test)**

$$\frac{p(x|\mathcal{C}_1)}{p(x|\mathcal{C}_2)} > \underbrace{\frac{p(\mathcal{C}_2)}{p(\mathcal{C}_1)}}_{\text{Decision threshold } \theta}$$

Recap: Bayes Decision Theory

- **Decision regions:** $\mathcal{R}_1, \mathcal{R}_2, \mathcal{R}_3, \ldots$



Recap: Classifying with Loss Functions

- We can formalize the intuition that different decisions have different weights by introducing a loss matrix L_{kj}

$$L_{kj} = loss\ for\ decision\ \mathcal{C}_j\ if\ truth\ is\ \mathcal{C}_k.$$

- Example: cancer diagnosis

Decision

$$L_{cancer\ diagnosis} = \text{Truth} \begin{array}{c} \\ \text{cancer} \\ \text{normal} \end{array} \begin{array}{c} \begin{array}{cc} \text{cancer} & \text{normal} \end{array} \\ \left(\begin{array}{cc} 0 & 1000 \\ 1 & 0 \end{array} \right) \end{array}$$

Recap: Minimizing the Expected Loss

- Optimal solution is the one that minimizes the loss.
  - But: loss function depends on the true class, which is unknown.

- Solution: Minimize the expected loss

$$\mathbb{E}[L] = \sum_k \sum_j \int_{\mathcal{R}_j} L_{kj} p(\mathbf{x}, \mathcal{C}_k) \, \mathrm{d}\mathbf{x}$$

- This can be done by choosing the regions $\mathcal{R}_j$ such that

$$\mathbb{E}[L] = \sum_k L_{kj} p(\mathcal{C}_k | \mathbf{x})$$

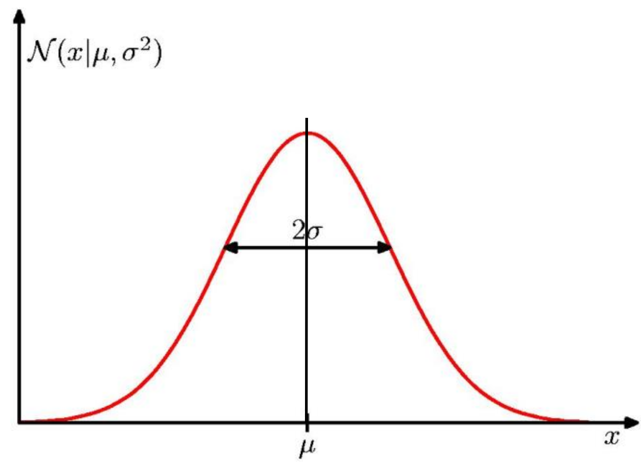
⇒ Adapted decision rule:

$$\frac{p(\mathbf{x}|\mathcal{C}_1)}{p(\mathbf{x}|\mathcal{C}_2)} > \frac{(L_{21} - L_{22})}{(L_{12} - L_{11})} \frac{p(\mathcal{C}_2)}{p(\mathcal{C}_1)}$$

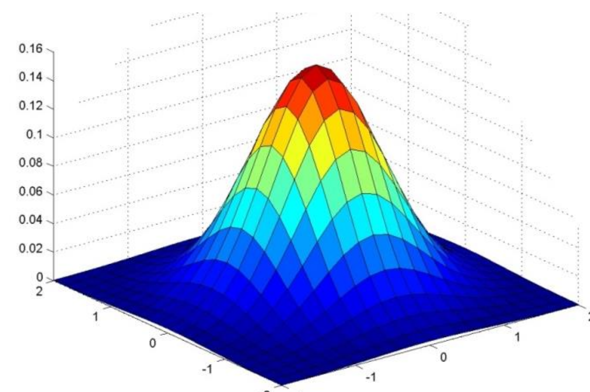
Recap: Gaussian (or Normal) Distribution

- **One-dimensional case**
  - **Mean** μ
  - **Variance** σ^2

$$\mathcal{N}(x|\mu,\sigma^2) = \frac{1}{\sqrt{2\pi\sigma}} \exp\left\{-\frac{(x-\mu)^2}{2\sigma^2}\right\}$$



- **Multi-dimensional case**
  - **Mean** $\boldsymbol{\mu}$
  - **Covariance** Σ



$$\mathcal{N}(\mathbf{x}|\boldsymbol{\mu},\boldsymbol{\Sigma}) = \frac{1}{(2\pi)^{D/2}|\boldsymbol{\Sigma}|^{1/2}} \exp\left\{-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^{\mathrm{T}}\boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu})\right\}$$

Image source: C.M. Bishop, 2006

Recap: Maximum Likelihood Approach

- **Computation of the likelihood**
  - Single data point: $p(x_n|\theta)$
  - Assumption: all data points $X = \{x_1, \ldots, x_n\}$ are independent

$$L(\theta) = p(X|\theta) = \prod_{n=1}^{N} p(x_n|\theta)$$

  - Log-likelihood

$$E(\theta) = -\ln L(\theta) = -\sum_{n=1}^{N} \ln p(x_n|\theta)$$

- **Estimation of the parameters θ (Learning)**
  - Maximize the likelihood (=minimize the negative log-likelihood)

  $\Rightarrow$ Take the derivative and set it to zero.

$$\frac{\partial}{\partial\theta} E(\theta) = -\sum_{n=1}^{N} \frac{\frac{\partial}{\partial\theta} p(x_n|\theta)}{p(x_n|\theta)} \stackrel{!}{=} 0$$

