Nonparametric Methods for Density Estimation
Nearest Neighbour Classification

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Probability Density Estimation

Parametric Methods for Density Estimation

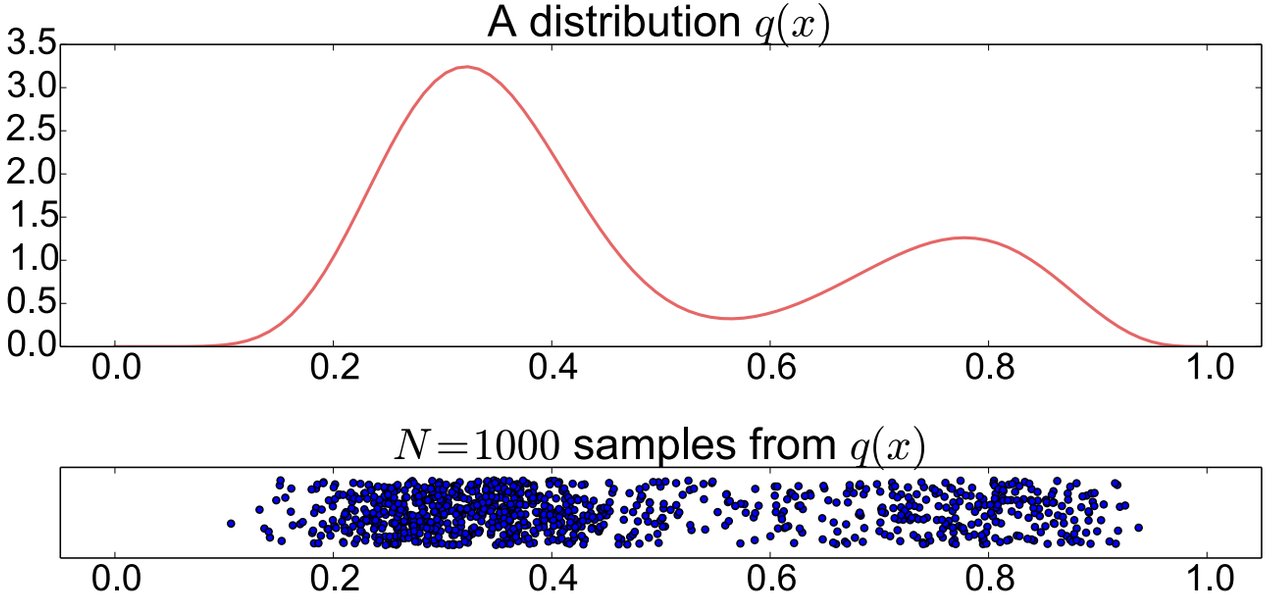
- Have been dealt with in the previous lecture
- Advantage: Low number of parameters to estimate
- Disadvantage: The resulting estimated density can be arbitrarily wrong if the underlying distribution does not agree with the assumed parametric model.

Non-Parametric Methods for Density Estimation

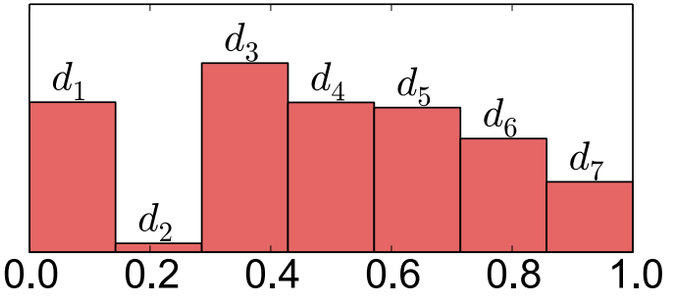
- Histogram
- Nearest Neighbor approach

Histogram as piecewise constant density estimate: Task formulation

Consider the following distribution $q(x)$ 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 width. For a given B, the parameters of this piecewise-constant function are the heights $d_1, d_2, ..., d_B$ of the individual bins. This function is denoted $p(x|\{d_1, d_2, ..., d_B\})$.



$p(x|\{d_1, d_2, .., d_B\})$ to be estimated



For the given number of bins B, $d_1, d_2, ..., d_B$ must conform to the constraint that the area under the function must sum up to one,

$$1 = \int_{-\infty}^{\infty} p(x|\{d_1, d_2, ..., d_B\})\mathrm{d}x = \sum_{i=1}^{B} \int_{\frac{i-1}{B}}^{\frac{i}{B}} d_i \,\mathrm{d}x = \sum_{i=1}^{B} d_i \overset{\text{bin width}}{\overset{\downarrow}{w}} = \sum_{i=1}^{B} \frac{d_i}{B}\,. \qquad (1)$$

Histogram as piecewise constant density estimate: Finding d_i's using Maximum Likelihood

Let us estimate $\{d_i, i = 1, 2, ..., B\}$ 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 $L(\mathcal{T})$ of observing the samples $\mathcal{T} = \{x_1, x_2, ..., x_N\}$ given the parameters $\boldsymbol{\theta} = \{d_1, d_2, ..., d_B\}$ is

$$L(\mathcal{T}) = p(\mathcal{T}|\boldsymbol{\theta}) = \prod_{i=1}^{N} p(x_i|\boldsymbol{\theta}) = \prod_{j=1}^{B} \overbrace{\left(\prod_{k=1}^{N_j} d_j \right)}^{\text{points in } j\text{-th bin}} = \prod_{j=1}^{B} d_j^{N_j} \,. \tag{2}$$

The maximization task is then

$$\ell(\mathcal{T}) = \sum_{j=1}^{B} N_j \log d_j \to \max \,, \qquad \text{subject to } \frac{1}{B} \sum_{j=1}^{B} d_j = 1 \,, \tag{3}$$

