Nonparametric Methods for Density Estimation
Nearest Neighbour Classification

Lecturer:
Jiří Matas

Authors:
Ondřej Drbohlav, Jiří Matas

Centre for Machine Perception
Czech Technical University, Prague
http://cmp.felk.cvut.cz

Lecture date: 24.10.2016

Last update: 25.10.2016

Probability Density Estimation

Parametric Methods for Density Estimation

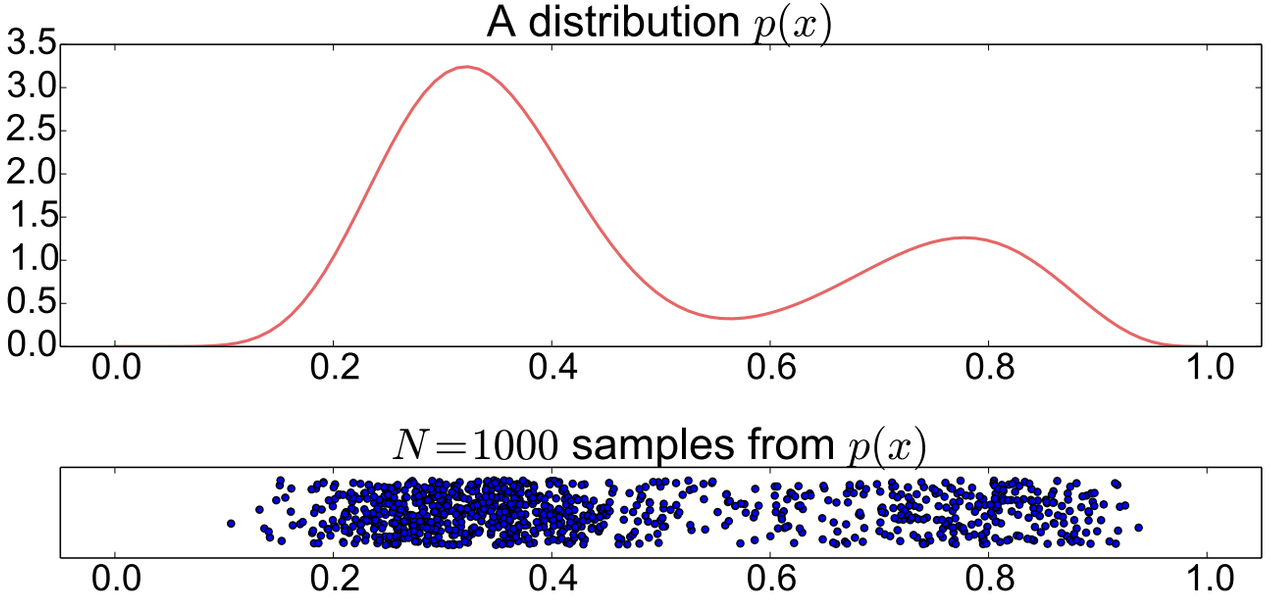
- Have been dealt with in the previous lecture
- Advantarge: Low number of parameters to estimate
- Disadvantage: The resulting estimated density can be arbitrarily wrong if the underlying distribution does not agree with the assumed parametric model.

Non-Parametric Methods for Density Estimation

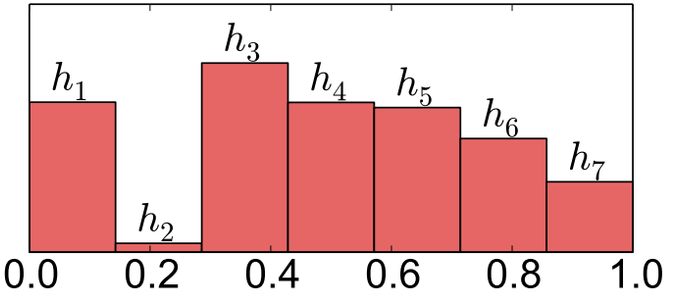
- Histogram
- Nearest Neighbor approach

Histogram (1)

Consider the following distribution on the interval $[0, 1]$, and i.i.d. sampling from it.
We will fit the distribution by a 'histogram' with B bins. More precisely, we will estimate a piecewise-constant function on the interval $[0, 1]$ with B segments of the same length.
For a given B, the parameters of this piecewise-constant function are the heights $h_1, h_2, ..., h_B$ of the individual bins. This function is denoted $p(x|\{h_1, h_2, ..., h_B\})$.



$p(x|\{h_1, h_2, .., h_B\})$ to be estimated



For the given number of bins B, $h_1, h_2, ..., h_B$ must conform to the constraint that the area under the function must sum up to one,

$$\frac{1}{B}\sum_{i=1}^{B} h_i = 1\,, \qquad (h_i \geq 0.) \tag{1}$$

Histogram (2)

Let us estimate $\{h_i, i = 1, 2, ..., B\}$ by Maximum Likelihood (ML) approach. Let N_i denote the number of samples which belong the i-th bin (thus clearly, $\sum_{i=1}^{B} N_i = N$). The likelihood $p(\mathcal{T}|\boldsymbol{\theta})$ of observing the samples $\mathcal{T} = \{x_1, x_2, ..., x_N\}$ given the parameters $\boldsymbol{\theta} = \{h_1, h_2, ..., h_B\}$ is

$$p(\mathcal{T}|\boldsymbol{\theta}) = \prod_{j=1}^{B} h_j^{N_j} \,. \tag{2}$$

The maximization task is then

$$\sum_{j=1}^{B} N_j \log h_j \to \max \,, \qquad \text{subject to } \frac{1}{B}\sum_{j=1}^{B} h_j = 1 \,, \tag{3}$$

where maximization has been formulated using the log-likelihood. The Lagrangian of the optimization task and the conditions of optimality (using the derivative $\partial/\partial h_k$) are then:

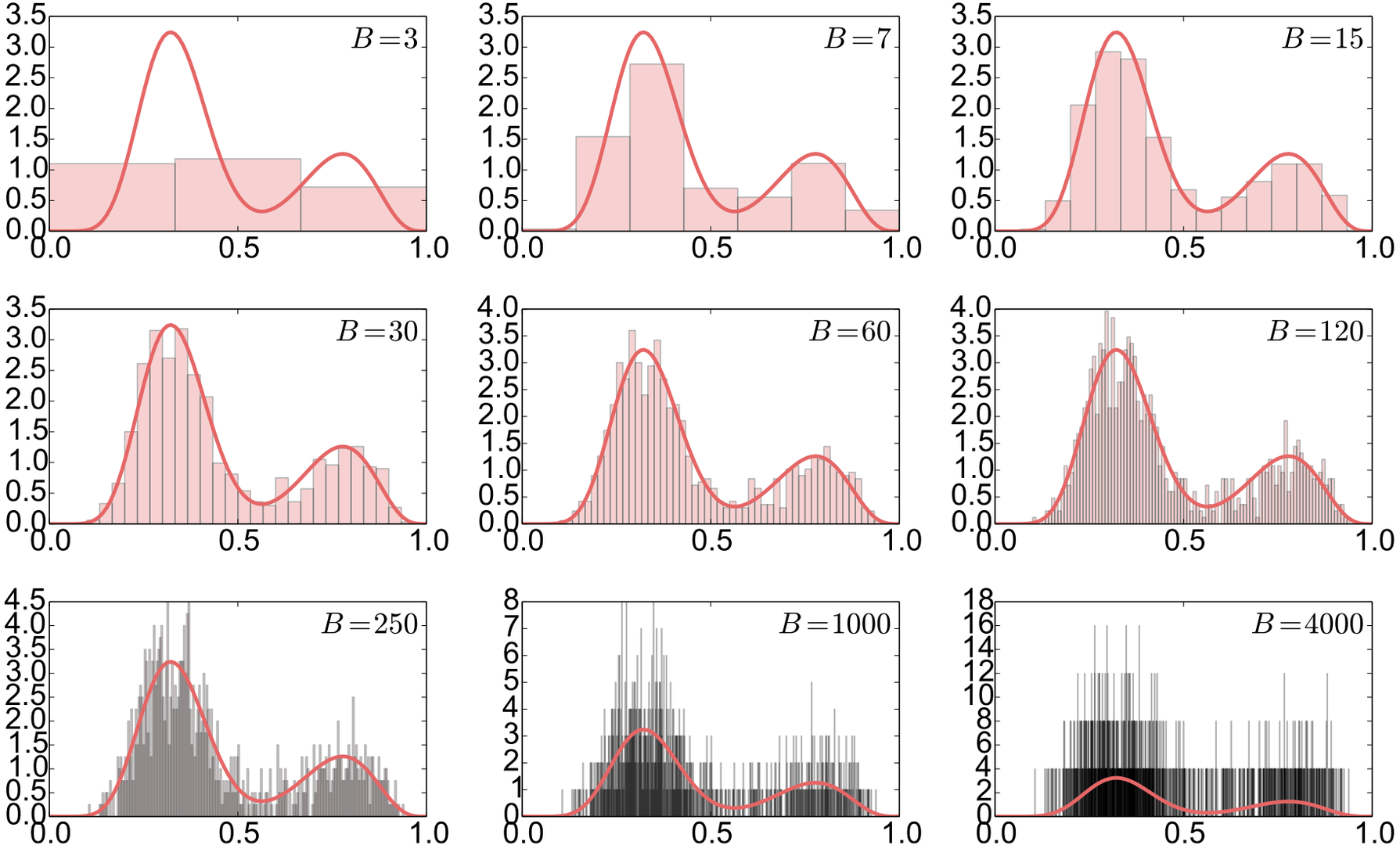
$$\text{Lagrangian: } \sum_{j=1}^{B} N_j \log h_j + \lambda \left(\frac{1}{B}\sum_{j=1}^{B} h_j - 1 \right) \tag{4}$$