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- Parametric Methods
  - Recap: Maximum Likelihood approach
  - Bayesian Learning
- Non-Parametric Methods
  - Histograms
  - Kernel density estimation
  - K-Nearest Neighbors
  - k-NN for Classification
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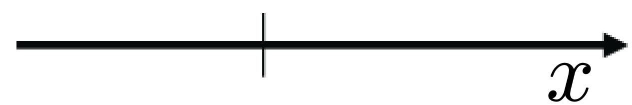
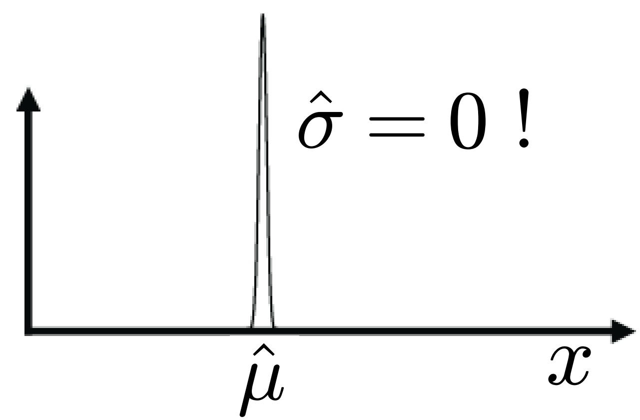
Recap: Maximum Likelihood – Limitations

- **Maximum Likelihood has several significant limitations**
  - **It systematically underestimates the variance of the distribution!**
  - **E.g. consider the case**

$$N = 1, X = \{x_1\}$$



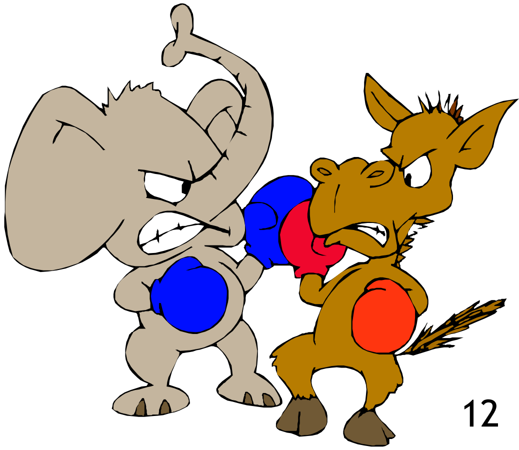
⇒ Maximum-likelihood estimate:



  - **We say ML *overfits to the observed data*.**
  - **We will still often use ML, but it is important to know about this effect.**

Deeper Reason

- Maximum Likelihood is a Frequentist concept
  - In the Frequentist view, probabilities are the frequencies of random, repeatable events.
  - These frequencies are fixed, but can be estimated more precisely when more data is available.
- This is in contrast to the Bayesian interpretation
  - In the Bayesian view, probabilities quantify the uncertainty about certain states or events.
  - This uncertainty can be revised in the light of new evidence.
- Bayesians and Frequentists do not like each other too well…



Bayesian vs. Frequentist View

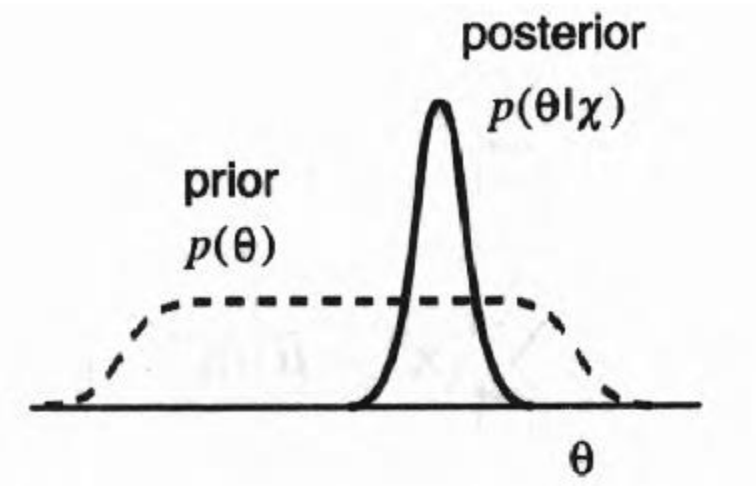
- To see the difference…
  - Suppose we want to estimate the uncertainty whether the Arctic ice cap will have disappeared by the end of the century.
  - This question makes no sense in a Frequentist view, since the event cannot be repeated numerous times.
  - In the Bayesian view, we generally have a prior, e.g. from calculations how fast the polar ice is melting.
  - If we now get fresh evidence, e.g. from a new satellite, we may revise our opinion and update the uncertainty from the prior.

$$Posterior \propto Likelihood \times Prior$$

  - This generally allows to get better uncertainty estimates for many situations.
- Main Frequentist criticism
  - The prior has to come from somewhere and if it is wrong, the result will be worse.

Bayesian Approach to Parameter Learning

- Conceptual shift
  - Maximum Likelihood views the true parameter vector θ to be unknown, but fixed.
  - In Bayesian learning, we consider θ to be a random variable.
- This allows us to use knowledge about the parameters θ
  - i.e., to use a prior for θ
  - Training data then converts this prior distribution on θ into a posterior probability density.



  - The prior thus encodes knowledge we have about the type of distribution we expect to see for θ.

Bayesian Learning Approach

- **Bayesian view:**
  - Consider the parameter vector θ as a random variable.
  - When estimating the parameters from a dataset X, we compute

$$p(x|X) = \int p(x, \theta|X) d\theta$$

Assumption: given θ, this doesn't depend on X anymore

$$p(x, \theta|X) = p(x|\theta, \cancel{X}) p(\theta|X)$$

$$p(x|X) = \int \underbrace{p(x|\theta)} p(\theta|X) d\theta$$

This is entirely determined by the parameter θ (i.e., by the parametric form of the pdf).

Bayesian Learning Approach

$$p(x|X) = \int p(x|\theta)\underbrace{p(\theta|X)}d\theta$$

$$p(\theta|X) = \frac{p(X|\theta)p(\theta)}{p(X)} = \frac{p(\theta)}{\underbrace{p(X)}}L(\theta)$$

$$p(X) = \int p(X|\theta)p(\theta)d\theta = \int L(\theta)p(\theta)d\theta$$

- **Inserting this above, we obtain**

$$p(x|X) = \int \frac{p(x|\theta)L(\theta)p(\theta)}{p(X)}d\theta = \int \frac{p(x|\theta)L(\theta)p(\theta)}{\int L(\theta)p(\theta)d\theta}d\theta$$

Bayesian Learning Approach

- Discussion

Likelihood of the parametric form θ given the data set X.