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

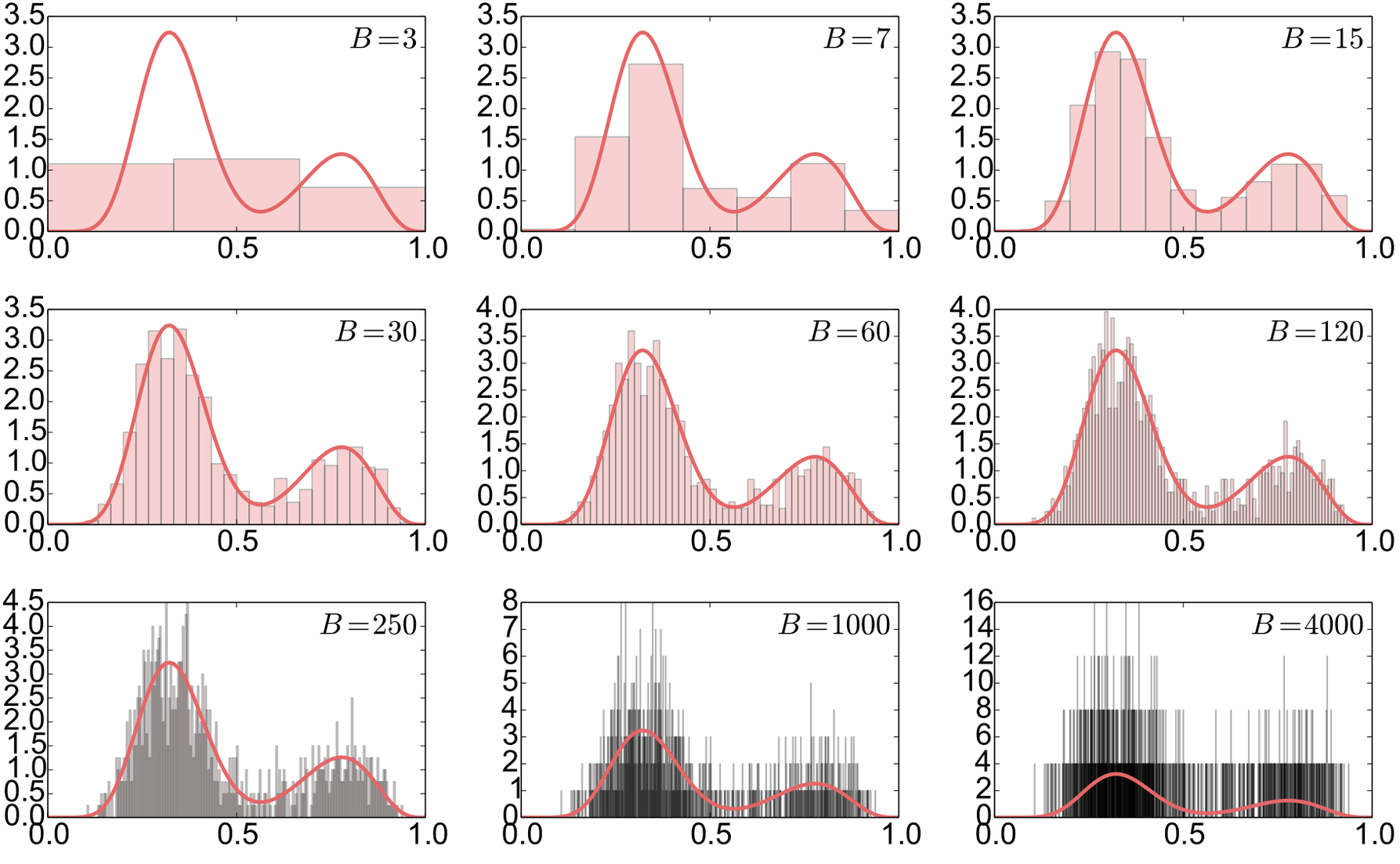
$$\text{Lagrangian: } \sum_{j=1}^{B} N_j \log d_j + \lambda \left(\frac{1}{B} \sum_{j=1}^{B} d_j - 1 \right) \tag{4}$$

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

Histogram as piecewise constant density estimate: Example, different number of bins

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

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



Histogram as piecewise constant density estimate: What number of bins produces closest pdf approximation?

Let us measure the differences between the (actual) source distribution $q(x)$ and the piecewise-constant density estimate $p(x) = p(x|\{d_1, d_2, ..., d_B\})$ from the $N = 1000$ samples, using B bins.

Measures used:

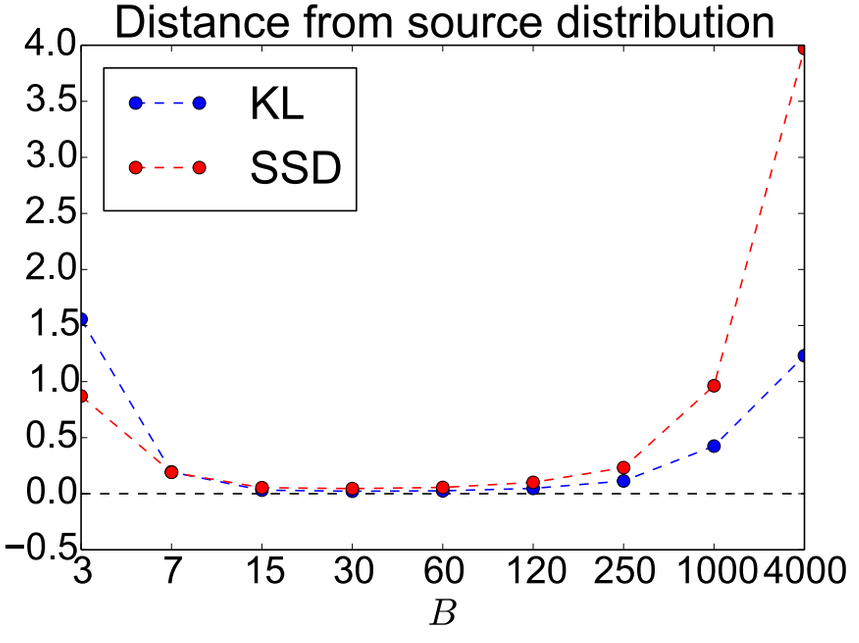
Kullback-Leibler divergence D_{KL}:

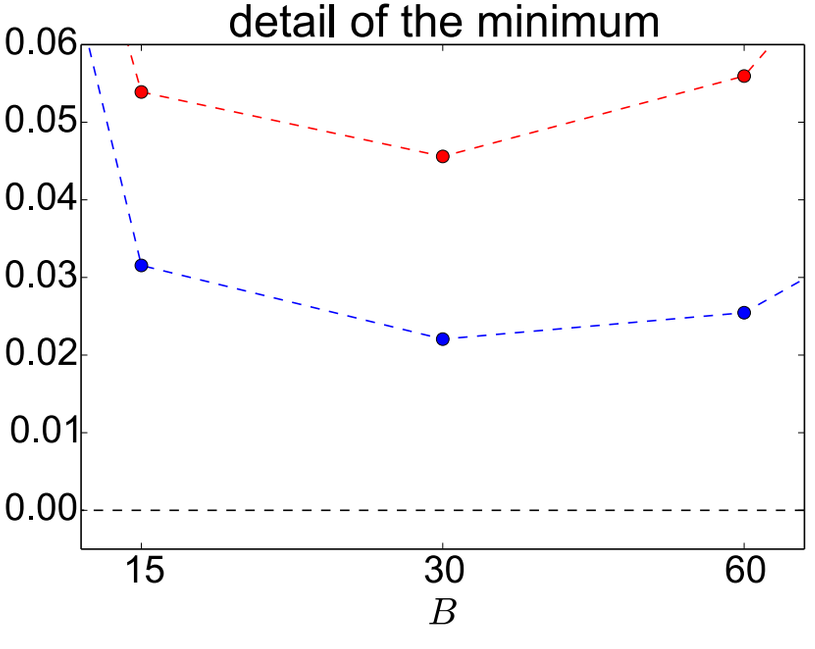
$$D_{\mathrm{KL}}(p\|q) = \int_{-\infty}^{\infty} p(x) \log \frac{p(x)}{q(x)} \mathrm{d}x \,. \tag{7}$$

(Note that KL div. is not a metric.)

Sum of squared differences D_{SSD}:

$$D_{\mathrm{SSD}}(p, q) = \int_{-\infty}^{\infty} (p(x) - q(x))^2 \mathrm{d}x \,. \tag{8}$$