$$\frac{N_k}{h_k} + \frac{\lambda}{B} = 0 \Rightarrow \frac{h_k}{N_k} = \text{const.} \Rightarrow \quad h_k = B\frac{N_k}{N} \quad . \tag{5}$$

Histogram (3)

$$h_k = B\frac{N_k}{N} \qquad (6)$$

This result is in line with the common use of histograms for approximating pdf's. Results for different B's:



Histogram: MAP and Bayes estimation

The ML estimation of h_i's suffers from similar problems as e.g. the Binomial Distribution estimation (recall estimating π, the fraction of red socks) in the last lecture.
MAP and Bayes estimation of h_i's need a suitable prior. The conjugate prior in this case is the Dirichlet Distribution, with the pdf $p(h_1, h_2, ..., h_B|\alpha_1, \alpha_2, ..., \alpha_B) \sim \prod h_i^{\alpha_i - 1}$.

MAP Estimation:

$$h_i = B\frac{N_i + \alpha_i - 1}{N + \sum_{i=1}^{B} \alpha_i - B} \tag{7}$$

Bayes Estimation:

$$h_i = B\frac{N_i + \alpha_i}{N + \sum_{i=1}^{B} \alpha_i} \tag{8}$$

Interpretation: The parameters α_i's again can be interpreted as 'virtual' observations, as if α_k points have already been assigned to the k-th bin.

Example: Take $\alpha_i = 2$ for all $i = 1, 2, ..., B$.

MAP:

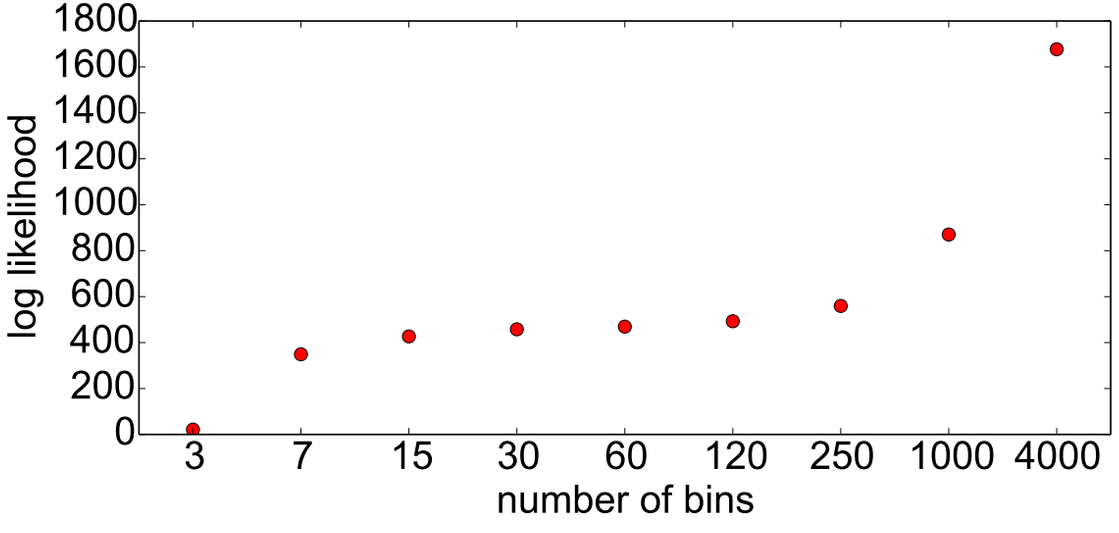
$$h_i = B\frac{N_i + 1}{N + B} \tag{9}$$

Bayes:

$$h_i = B\frac{N_i + 2}{N + 2B} \tag{10}$$

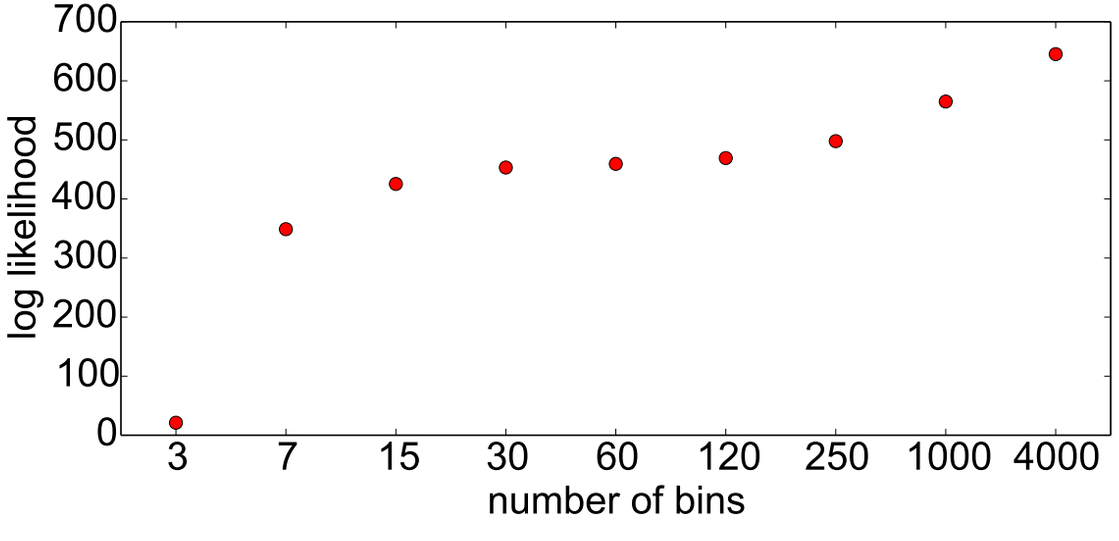
Histogram: Choosing the number of bins B (1)