Estimate for x based on parametric form θ

Prior for the parameters θ

$$p(x|X) = \int \frac{p(x|\theta)L(\theta)p(\theta)}{\underbrace{\int L(\theta)p(\theta)d\theta}} d\theta$$

Normalization: integrate over all possible values of θ

  - If we now plug in a (suitable) prior $p(\theta)$, we can estimate $p(x|X)$ from the data set X.

Bayesian Density Estimation

- **Discussion**

$$p(x|X) = \int p(x|\theta)p(\theta|X)d\theta = \int \frac{p(x|\theta)L(\theta)p(\theta)}{\int L(\theta)p(\theta)d\theta}d\theta$$

  - The probability $p(\theta|X)$ makes the dependency of the estimate on the data explicit.
  - If $p(\theta|X)$ is very small everywhere, but is large for one $\hat{\theta}$, then

$$p(x|X) \approx p(x|\hat{\theta})$$

$\Rightarrow$ In this case, the estimate is determined entirely by $\hat{\theta}$.

$\Rightarrow$ The more uncertain we are about θ, the more we average over all parameter values.

Bayesian Density Estimation

- Problem
  - In the general case, the integration over θ is not possible (or only possible stochastically).

- Example where an analytical solution is possible
  - Normal distribution for the data, σ^2 assumed known and fixed.
  - Estimate the distribution of the mean:

$$p(\mu|X) = \frac{p(X|\mu)p(\mu)}{p(X)}$$

  - Prior: We assume a Gaussian prior over μ,

$$p(\mu) = \mathcal{N}\left(\mu|\mu_0, \sigma_0^2\right).$$

Bayesian Learning Approach

- **Sample mean:** $\bar{x} = \frac{1}{N} \sum_{n=1}^{N} x_n$

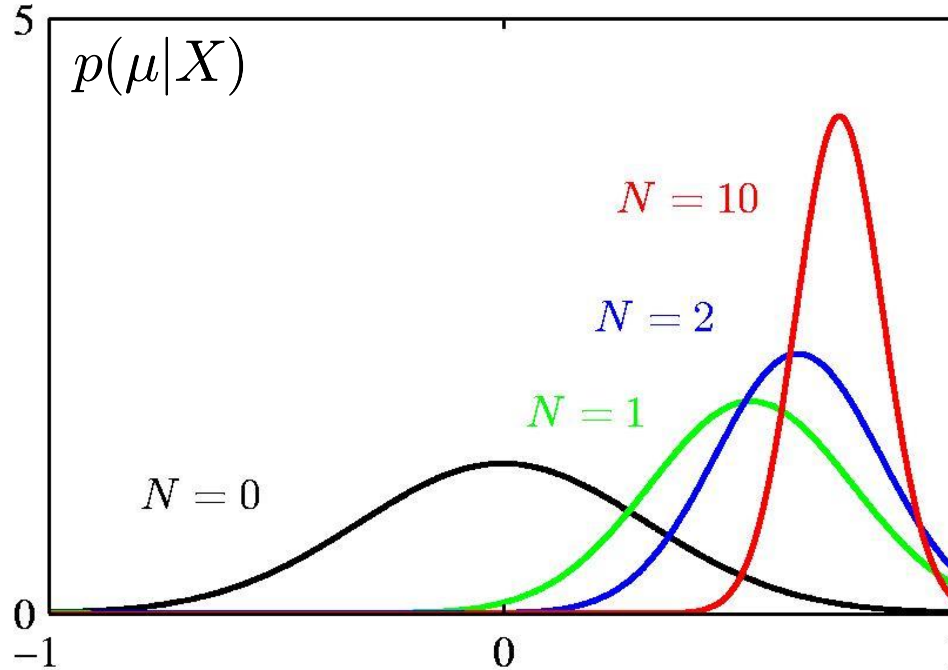
- **Bayes estimate:**

$$\mu_N = \frac{\sigma^2 \mu_0 + N\sigma_0^2 \bar{x}}{\sigma^2 + N\sigma_0^2}$$

$$\frac{1}{\sigma_N^2} = \frac{1}{\sigma_0^2} + \frac{N}{\sigma^2}$$

- **Note:**

	$N = 0$	$N \to \infty$
μ_N	μ_0	μ_{ML}
σ_N^2	σ_0^2	0



$\mu_0 = 0$

Image source: C.M. Bishop, 2006

Summary: ML vs. Bayesian Learning

- Maximum Likelihood
  - Simple approach, often analytically possible.
  - Problem: estimation is biased, tends to overfit to the data.

    $\Rightarrow$ Often needs some correction or regularization.
  - But:
    - Approximation gets accurate for $N \to \infty$.

- Bayesian Learning
  - General approach, avoids the estimation bias through a prior.
  - Problems:
    - Need to choose a suitable prior (not always obvious).
    - Integral over θ often not analytically feasible anymore.
  - But:
    - Efficient stochastic sampling techniques available.

(In this lecture, we'll use both concepts wherever appropriate)

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- Parametric Methods
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  - Bayesian Learning
- Non-Parametric Methods
  - Histograms
  - Kernel density estimation
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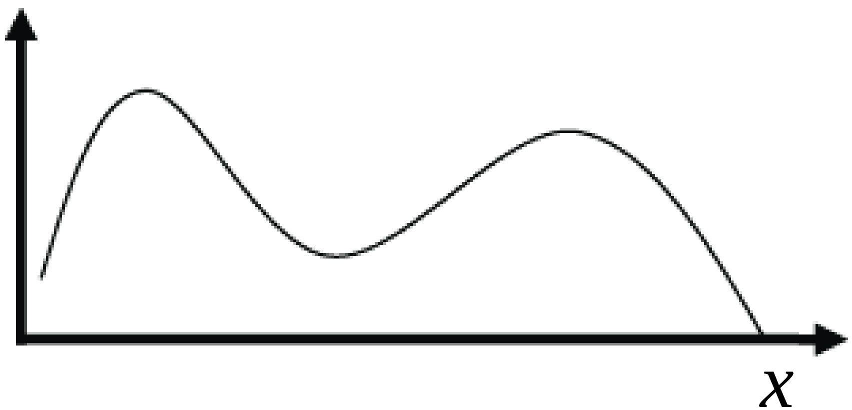
Non-Parametric Methods