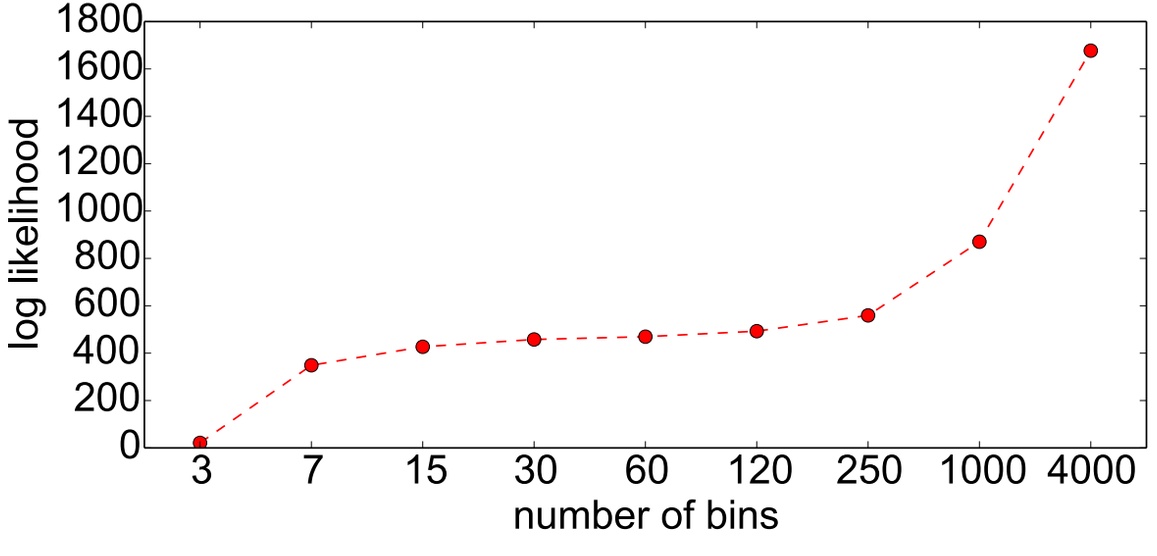
Histogram as piecewise constant density estimate: Choosing the number of bins B by ML

How can we find the optimal number of bins B? Let us try to employ the ML approach again: find the B which maximizes the likelihood. Recall that:

$$\text{parameters } d_j: \quad d_j = B\frac{N_j}{N} \quad \text{(ML estimate)} \tag{9}$$

$$\text{likelihood } L(\mathcal{T}): \quad L(\mathcal{T}) = p(\mathcal{T}|\{d_1, d_2, ..., d_B\}) = \prod_{j=1}^{B} d_j^{N_j} = \prod_{j=1}^{B} \left(\frac{BN_j}{N}\right)^{N_j} \tag{10}$$

$$\text{log-likelihood } \ell(\mathcal{T}): \quad \ell(\mathcal{T}) = \sum_{j=1}^{B} N_j \log d_j = \sum_{j=1}^{B} N_j \log \frac{BN_j}{N} \tag{11}$$



For $B = 4000$, the log-likelihood ℓ is the highest.

But the pdf estimate with this B is poor, and very different from the source distribution as measured by D_{KL} or D_{SSD}.

For $B = 10^5$, $\ell(\mathcal{T}) \sim 4600$.

What went wrong?

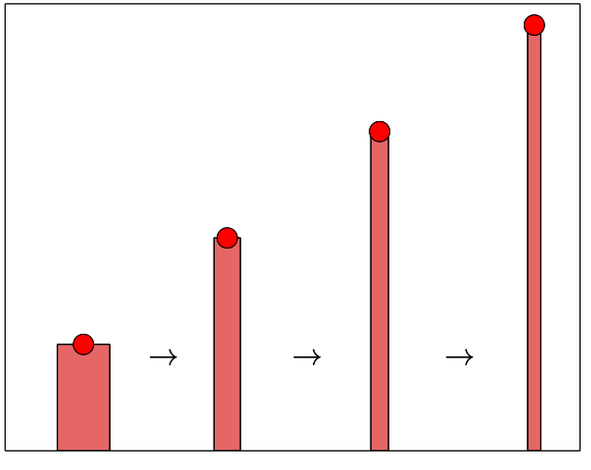
Histogram, choosing the number of bins B: ML overfits and produces $B = \infty$

When B grows, eventually it will reach a number $\hat{B}$ such that there is either *no* or *one* point in every bin (assuming no two points in the data are identical), and this will stay true for any $B > \hat{B}$.

In such cases,

$$d_j = \begin{cases} \frac{B}{N} \text{ if the bin is populated by a point,} \\ 0 \text{ if the bin is not populated.} \end{cases} \tag{12}$$

As the number of bins B grows, the widths of occupied bins get narrower and the heights d_j's higher. If $B \to \infty$ then also $d_j \to \infty$ for the occupied bins, and therefore also $\ell(\mathcal{T}) \to \infty$. Thus, such an approach cannot produce a "reasonable" answer to choosing B, as the solution it provides is $B = \infty$.



The problem is that the log-likelihood ℓ is computed using the same data used for fitting the model (computing d_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.

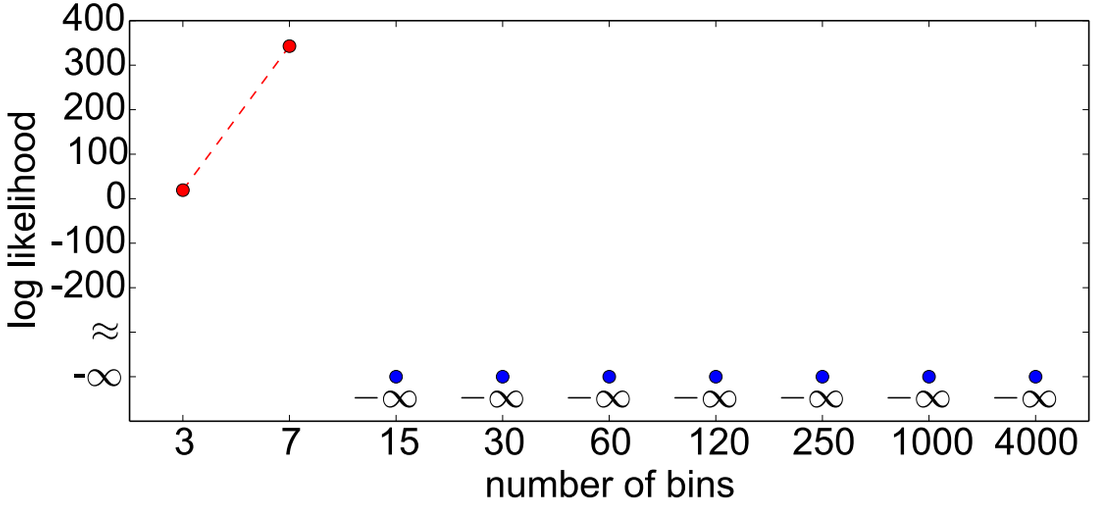
Histogram, choosing the number of bins B: Employing cross-validation

Let us compute the log likelihood using the following procedure: remove a given point from the dataset for computing d_i's and evaluate its contribution to the log-likelihood. Do this for all the points. This approach is related to cross-validation technique (leave-one-out) for choosing parameters of a classifier.

Let the point in question belong to the j-th bin. The ML estimate for d_j, after removing this point from the dataset, is

$$d_j = B\frac{N_j - 1}{N - 1}\,, \qquad (N_j \geq 1)\,, \tag{13}$$

where the subtractions of 1 reflect the fact that the considered point is not used for estimating d_j. Computing the log likelihood ℓ this way produces the following result:



$$\ell = \sum_{\substack{j=1 \\ N_j \geq 1}}^{B} N_j \log d_j,$$

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

The 'failure' for $B > 7$ is caused by singly-occupied bins ($N_j = 1$) for which the modified ML estimate for d_j becomes zero. This will be fixed by using different estimates for d_j's.

Histogram, choosing the number of bins B: More suitable estimates for d_j's

The problem of d_i being estimated as 0 is similar to the one encountered previously: Recall the example of tossing a coin three times, always getting *heads* ($\mathcal{T} = \{H, H, H\}$). The ML estimate is a fully unfair coin (probability of getting *heads* is 1, $\pi_{\text{head}} = 1$), thus making the likelihood of any sequence containing *tails* zero. We have seen before that employing the prior for the parameters to be estimated can mitigate this problem.

A (conjugate) prior for the histogram bin counts is the Dirichlet Distribution, with the pdf $p(d_1, d_2, ..., d_B|\alpha_1, \alpha_2, ..., \alpha_B) \sim \prod d_i^{\alpha_i - 1}$.