Let us again employ the ML approach, this time for choosing the number of bins B:



$$\ell = \sum_{j=1}^{B} N_j \log h_j,$$

with $h_j = B\frac{N_j}{N}$



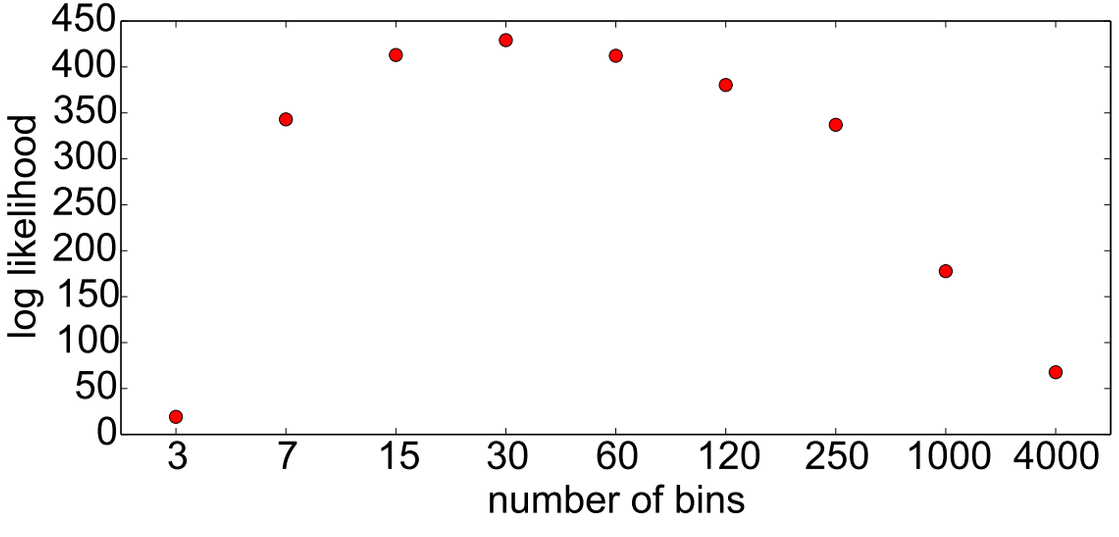
$$\ell = \sum_{j=1}^{B} N_j \log h_j,$$

with $h_j = B\frac{N_j+1}{N+B}$

Histogram: Choosing the number of bins B, cross-validation

The problem is that the log-likelihood ℓ is computed using the same data used for fitting the model (computing h_i's). This is a similar concept to training a classifier on certain data and testing on the same data, which is prone to over-fitting and poor generalization.

Let us compute the log likelihood using the following procedure: remove a given point from the dataset for computing h_i's and evaluate its contribution to the log-likelihood. Do this for all the points. If we start from e.g. $h_j = B\frac{N_j+1}{N+B}$, the modified estimation of h_j (omitting the point in question) will become $h_j = B\frac{N_j}{N-1+B}$. This leads to the following result:



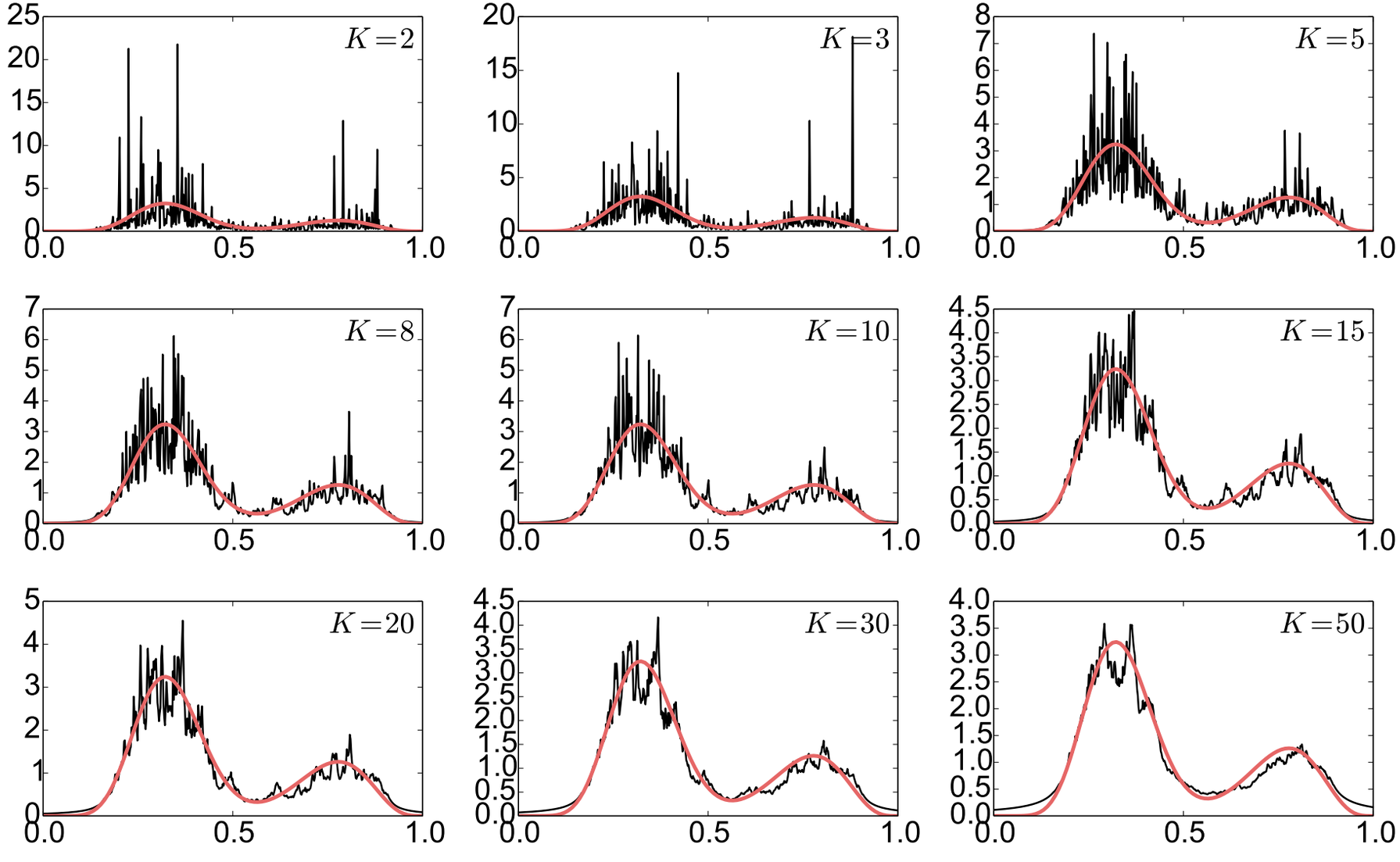
$$\ell = \sum_{j=1}^{B} N_j \log h_j,$$

with $h_j = B\frac{N_j}{N+B-1}$

This approach is related to cross-validation technique (leave-one-out) for choosing parameters of a classifier.

K-Nearest Neighbor Approach to Density Estimation

Find K neighbors, the density estimate is then $p \sim 1/V$ where V is the volume of a minimum cell containing K NNs. Example ($p \sim$ inverse distance to K-th NN, same 1000 samples as before):



K-Nearest Neighbor Approach to Classification

Outline:

- Definition
- Properties
- Asymptotic error of NN classifier
- Error reduction by edit operation on the training class
- Fast NN search

K-NN Classification Definition

Assumption:

- Training set $\mathcal{T} = \{(x_1, k_1), (x_2, k_2), ..., (x_N, k_N)\}$. There are R classes (letter K is reserved for KNN in this lecture)
- A distance function $d : X \times X \mapsto \mathbb{R}_0^+$

Algorithm:

1. Given x, find K points $S = \{(x'_1, k'_1), (x'_2, k'_2), ..., (x'_K, k'_K)\}$ from the training set $\mathcal{T}$ which are closest to x in the metric d:

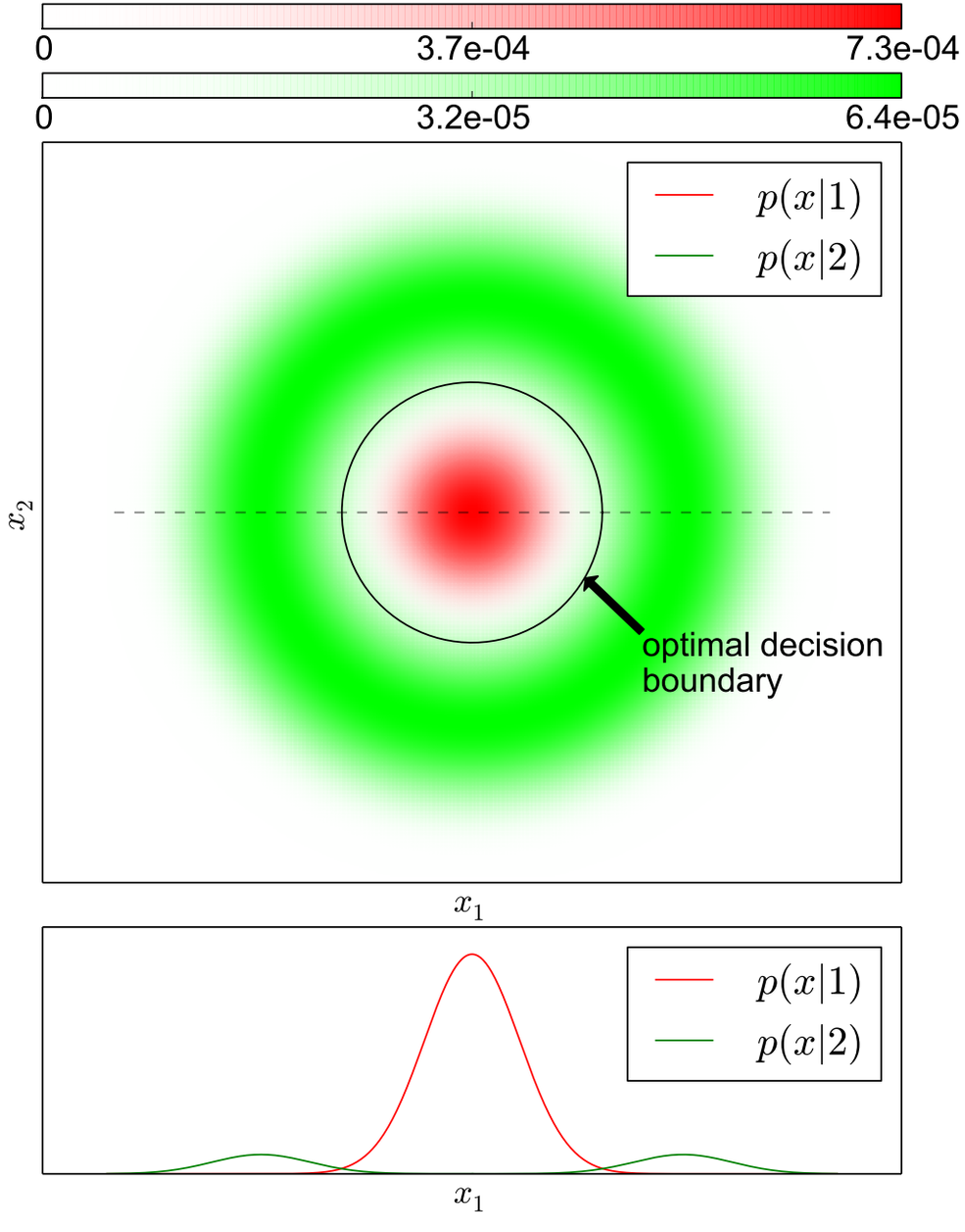
$$S = \{(x'_1, k'_1), (x'_2, k'_2), ..., (x'_K, k'_K)\} \equiv \{(x_{r_1}, k_{r_1}), (x_{r_2}, k_{r_2}), ..., (x_{r_K}, k_{r_K})\} \quad (11)$$

$$r_i\text{: the rank of } (x_i, k_i) \in \mathcal{T} \text{ as given by the ordering } d(x, x_i) \quad (12)$$

2. Classify x to the class k which has majority in S:

$$k = \underset{l \in R}{\text{argmax}} \sum_{i=1}^{K} [\![k'_i = l]\!] \qquad (x'_i, k'_i) \in S \quad (13)$$

K-NN Example (1)



Consider the two distributions shown. The priors are assumed to be the same,

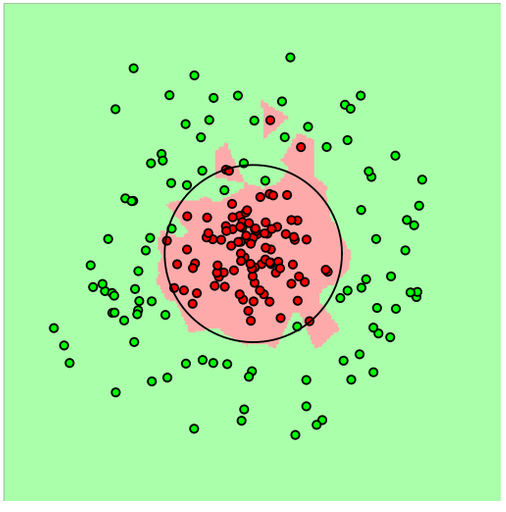
$$p(1) = p(2) = 0.5.$$

Bayesian optimal decision boundary is shown by the black circle.

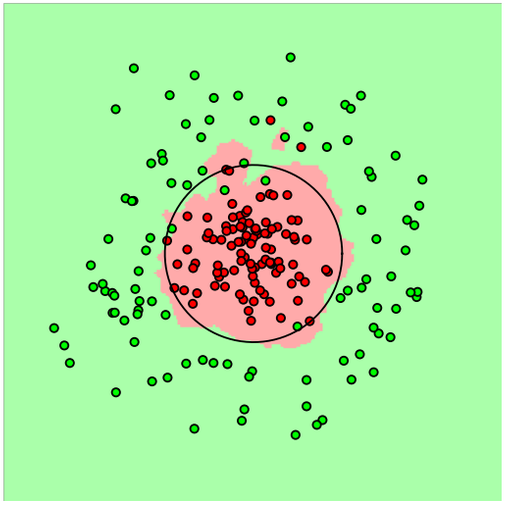
Bayesian error is $\epsilon_B = 0.026$.

K-NN Example (2)