- Non-parametric representations
  - Often the functional form of the distribution is unknown

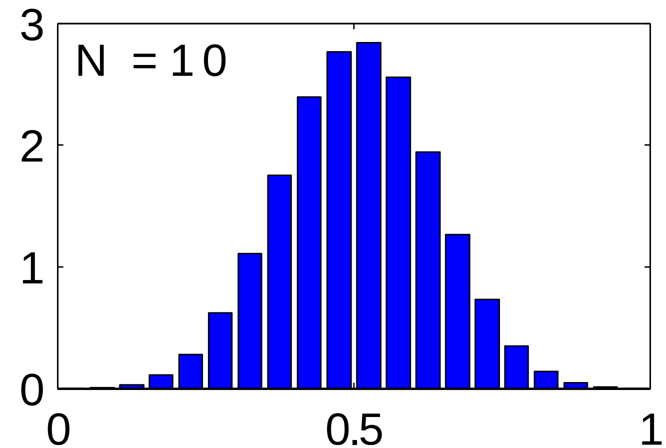


- Estimate probability density from data
  - Histograms
  - Kernel density estimation (Parzen window / Gaussian kernels)
  - k-Nearest-Neighbor

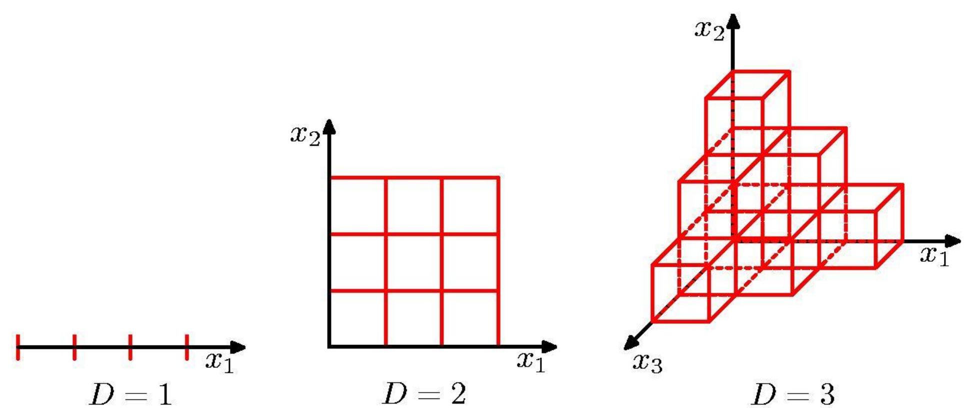
Histograms

- **Basic idea:**
  - **Partition the data space into distinct bins with widths Δ_i and count the number of observations, n_i, in each bin.**

$$p_i = \frac{n_i}{N\Delta_i}$$



  - **Often, the same width is used for all bins, $\Delta_i = \Delta$.**
  - **This can be done, in principle, for any dimensionality D...**



...but the required number of bins grows exponentially with D!

Image source: C.M. Bishop, 2006

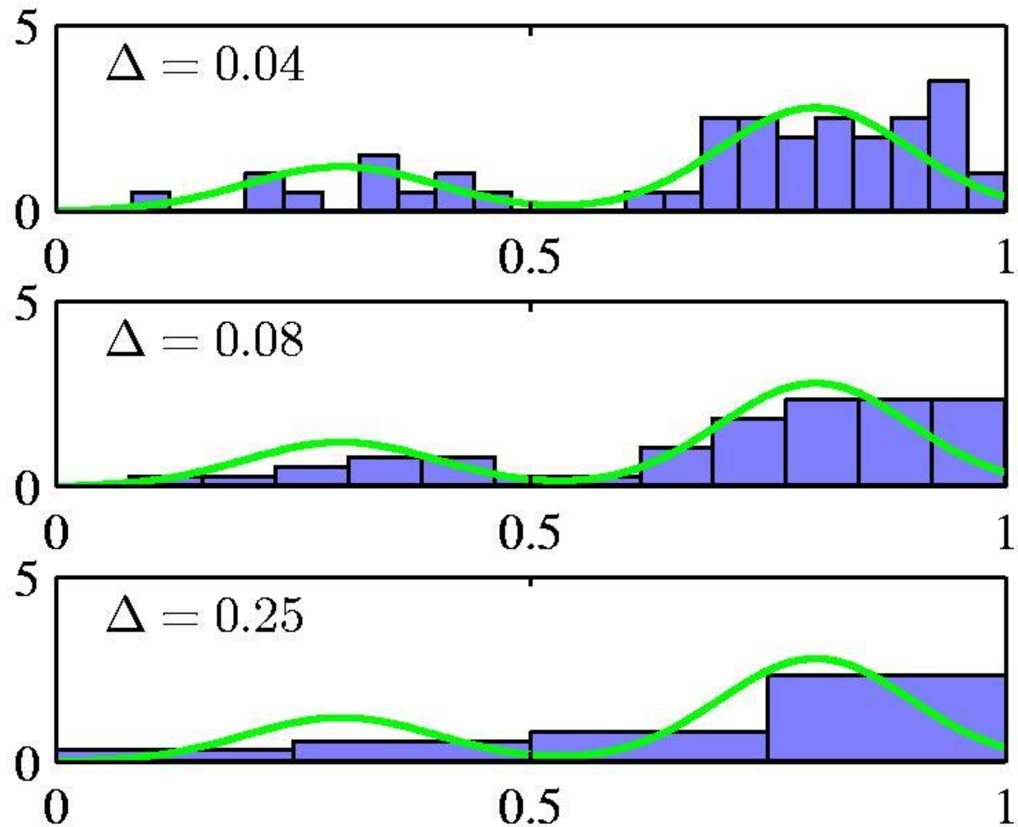
Histograms

- **The bin width Δ acts as a smoothing factor.**

not smooth enough

about OK

too smooth



Machine Learning Summer '15

Image source: C.M. Bishop, 2006

Summary: Histograms

- Properties
  - Very general. In the limit ($N \to \infty$), every probability density can be represented.
  - No need to store the data points once histogram is computed.
  - Rather brute-force
- Problems
  - High-dimensional feature spaces
    - D-dimensional space with M bins/dimension will require M^D bins!