MAP Estimate:

$$d_i = B\frac{N_i + \alpha_i - 1}{N + \sum_{i=1}^{B} \alpha_i - B} \qquad (14)$$

Bayes Estimate:

$$d_i = B\frac{N_i + \alpha_i}{N + \sum_{i=1}^{B} \alpha_i} \qquad (15)$$

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

Example: The Bayes estimate using $\alpha_i = 1$ for all $i = 1, 2, ..., B$ is

$$d_i = B\frac{N_i+1}{N+B}. \qquad (16)$$

Using this estimate will enable us to make reasonable computation of likelihood for all B's.

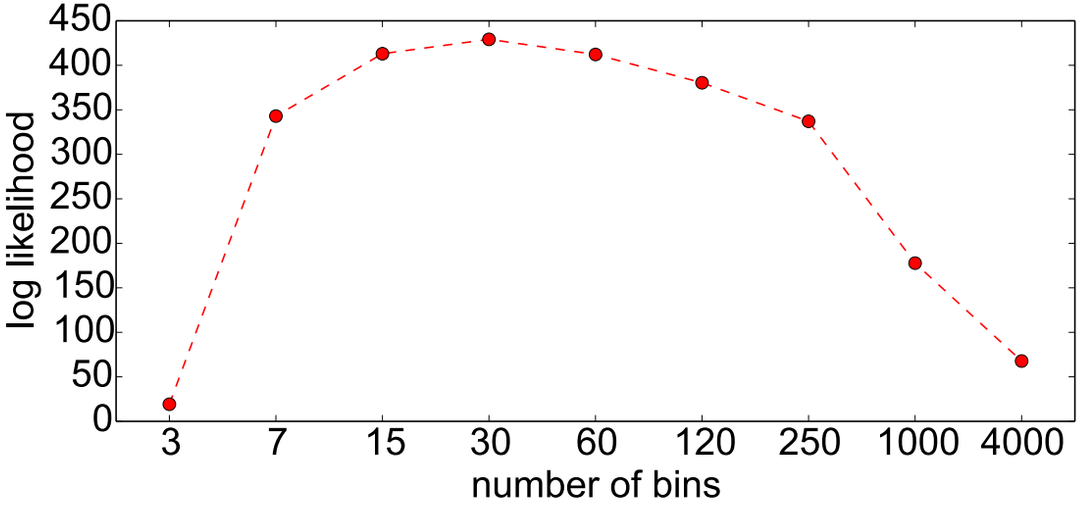
Histogram, choosing the number of bins B: ML to find B, cross-validation, Bayes esimate for d_j's

Let us now return to the previous task. Compute the log likelihood using the following procedure: remove a given point from the dataset for computing d_i's and evaluate its contribution to the log-likelihood. Do this for all the points.

Use the Bayes estimate for d_j from the previous example, $d_j = B\frac{N_j+1}{N+B}$. The modified estimation of d_j (omitting the point in question) will become

$$d_j = B\frac{N_j}{N-1+B}\,. \tag{17}$$

This leads to the following result:



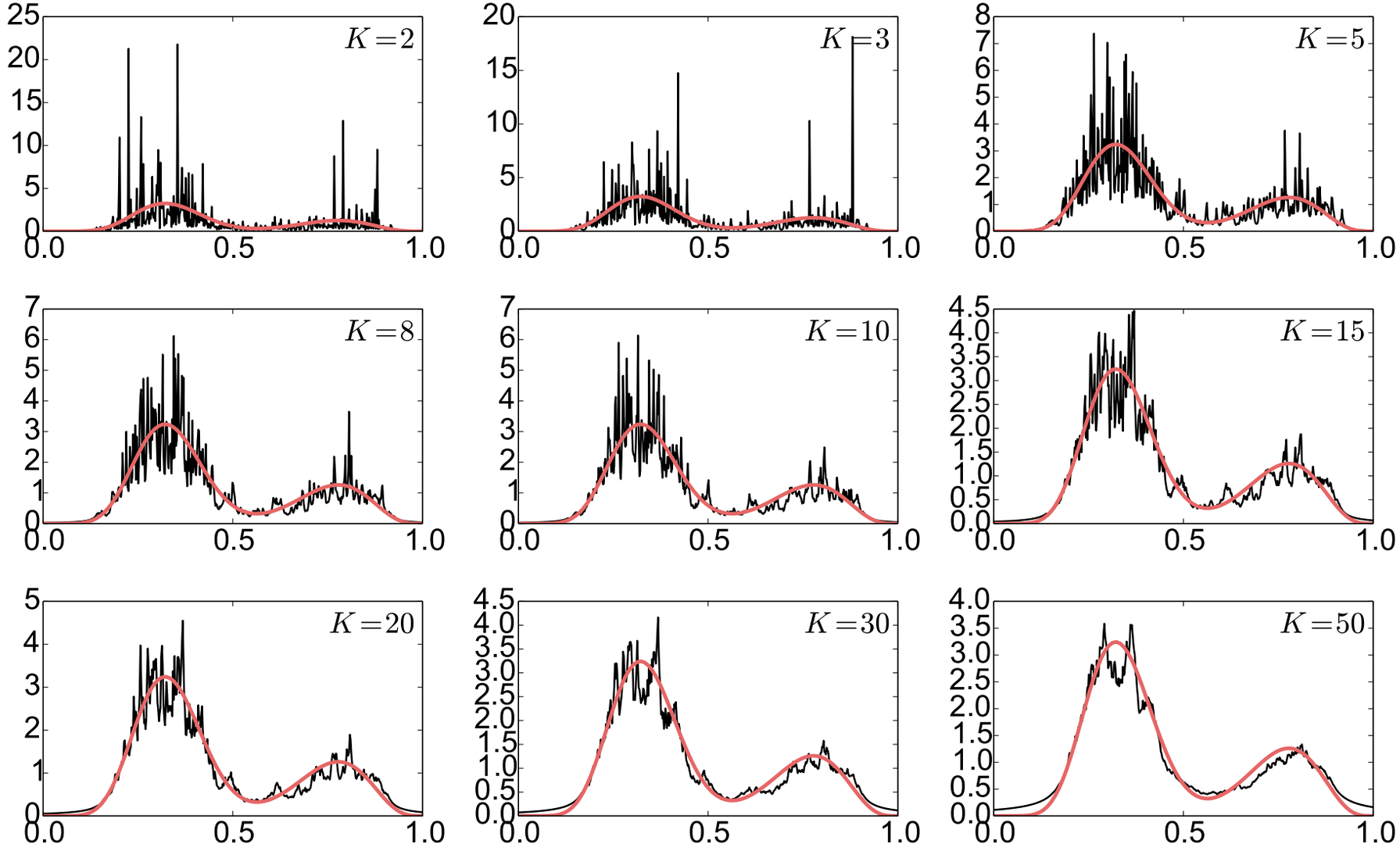
$$\ell = \sum_{j=1}^{B} N_j \log d_j,$$

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

This result is in agreement with distribution differences as measured by D_{KL} or D_{SSD}. In particular, $B = 30$ is identified as the best-approximating number of bins.