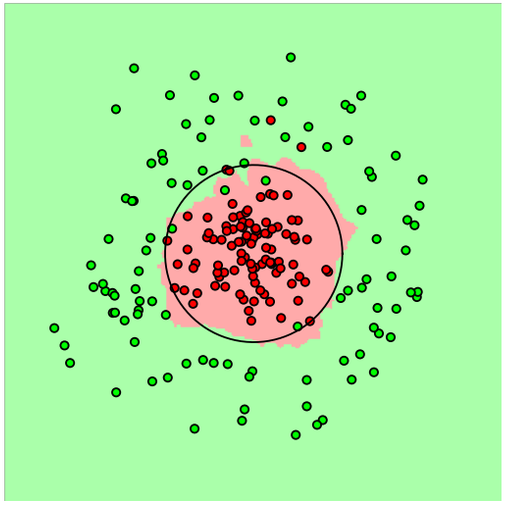
K = 1, error $\epsilon = 0.044$



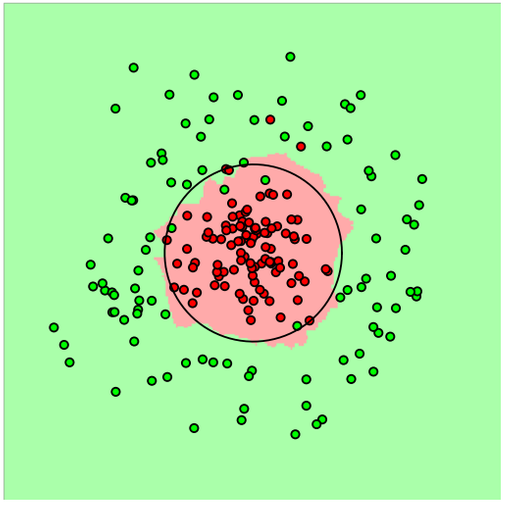
K = 3, error $\epsilon = 0.034$



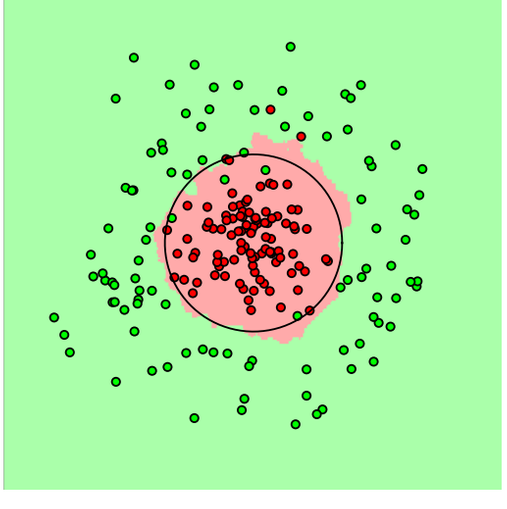
K = 5, error $\epsilon = 0.032$



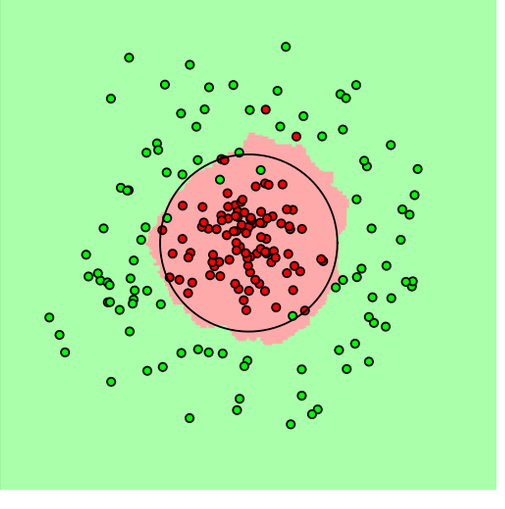
K = 7, error $\epsilon = 0.030$



K = 9, error $\epsilon = 0.031$



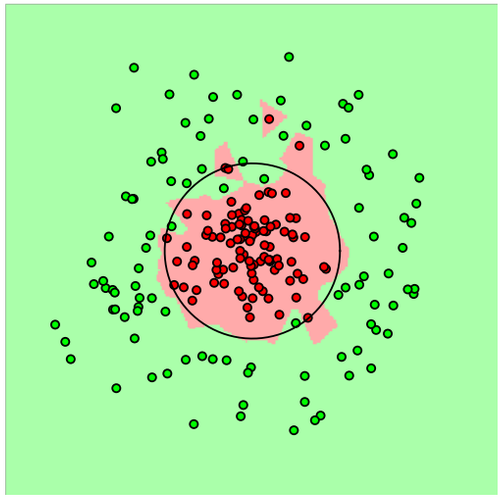
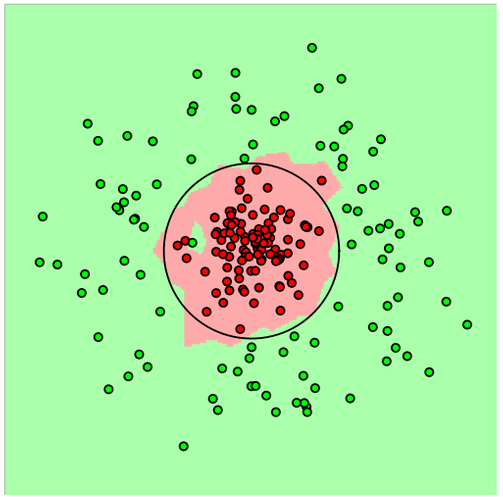
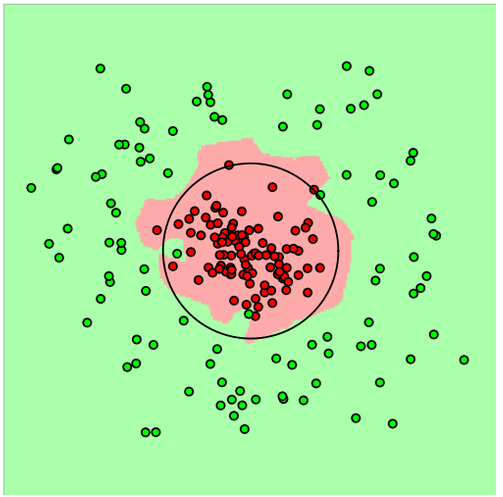
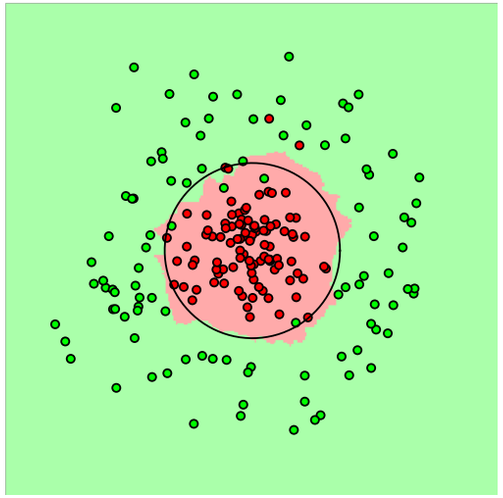
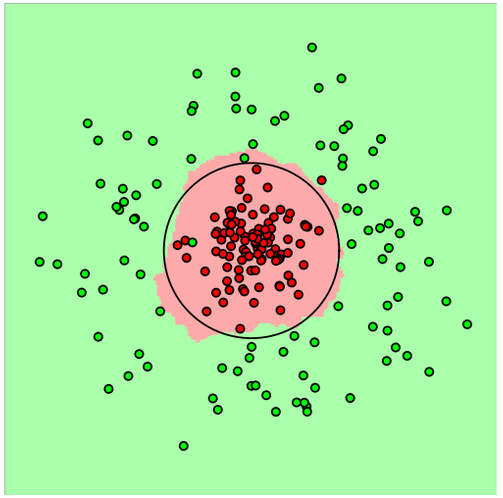
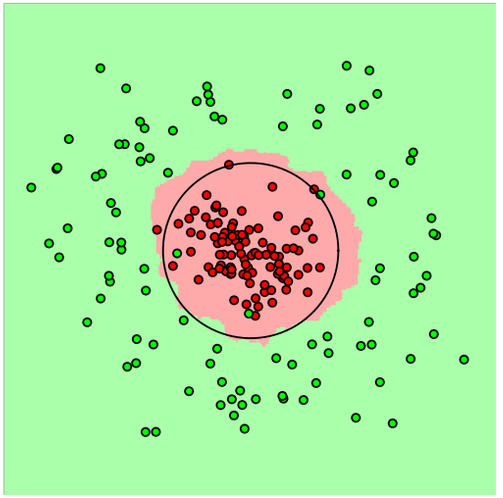
K = 11, error $\epsilon = 0.032$



$N = 100$ samples for each class. Bayes error $\epsilon_B = 0.026$.

K-NN Example (3)

The results depend on the training set (result of a random process.)
Each of the training sets $\mathcal{T}_1$, $\mathcal{T}_2$, $\mathcal{T}_3$ contain 100 points for each class.

$\mathcal{T}_1$	$\mathcal{T}_2$	$\mathcal{T}_3$
K = 1, error $\epsilon = 0.044$	K = 1, error $\epsilon = 0.038$	K = 1, error $\epsilon = 0.043$
		
K = 7, error $\epsilon = 0.030$	K = 7, error $\epsilon = 0.031$	K = 7, error $\epsilon = 0.036$
		

K-NN Properties

- Trivial implementation ($\rightarrow$ good baseline method)
- 1-NN: Bayes error ϵ_B is the lower bound on error of classification ϵ_{NN} (in the asymptotic case $N \rightarrow \infty$.) Higher bounds can also be constructed, e.g. $\epsilon_{NN} \leq 2\epsilon_B$
- Slow when implemented naively, but can be sped up (Voronoi, k-D trees)
- High computer memory requirements (but training set can be edited and its cardinality decreased)
- How to construct the metric d? (problem of scales in different axes)

K-NN : Speeding Up the Classification

- Sophisticated algorithms for NN search:
  - Classical problem in Comp. Geometry
  - k-D trees
- Removing the samples from the training class $\mathcal{T}$ which do not change the result of classification
  - Exactly: using Voronoi diagram
  - Approximately: E.g. use Gabriel graph instead of Voronoi
  - Condensation algorithm: iterative, also approximate.