    $\Rightarrow$ Requires an exponentially growing number of data points

    $\Rightarrow$ "Curse of dimensionality"
  - Discontinuities at bin edges
  - Bin size?
    - too large: too much smoothing
    - too small: too much noise

Statistically Better-Founded Approach

- Data point $\mathbf{x}$ comes from pdf $p(\mathbf{x})$
  - Probability that x falls into small region $\mathcal{R}$

$$P = \int_{\mathcal{R}} p(y)dy$$

- If $\mathcal{R}$ is sufficiently small, $p(\mathbf{x})$ is roughly constant
  - Let V be the volume of $\mathcal{R}$

$$P = \int_{\mathcal{R}} p(y)dy \approx p(\mathbf{x})V$$

- If the number N of samples is sufficiently large, we can estimate P as

$$P = \frac{K}{N} \qquad \Rightarrow p(\mathbf{x}) \approx \frac{K}{NV}$$

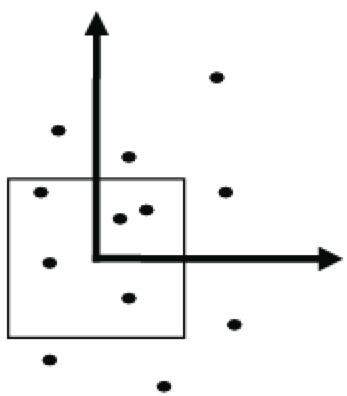
Statistically Better-Founded Approach

$$p(\mathbf{x}) \approx \frac{K}{NV}$$

fixed V
determine K → **Kernel Methods**

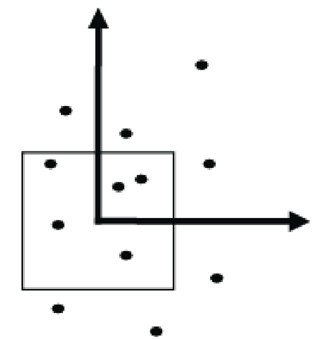
fixed K
determine V → **K-Nearest Neighbor**

- **Kernel methods**
  - Example: Determine the number K of data points inside a fixed window...



Kernel Methods

- **Parzen Window**
  - **Hypercube of dimension D with edge length h:**



$$k(\mathbf{u}) = \begin{cases} 1, & |u_i \cdot \quad \frac{1}{2}, \quad i = 1, \ldots, D \\ 0, & else \end{cases}$$

"Kernel function"

$$K = \sum_{n=1}^{N} k\left(\frac{\mathbf{x} - \mathbf{x}_n}{h}\right) \qquad V = \int k(\mathbf{u}) d\mathbf{u} = h^d$$

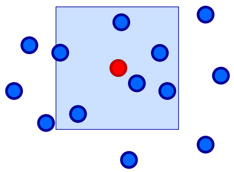
  - **Probability density estimate:**

$$p(\mathbf{x}) \approx \frac{K}{NV} = \frac{1}{Nh^D} \sum_{n=1}^{N} k\left(\frac{\mathbf{x} - \mathbf{x}_n}{h}\right)$$

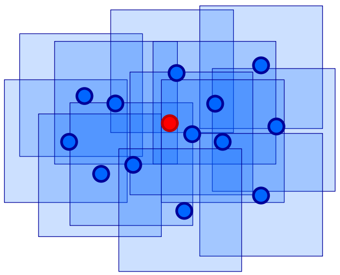
Slide credit: Bernt Schiele

Kernel Methods: Parzen Window

- Interpretations
  1. We place a *kernel window* k *at location* $\mathbf{x}$ and count how many data points fall inside it.



  2. We place a *kernel window* k *around each data point* $\mathbf{x}_n$ and sum up their influences at location $\mathbf{x}$.



  $\Rightarrow$ Direct visualization of the density.

- Still, we have artificial discontinuities at the cube boundaries…
  - We can obtain a smoother density model if we choose a smoother kernel function, e.g. a Gaussian

Kernel Methods: Gaussian Kernel

- **Gaussian kernel**
  - Kernel function

$$k(\mathbf{u}) = \frac{1}{(2\pi h^2)^{1/2}} \exp\left\{-\frac{\mathbf{u}^2}{2h^2}\right\}$$

$$K = \sum_{n=1}^{N} k(\mathbf{x} - \mathbf{x}_n) \qquad V = \int k(\mathbf{u}) d\mathbf{u} = 1$$