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 K-NN 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:

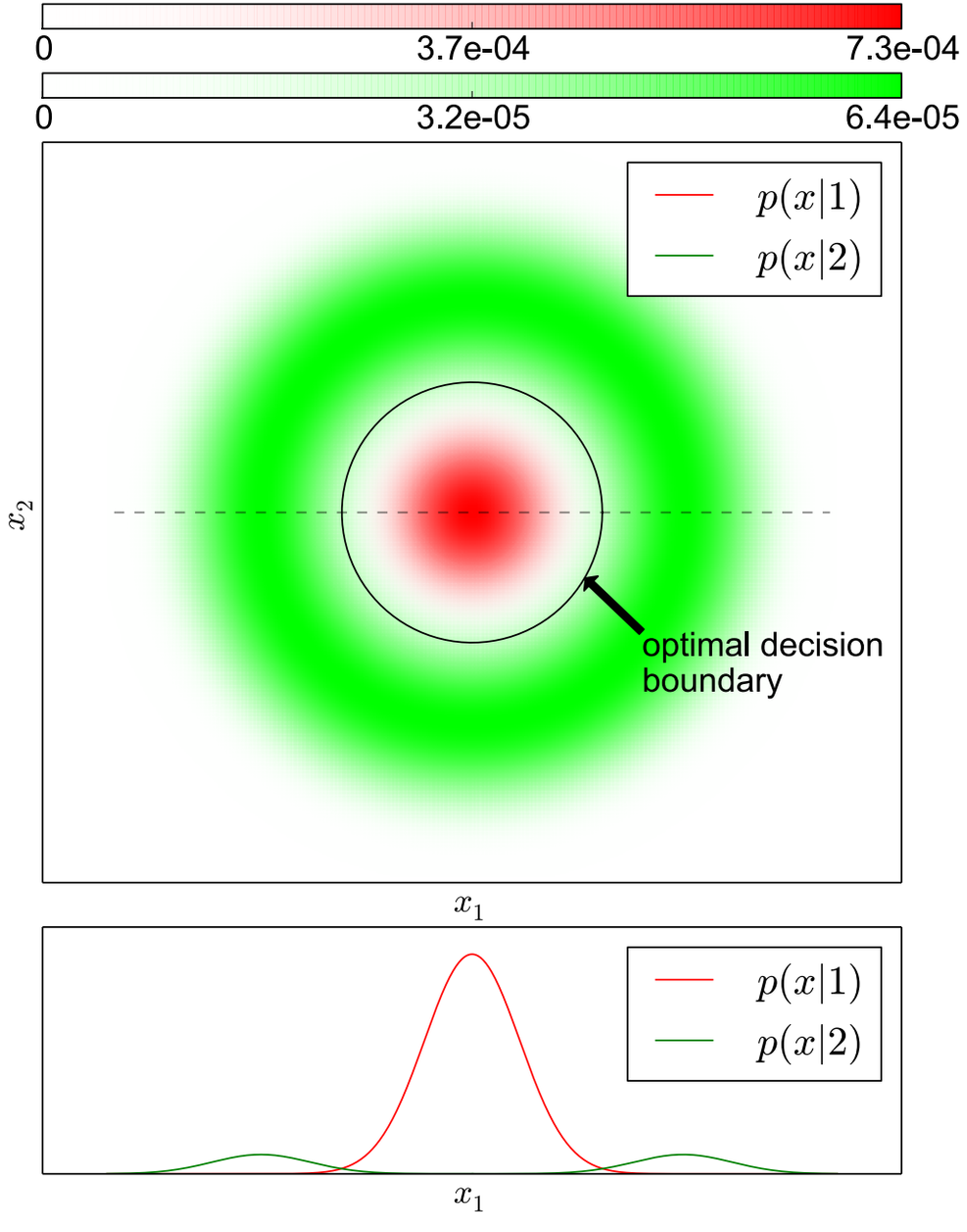
$$S = \{(x'_1, k'_1), (x'_2, k'_2), ..., (x'_K, k'_K)\} \equiv \{(x_{r_1}, k_{r_1}), (x_{r_2}, k_{r_2}), ..., (x_{r_K}, k_{r_K})\} \quad (18)$$

$$r_i\text{: the rank of } (x_i, k_i) \in \mathcal{T} \text{ as given by the ordering } d(x, x_i) \quad (19)$$

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

$$k = \underset{l \in R}{\text{argmax}} \sum_{i=1}^{K} [\![k'_i = l]\!] \qquad (x'_i, k'_i) \in S \quad (20)$$

K-NN Example (1)



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

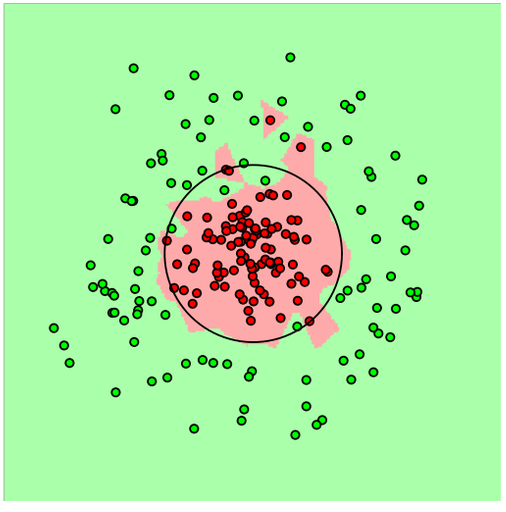
$$p(1) = p(2) = 0.5.$$

Bayesian optimal decision boundary is shown by the black circle.

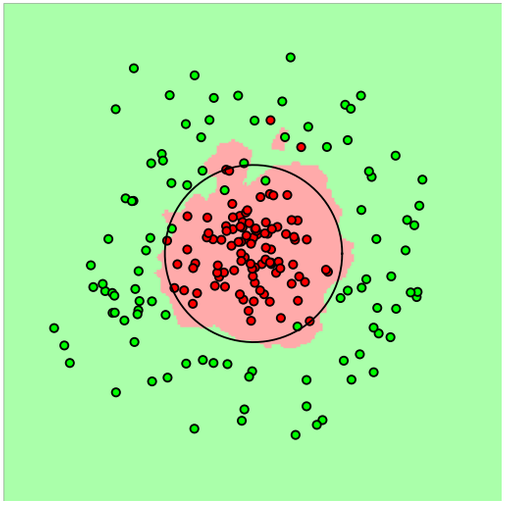
Bayesian error is $\epsilon_B = 0.026$.

K-NN Example (2)