Condensation Algorithm

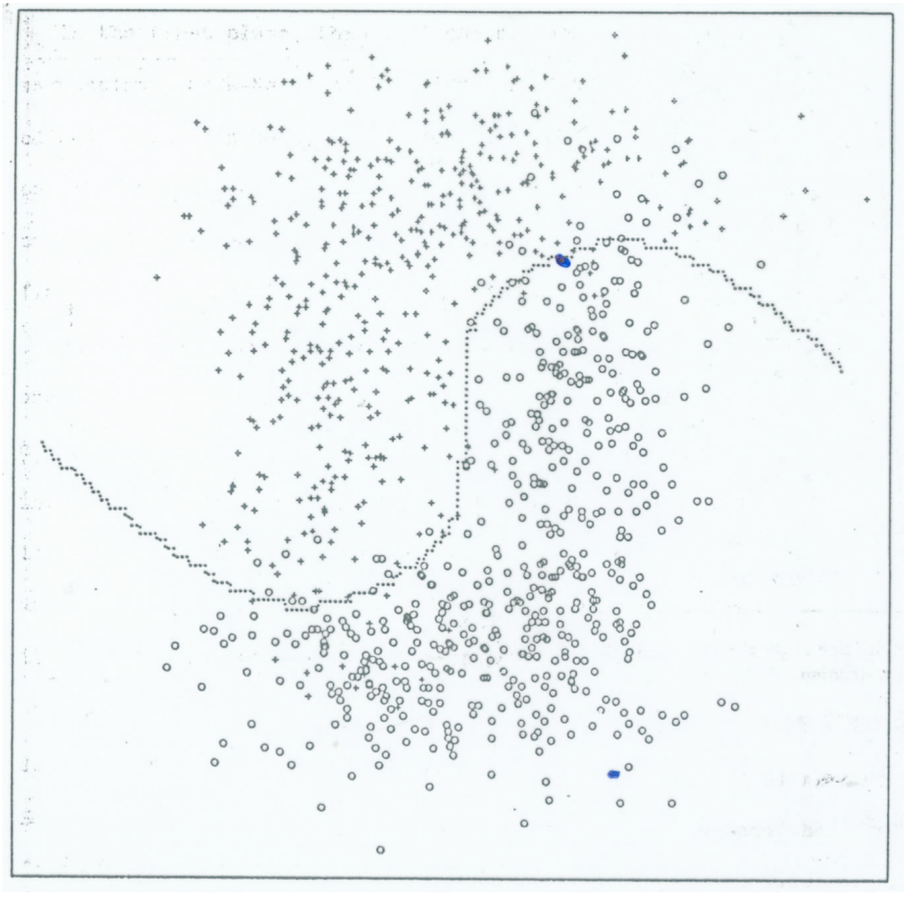
Input: The training set $\mathcal{T}$.

Algorithm

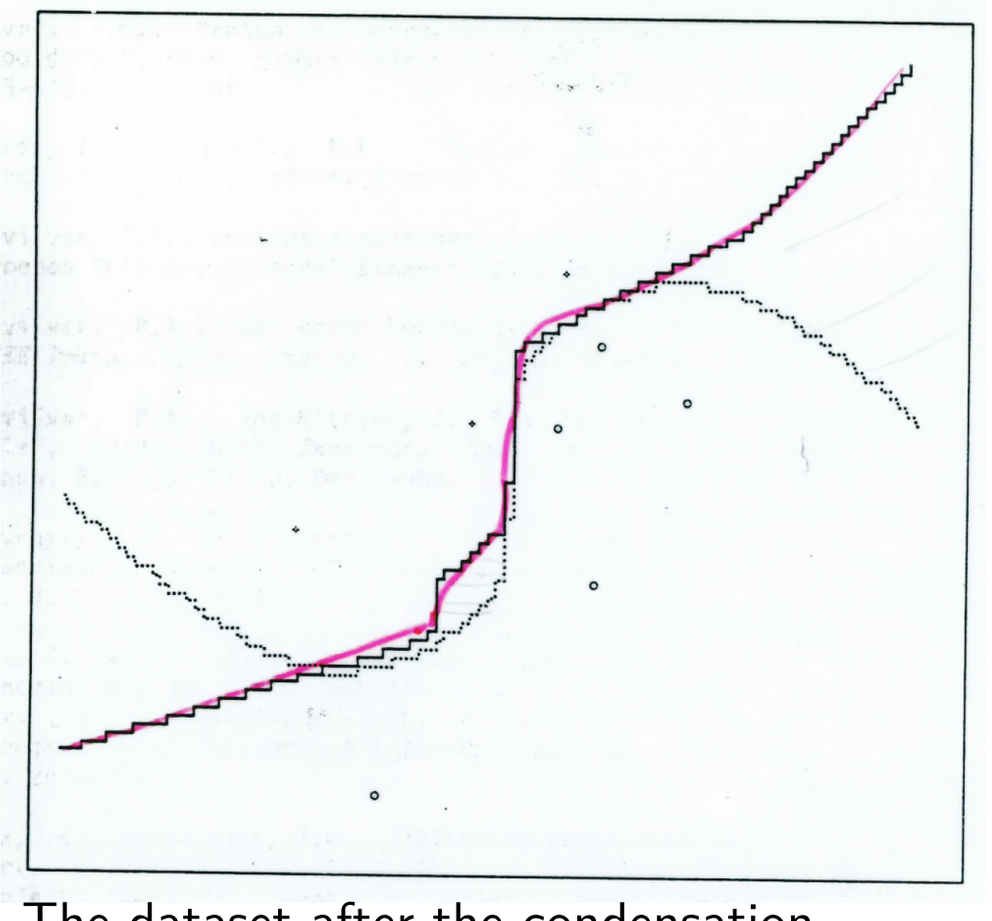
1. Create two lists, A and B. Insert a randomly selected sample from $\mathcal{T}$ to A. Insert the rest of the training samples to B.
2. Classify samples from B using 1NN with training set A. If an $x \in B$ is mis-classified, move it from B to A.
3. If a move has been triggered in Step 2., goto Step 2.

Output: A (the condensed training set for 1NN classification)

Condensation Algorithm, Example



The training dataset



The dataset after the condensation.
Shown with the new decision boundary.

1-NN Classification Error

Recall that a classification error $\bar{\epsilon}$ for strategy $q\colon X \to R$ is computed as

$$\bar{\epsilon} = \int \sum_{k:q(x)\neq k} p(x,k)\mathrm{d}x = \int \underbrace{\sum_{k:q(x)\neq k} p(k|x)}_{\epsilon(x)} p(x)\mathrm{d}x = \int \epsilon(x)p(x)\mathrm{d}x\,. \tag{14}$$

We know that the Bayesian strategy q_B decides for the highest posterior probability $q(x) = \mathrm{argmax}_k\, p(k|x)$, thus the partial error $\epsilon_B(x)$ for a given x is