  - Probability density estimate

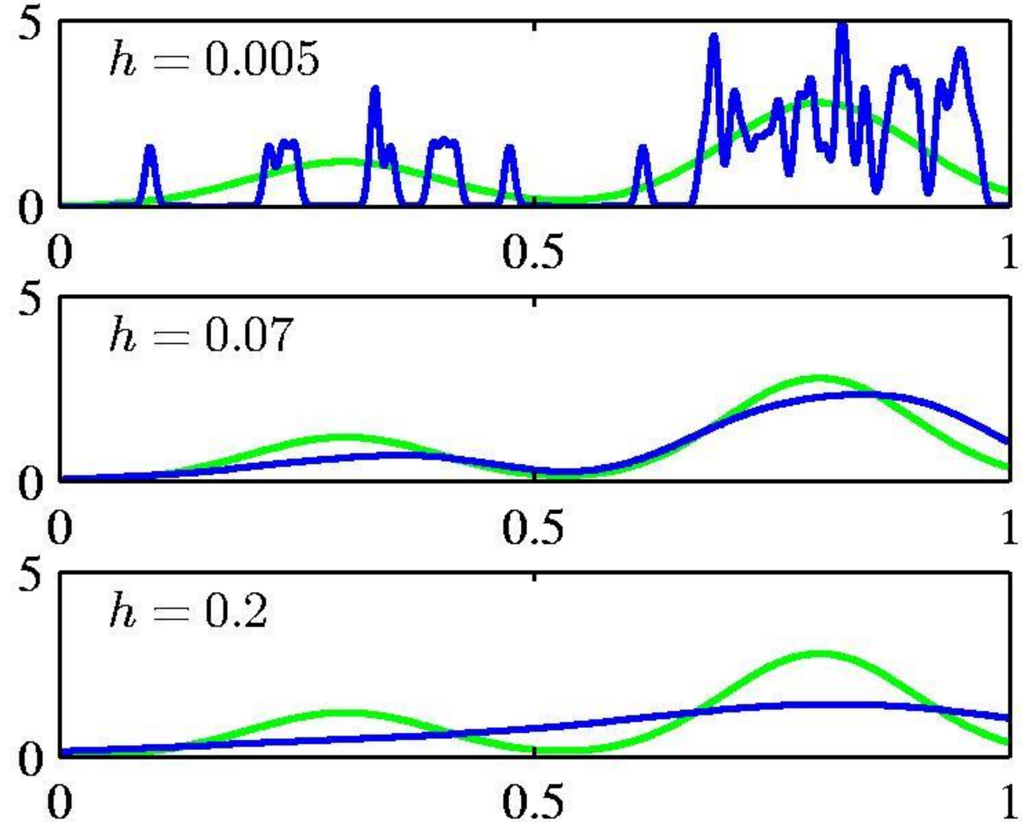
$$p(\mathbf{x}) \approx \frac{K}{NV} = \frac{1}{N} \sum_{n=1}^{N} \frac{1}{(2\pi)^{D/2} h} \exp\left\{-\frac{||\mathbf{x} - \mathbf{x}_n||^2}{2h^2}\right\}$$

Gauss Kernel: Examples

not smooth enough

about OK

too smooth



h **acts as a smoother.**

Image source: C.M. Bishop, 2006

Kernel Methods

- **In general**
  - Any kernel such that

$$k(\mathbf{u}) \geqslant 0, \qquad \int k(\mathbf{u})\,\mathrm{d}\mathbf{u} = 1$$

can be used. Then

$$K = \sum_{n=1}^{N} k(\mathbf{x} - \mathbf{x}_n)$$

  - And we get the probability density estimate

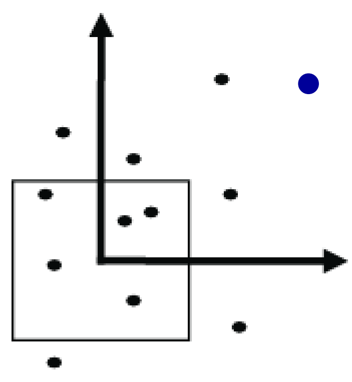
$$p(\mathbf{x}) \approx \frac{K}{NV} = \frac{1}{N} \sum_{n=1}^{N} k(\mathbf{x} - \mathbf{x}_n)$$

Statistically Better-Founded Approach

$$p(\mathbf{x}) \approx \frac{K}{NV}$$

fixed V
determine K
→ **Kernel Methods**

fixed K
determine V
→ **K-Nearest Neighbor**

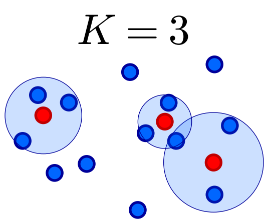


- **K-Nearest Neighbor**
  - **Increase the volume V until the K next data points are found.**

K-Nearest Neighbor

- **Nearest-Neighbor density estimation**
  - Fix K, estimate V from the data.
  - Consider a hypersphere centred on $\mathbf{x}$ and let it grow to a volume $V^\star$ that includes K of the given N data points.
  - Then

$$p(\mathbf{x}) \simeq \frac{K}{NV^\star}.$$



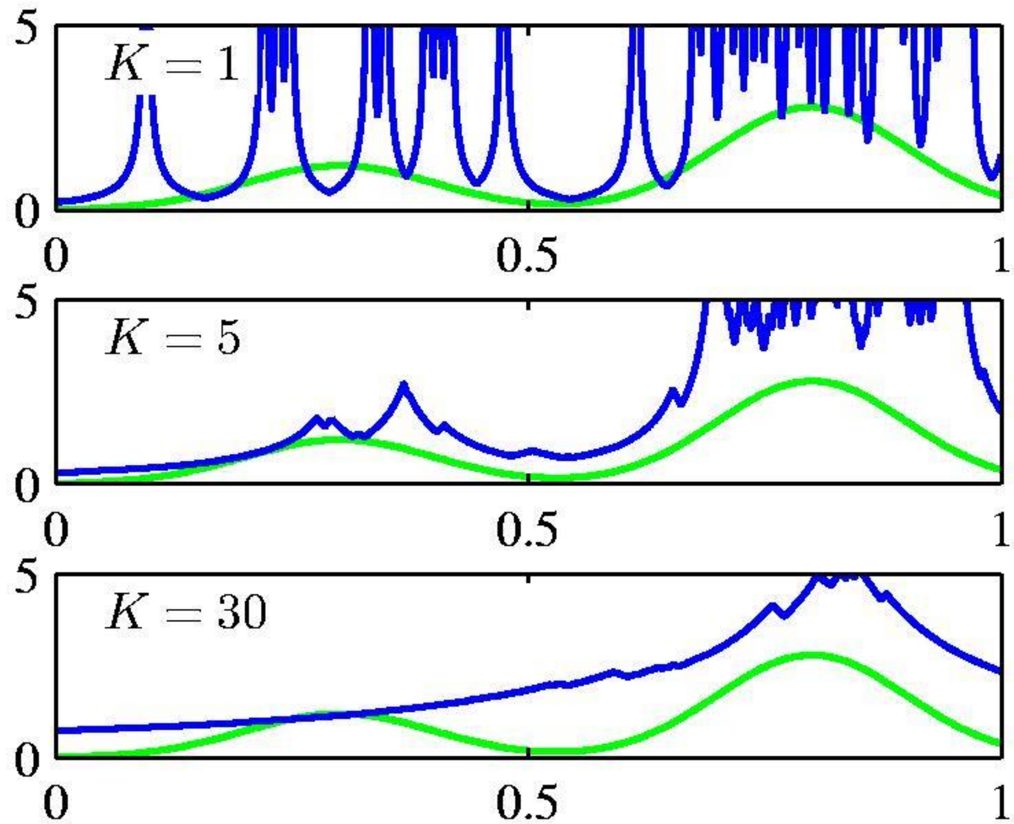
- **Side note**
  - Strictly speaking, the model produced by K-NN is not a true density model, because the integral over all space diverges.
  - E.g. consider $K = 1$ and a sample exactly on a data point $\mathbf{x} = x_j$.