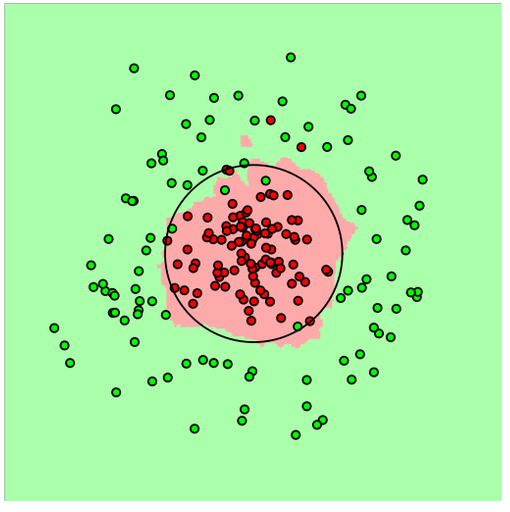
K = 1, error $\epsilon = 0.044$



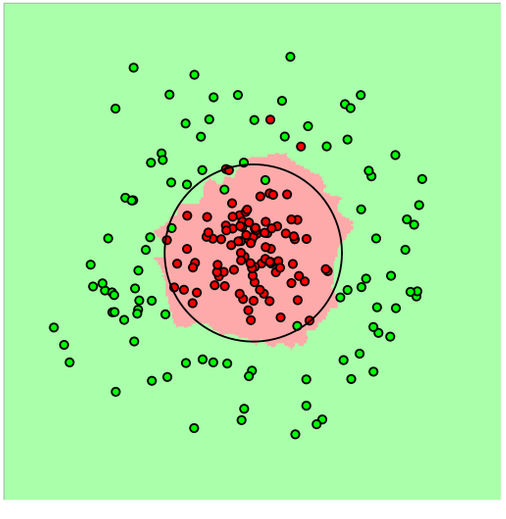
K = 3, error $\epsilon = 0.034$



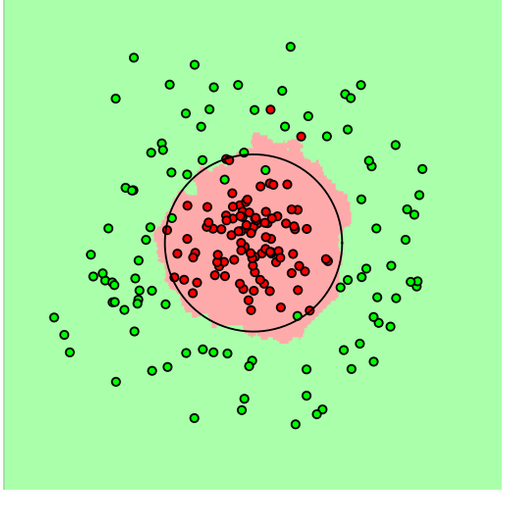
K = 5, error $\epsilon = 0.032$



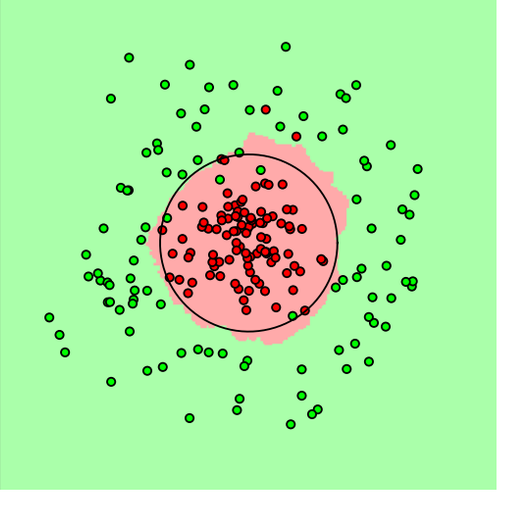
K = 7, error $\epsilon = 0.030$



K = 9, error $\epsilon = 0.031$

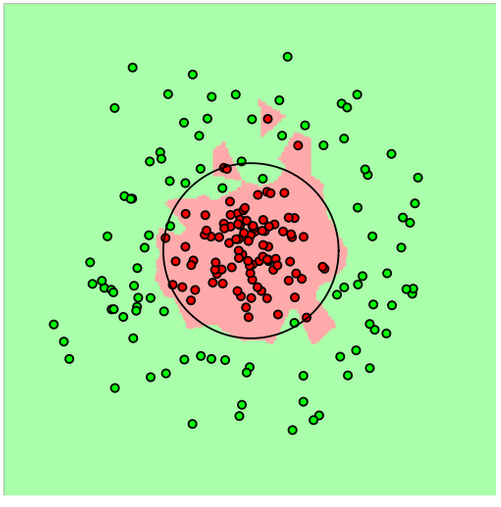
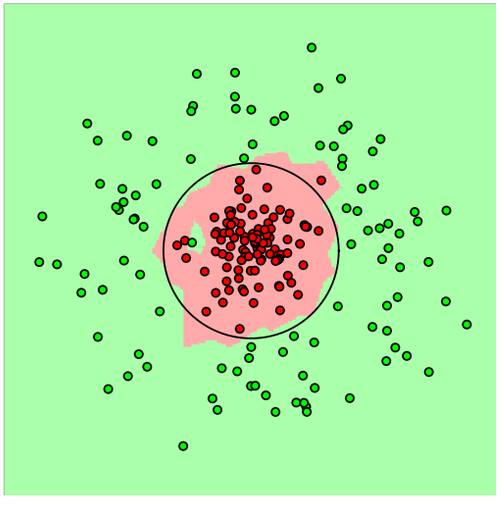
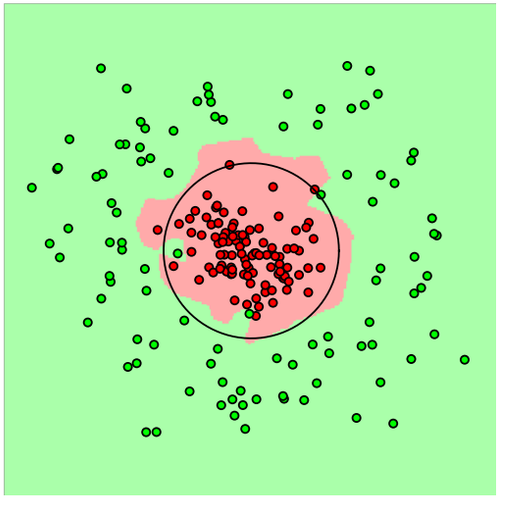
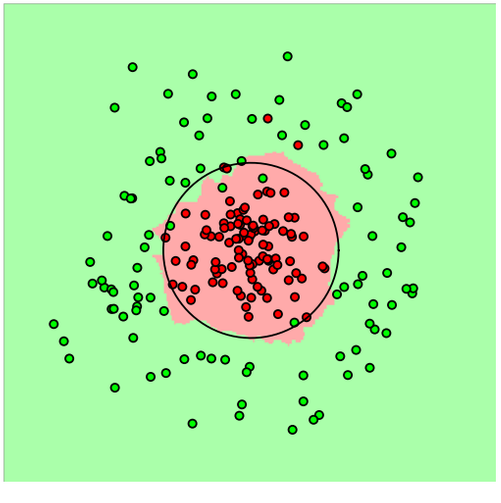
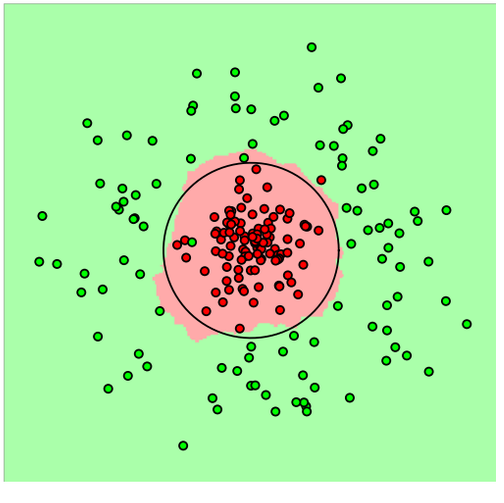
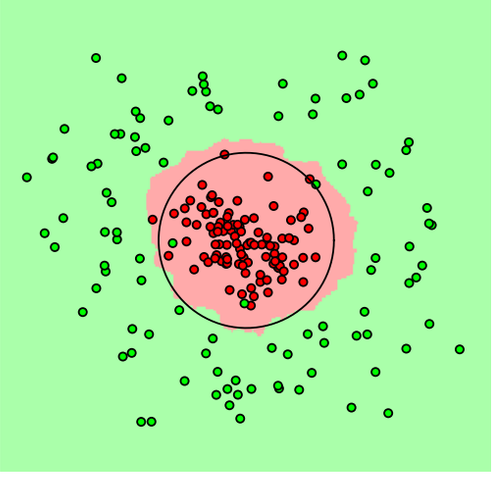