$$\epsilon_B(x) = 1 - \max_k p(k|x)\,. \tag{15}$$

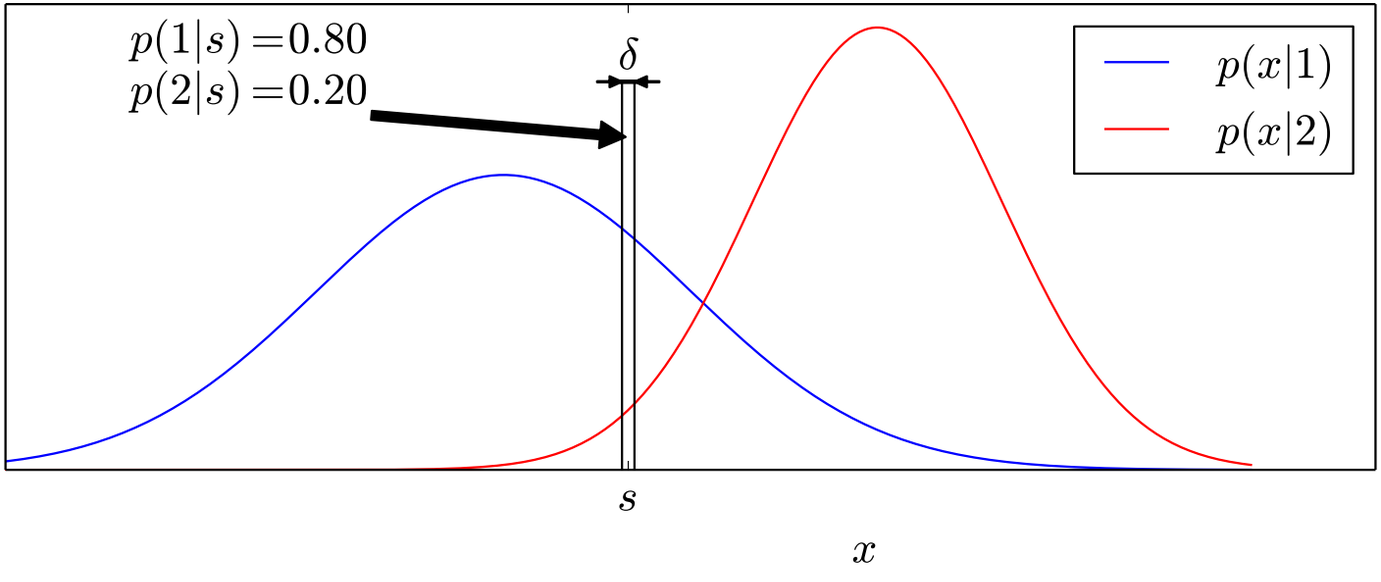
Assume the asymptotic case. We will show that the following bounds hold for the partial error $\epsilon_{NN}(x)$ and classification error $\bar{\epsilon}_{NN}$ in the 1-NN classification,

$$\epsilon_B(x) \leq \epsilon_{NN}(x) \leq 2\epsilon_B(x) - \tfrac{R}{R-1}\epsilon_B^2(x)\,, \tag{16}$$

$$\bar{\epsilon}_B \leq \bar{\epsilon}_{NN} \leq 2\bar{\epsilon}_B - \tfrac{R}{R-1}\bar{\epsilon}_B^2\,, \tag{17}$$

where $\bar{\epsilon}_B$ is the Bayes classification error and R is the number of classes.

1-NN Classification Error, Example (1)



Consider two distributions as shown, a small interval δ on an x-axis, and a point $s \in \delta$. Let the class priors be $p(1) = p(2) = 0.5$. Assume $\delta \to 0$ and number of samples $N \to \infty$.

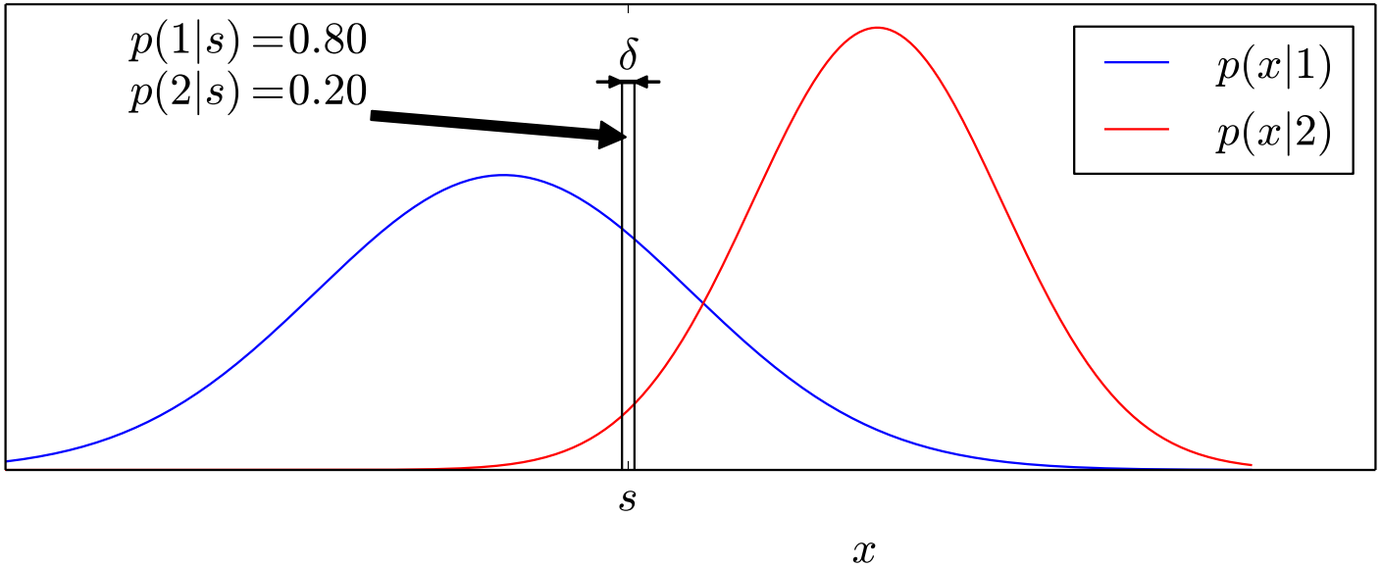
Observe the following:

$$p(1|s) = 0.8\,, \quad p(2|s) = 0.2\,, \tag{18}$$

$$p(NN=1|s) = p(1|s) = 0.8\,, \quad p(NN=2|s) = p(2|s) = 0.2\,, \tag{19}$$

where $p(NN=k|s)$ is the probability that the 1-NN of s is from class k ($k = 1, 2$) and thus s is classified as k.

1-NN Classification Error, Example (2)



The error $\epsilon_{NN}(s)$ at s is

$$\epsilon_{NN}(s) = p(1|s)\, p(NN=2|s) + p(2|s)\, p(NN=1|s) \tag{20}$$

$$= 1 - p(1|s)\, p(NN=1|s) - p(2|s)\, p(NN=2|s) \tag{21}$$

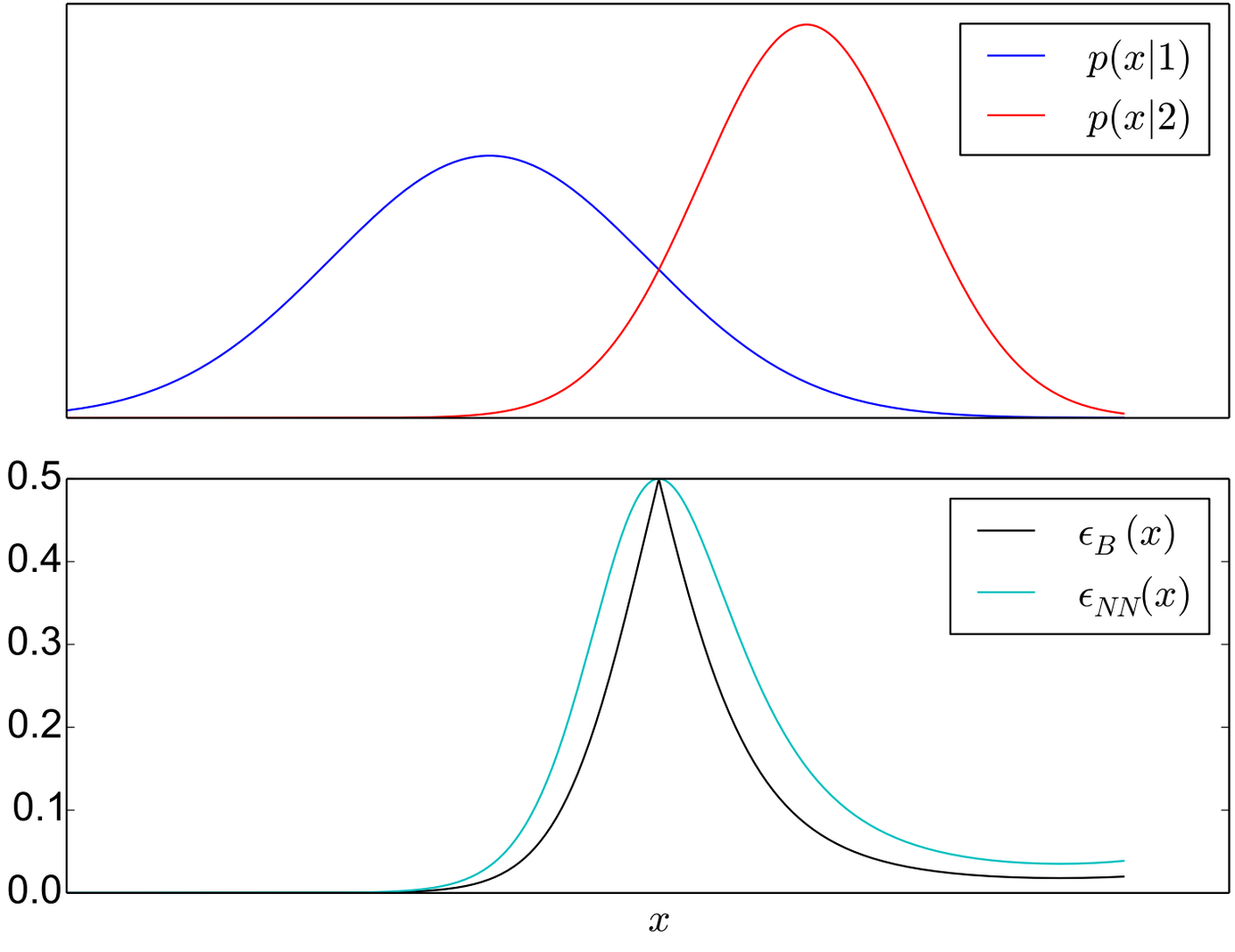
$$= 1 - p^2(1|s) - p^2(2|s)\,. \tag{22}$$