k-Nearest Neighbor: Examples

not smooth enough

about OK

too smooth



K acts as a smoother.

Image source: C.M. Bishop, 2006

Summary: Kernel and k-NN Density Estimation

- Properties
  - Very general. In the limit ($N \rightarrow \infty$), every probability density can be represented.
  - No computation involved in the training phase
  - $\Rightarrow$ Simply storage of the training set
- Problems
  - Requires storing and computing with the entire dataset.
  - $\Rightarrow$ Computational cost linear in the number of data points.
  - $\Rightarrow$ This can be improved, at the expense of some computation during training, by constructing efficient tree-based search structures.
  - Kernel size / K in K-NN?
    - Too large: too much smoothing
    - Too small: too much noise

K-Nearest Neighbor Classification

- **Bayesian Classification**

$$p(\mathcal{C}_j|\mathbf{x}) = \frac{p(\mathbf{x}|\mathcal{C}_j)p(\mathcal{C}_j)}{p(\mathbf{x})}$$

- **Here we have**

$$p(\mathbf{x}) \approx \frac{K}{NV}$$

$$p(\mathbf{x}|\mathcal{C}_j) \approx \frac{K_j}{N_j V} \longrightarrow p(\mathcal{C}_j|\mathbf{x}) \approx \frac{K_j}{N_j V}\frac{N_j}{N}\frac{NV}{K} = \frac{K_j}{K}$$

$$p(\mathcal{C}_j) \approx \frac{N_j}{N}$$

k-Nearest Neighbor classification

K-Nearest Neighbors for Classification

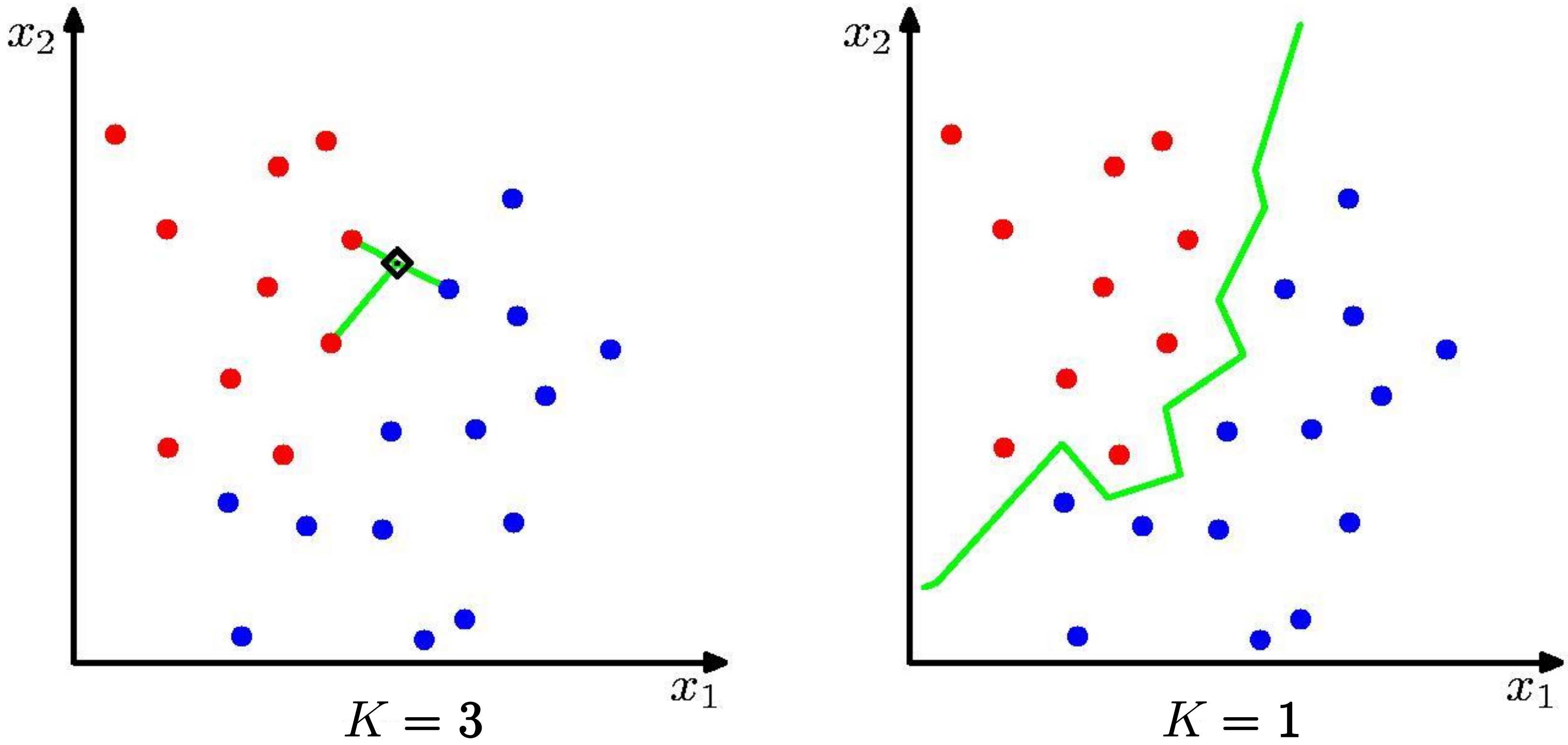
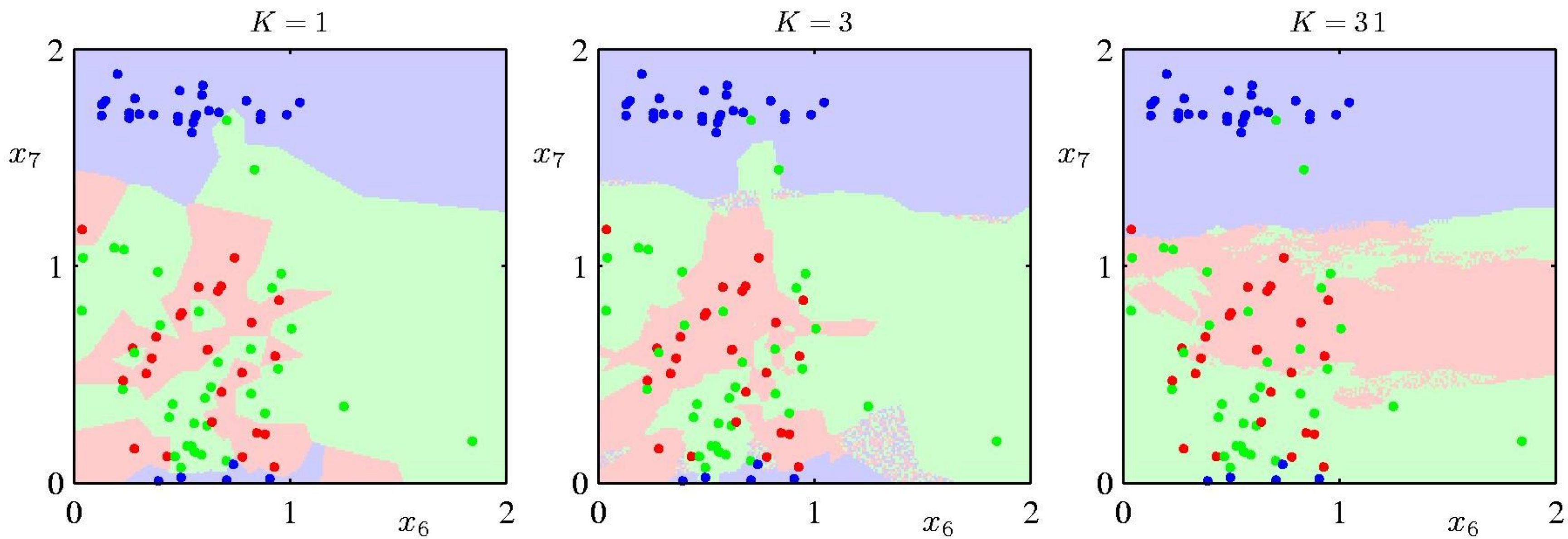