K = 11, error $\epsilon = 0.032$



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

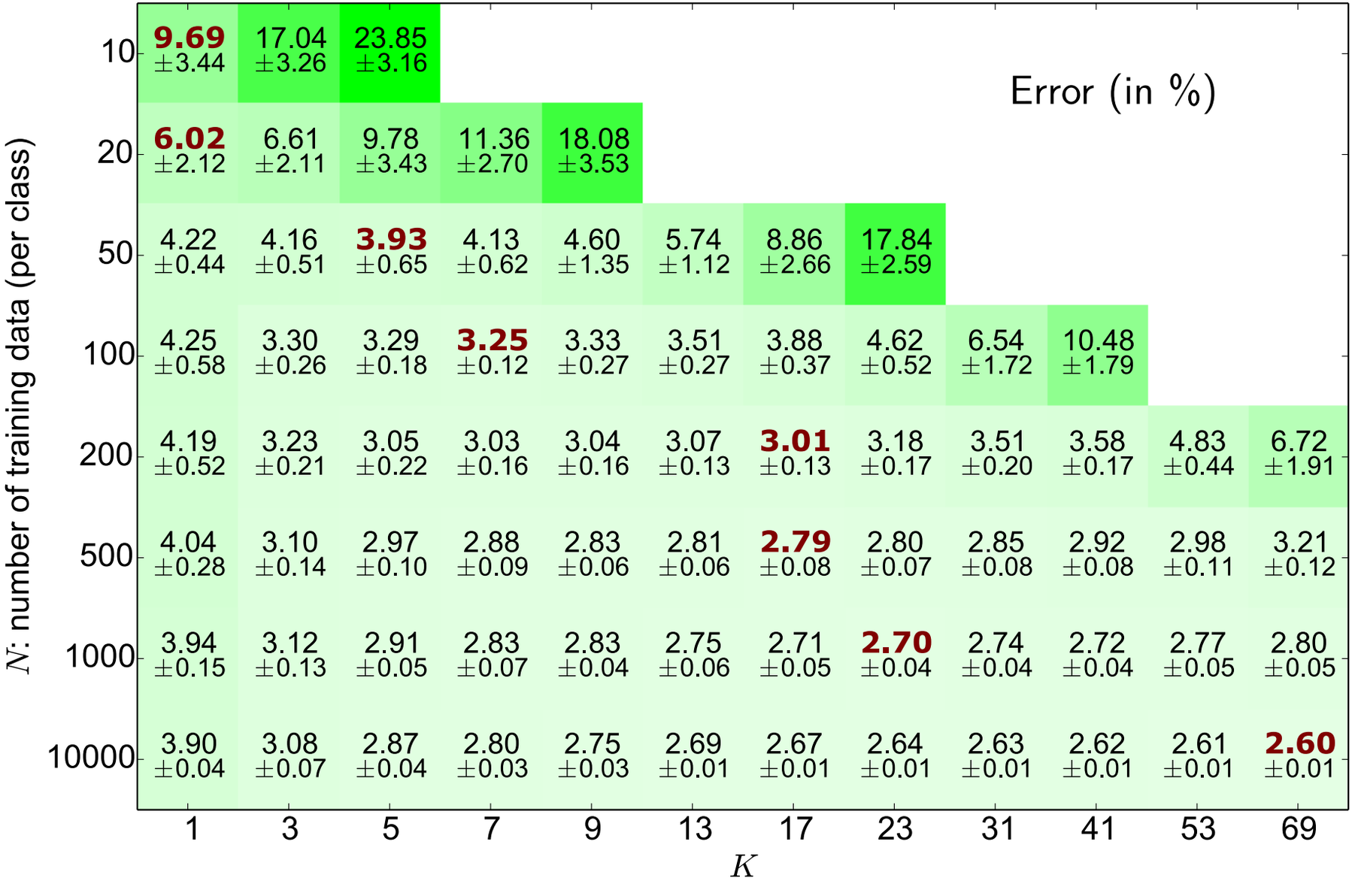
K-NN Example (3)

$\mathcal{T}_1$	$\mathcal{T}_2$	$\mathcal{T}_3$
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 $\epsilon = 0.036$ 

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.

K-NN Example (4)

K-NN error for different K and different sizes of the training set (N samples per class). 10 training sets have been generated randomly for each setting of K and N. Average error and its std is shown. Minimum average error is highligted for each N. Bayes err. $\epsilon_B = 2.58\%$.



K-NN Properties

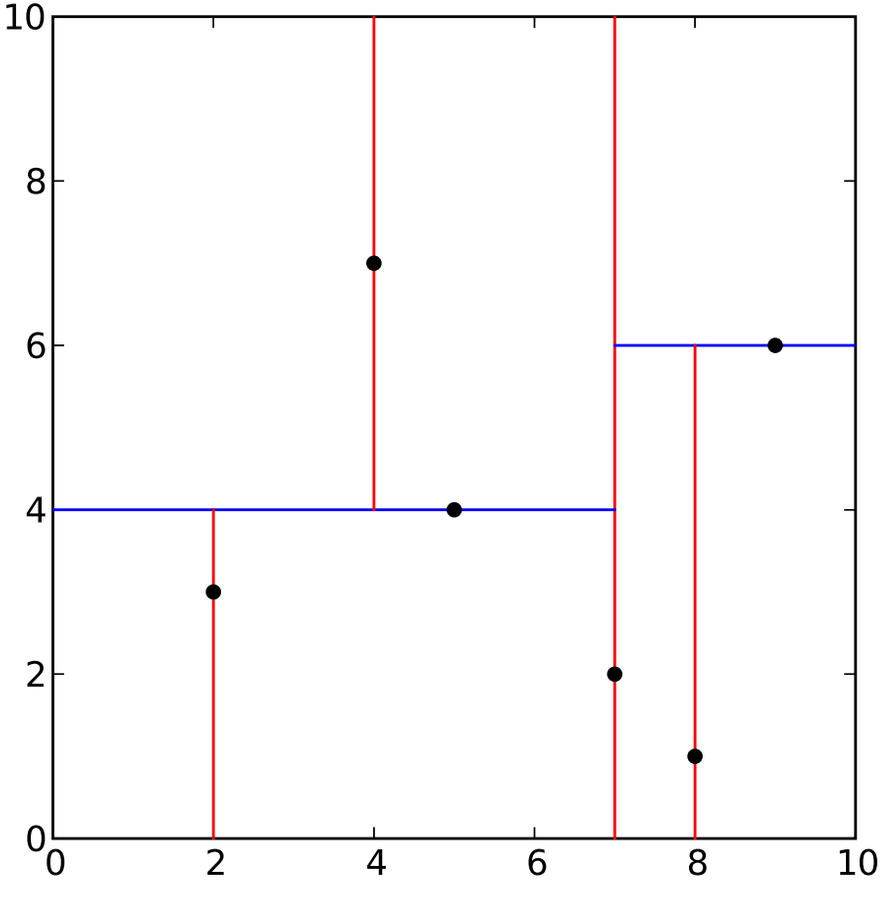
- Trivial implementation ($\rightarrow$ good baseline method)
- 1-NN: Bayes error ϵ_B is the lower bound on error of classification ϵ_{NN} (in the asymptotic case $N \rightarrow \infty$.) Upper bounds can also be constructed, e.g. $\epsilon_{NN} \leq 2\epsilon_B$
- Slow when implemented naively, but 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)

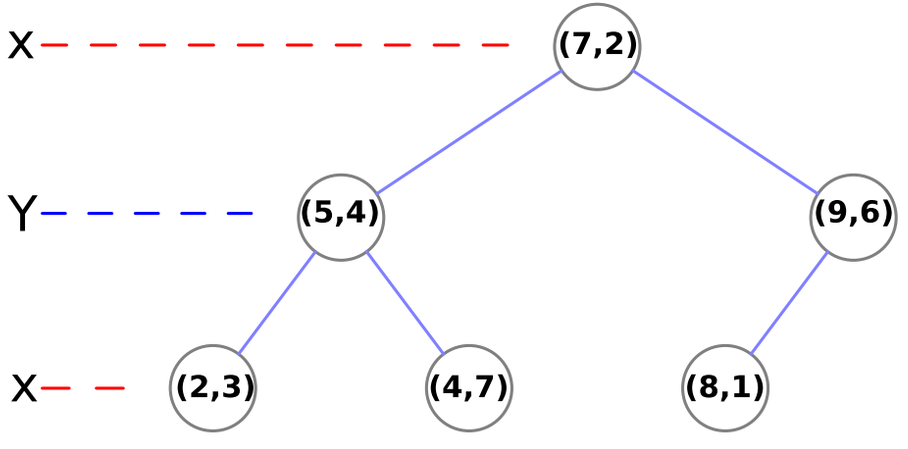
K-NN : Speeding Up the Classification

- 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.