Generally, for R classes, the error will be

$$\epsilon_{NN}(s) = 1 - \sum_{k \in R} p^2(k|s)\,. \tag{23}$$

1-NN Classification Error, Example (3)

The two distributions and the partial errors
(the Bayesian error $\epsilon_B(x)$ and the 1-NN error $\epsilon_{NN}(x)$)



1-NN Classification Error Bounds (1)

Let us now return to the inequalities and prove them:

$$\epsilon_B(x) \leq \epsilon_{NN}(x) \leq 2\epsilon_B(x) - \frac{R}{R-1}\epsilon_B^2(x)\,, \tag{24}$$

The **first** inequality follows from the fact that Bayes strategies are optimal.

To prove the **second** inequality, let $P(x)$ denote the maximum posterior for x:

$$P(x) = \max_k p(k|x) \tag{25}$$

$$\Rightarrow \quad \epsilon_B(x) = 1 - P(x)\,. \tag{26}$$

Let us rewrite the partial error $\epsilon_{NN}(x)$ using the Bayesian entities $P(x)$ and $q(x)$:

$$\epsilon_{NN}(x) = 1 - \sum_{k \in R} p^2(k|x) = 1 - P^2(x) - \sum_{k \neq q(x)} p^2(k|x)\,. \tag{27}$$

We know that $p(q(x)|x) = P(x)$, but the remaining posteriors can be arbitrary. Let us consider the worst case. i.e. set $p(k|x)$ for $k \neq q(x)$ such that Eq. (27) is maximized. This will provide the higher bound.

1-NN Classification Error Bounds (2)

There are the following constraints on $p(k|x)$ $(k \neq q(x))$:

$$\sum_{k \neq q(x)} p(k|x) + P(x) = 1 \qquad \text{(posteriors sum to 1)} \tag{28}$$

$$\sum_{k \neq q(x)} p^2(k|x) \to \min \tag{29}$$

It is easy to show that this optimization problem is solved by setting all the posteriors to the same number. Thus,

$$p(k|x) = \frac{1 - P(x)}{R - 1} = \frac{\epsilon_B(x)}{R - 1} \qquad (k \neq q(x)) \tag{30}$$

The higher bound can then be rewritten in terms of the Bayes partial error $\epsilon_B(x) = 1 - P(x)$:

$$\epsilon_{NN}(x) \leq 1 - P^2(x) - \sum_{k \neq q(x)} p^2(k|x) = 1 - (1 - \epsilon_B(x))^2 - (R - 1)\frac{\epsilon_B^2(x)}{(R - 1)^2}\,. \tag{31}$$

1-NN Classification Error Bounds (3)

$$\epsilon_{NN}(x) \leq 1 - P^2(x) - \sum_{k \neq q(x)} p^2(k|x) \; = 1 - (1 - \epsilon_B(x))^2 - \frac{\epsilon_B^2(x)}{R-1}\,. \tag{32}$$

After expanding this, we get

$$\epsilon_{NN}(x) \leq 1 - (1 - \epsilon_B(x))^2 - \frac{\epsilon_B^2(x)}{(R-1)} \tag{33}$$

$$= 1 - 1 + 2\epsilon_B(x) - \epsilon_B^2(x) - \epsilon_B^2(x)\frac{R}{R-1} \tag{34}$$

$$= \; 2\epsilon_B(x) - \epsilon_B^2(x)\tfrac{R}{R-1} \tag{35}$$

Note that for $R = 2$, the bound is tight because using $\epsilon_B(x) = 1 - P(x)$ in Eq. (32) gives

$$\epsilon_{NN}(x) \leq 1 - P^2(x) - \frac{(1 - P(x))^2}{1} = \epsilon_{NN}(x)\,. \tag{36}$$

1-NN Classification Error Bounds (4)

The inequality for the local errors has been proven:

$$\epsilon_{NN}(x) \leq 2\epsilon_B(x) - \epsilon_B^2(x)\frac{R}{R-1} \tag{37}$$

Is there a similar higher bound for the classification error $\bar{\epsilon}_{NN} = \int \epsilon_{NN}(x)p(x)\mathrm{d}x$, based on the Bayes error $\bar{\epsilon}_B = \int \epsilon_B(x)p(x)\mathrm{d}x$?

Multiplying Eq. (38) by $p(x)$, and integrating, gives

$$\bar{\epsilon}_{NN} \leq 2\bar{\epsilon}_B(x) - \frac{R}{R-1}\int \epsilon_B^2(x)p(x)\mathrm{d}x \tag{38}$$

Let us use the known identity and inequality (where $E(\cdot)$ is the expectation operator)

$$\mathrm{var}(x) = E\left(x^2\right) - E^2(x)\,,\ \mathrm{var}(x) \geq 0 \qquad \Rightarrow \qquad E(x^2) \geq E^2(x) \tag{39}$$

Thus, $\int \epsilon_B^2(x)p(x)\mathrm{d}x \geq \left(\int \epsilon_B(x)p(x)\mathrm{d}x\right)^2$, and

$$\bar{\epsilon}_{NN} \leq 2\bar{\epsilon}_B(x) - \frac{R}{R-1}\int \epsilon_B^2(x)p(x)\mathrm{d}x \leq \ 2\bar{\epsilon}_B(x) - \frac{R}{R-1}\bar{\epsilon}_B^2\ . \tag{40}$$

K-NN Classification Error Bound

It can be shown that for K-NN, the following inequality holds:

$$\bar{\epsilon}_{KNN} \leq \bar{\epsilon}_B + \bar{\epsilon}_{1NN}/\sqrt{K \text{ const}} \tag{41}$$

Edit algorithm

The primary goal of this method is to reduce the classification error (not the speed-up of classification.)

Input: The training set $\mathcal{T}$.

Algorithm

1. Partition $\mathcal{T}$ to two sets, A and B ($\mathcal{T} = A \cup B$, $A \cap B = \emptyset$.)
2. Classify samples in B using **K**NN with training set A. Remove all samples from B which have been mis-classified.

Output: B the training set for **1**NN classification.

Asymptotic property:

$$\bar{\epsilon}_{edit} = \bar{\epsilon}_B \frac{1 - \bar{\epsilon}_B}{1 - \bar{\epsilon}_{KNN}} \tag{42}$$

If $\bar{\epsilon}_{KNN}$ is small (e.g. 0.05) then the edited 1NN is quasi-Bayes (almost the same performance as Bayesian Classification.)