Image source: C.M. Bishop, 2006

K-Nearest Neighbors for Classification

- Results on an example data set



- K acts as a smoothing parameter.
- Theoretical guarantee
  - For $N \to \infty$, the error rate of the 1-NN classifier is never more than twice the optimal error (obtained from the true conditional class distributions).

Image source: C.M. Bishop, 2006

Bias-Variance Tradeoff

- Probability density estimation
  - Histograms: bin size?
    - Δ too large: too smooth
    - Δ too small: not smooth enough
  - Kernel methods: kernel size?
    - h too large: too smooth
    - h too small: not smooth enough
  - K-Nearest Neighbor: K?
    - K too large: too smooth
    - K too small: not smooth enough

Too much bias

Too much variance

- This is a general problem of many probability density estimation methods
  - Including parametric methods and mixture models

Discussion

- The methods discussed so far are all simple and easy to apply. They are used in many practical applications.
- However…
  - Histograms scale poorly with increasing dimensionality.

  ⇒ Only suitable for relatively low-dimensional data.
  - Both k-NN and kernel density estimation require the entire data set to be stored.

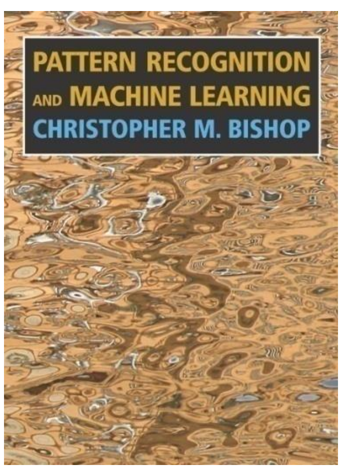
  ⇒ Too expensive if the data set is large.
  - Simple parametric models are very restricted in what forms of distributions they can represent.

  ⇒ Only suitable if the data has the same general form.
- We need density models that are efficient and flexible!

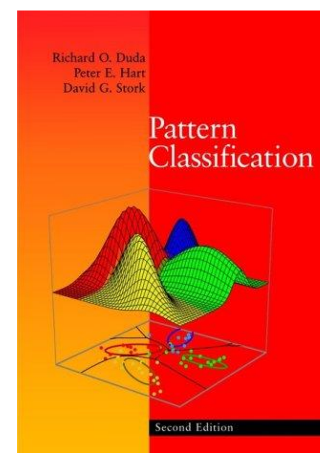
  ⇒ Next lecture…

References and Further Reading

- More information in Bishop's book
  - Gaussian distribution and ML: Ch. 1.2.4 and 2.3.1-2.3.4.
  - Bayesian Learning: Ch. 1.2.3 and 2.3.6.
  - Nonparametric methods: Ch. 2.5.
- Additional information can be found in Duda & Hart
  - ML estimation: Ch. 3.2
  - Bayesian Learning: Ch. 3.3-3.5
  - Nonparametric methods: Ch. 4.1-4.5



Christopher M. Bishop
Pattern Recognition and Machine Learning
Springer, 2006



R.O. Duda, P.E. Hart, D.G. Stork
Pattern Classification
2nd Ed., Wiley-Interscience, 2000