K-d Tree

k-d tree decomposition for the point set (2,3), (5,4), (9,6), (4,7), (8,1), (7,2)





Condensation Algorithm

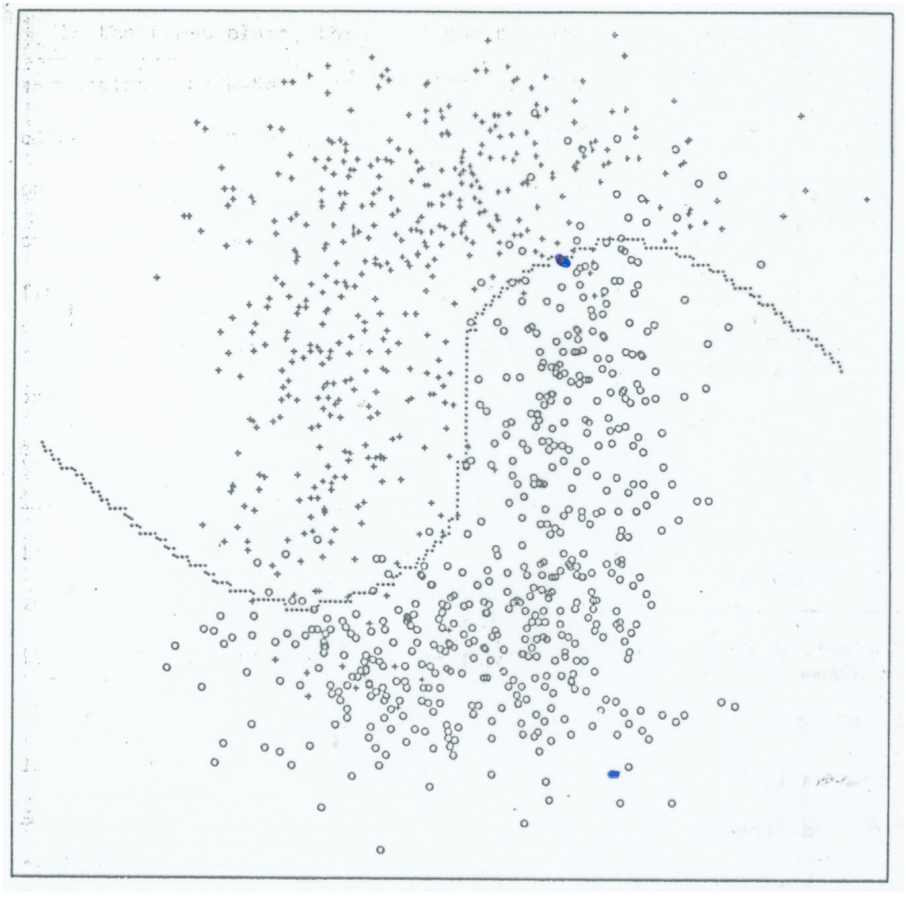
Input: The training set $\mathcal{T}$.

Algorithm

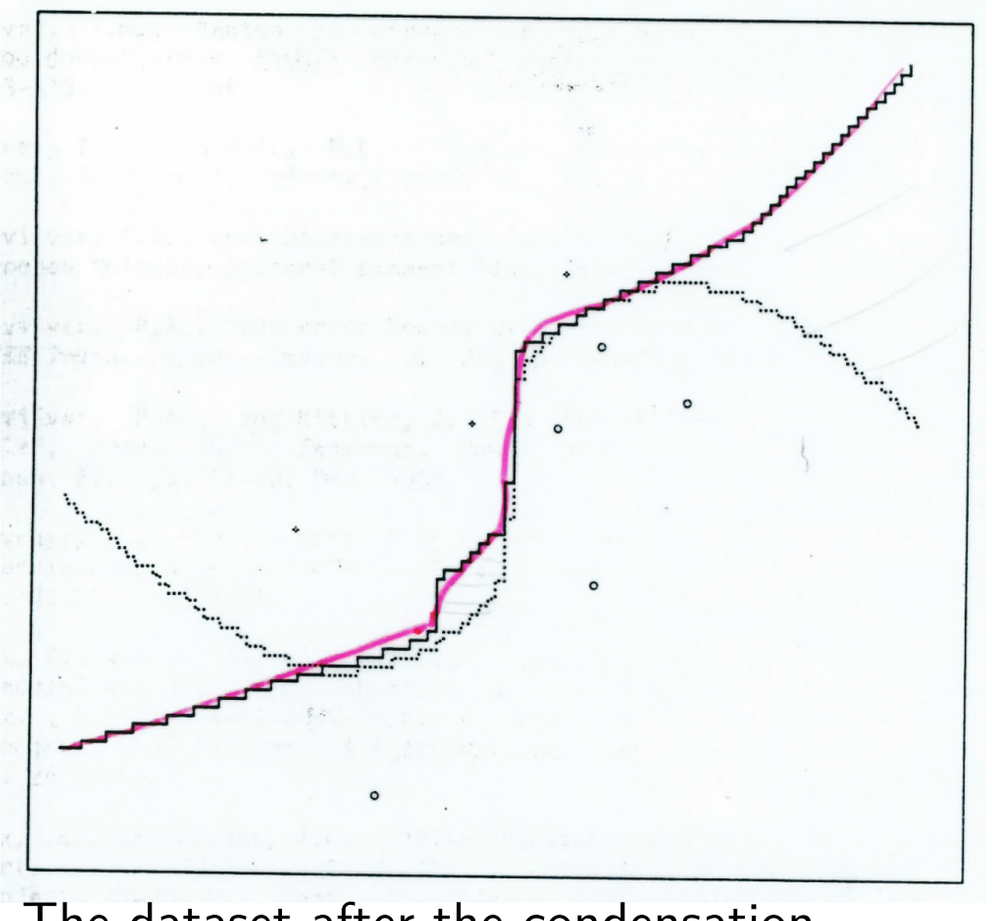
1. Create two lists, A and B. Insert a randomly selected sample from $\mathcal{T}$ to A. Insert the rest of the training samples to B.
2. Classify samples from B using 1NN with training set A. If an $x \in B$ is mis-classified, move it from B to A.
3. If a move has been triggered in Step 2., goto Step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

$$\bar{\epsilon} = \int \sum_{k:q(x)\neq k} p(x,k)\mathrm{d}x = \int \underbrace{\sum_{k:q(x)\neq k} p(k|x)}_{\epsilon(x)} p(x)\mathrm{d}x = \int \epsilon(x)p(x)\mathrm{d}x\,. \tag{21}$$

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

$$\epsilon_B(x) = 1 - \max_k p(k|x)\,. \tag{22}$$

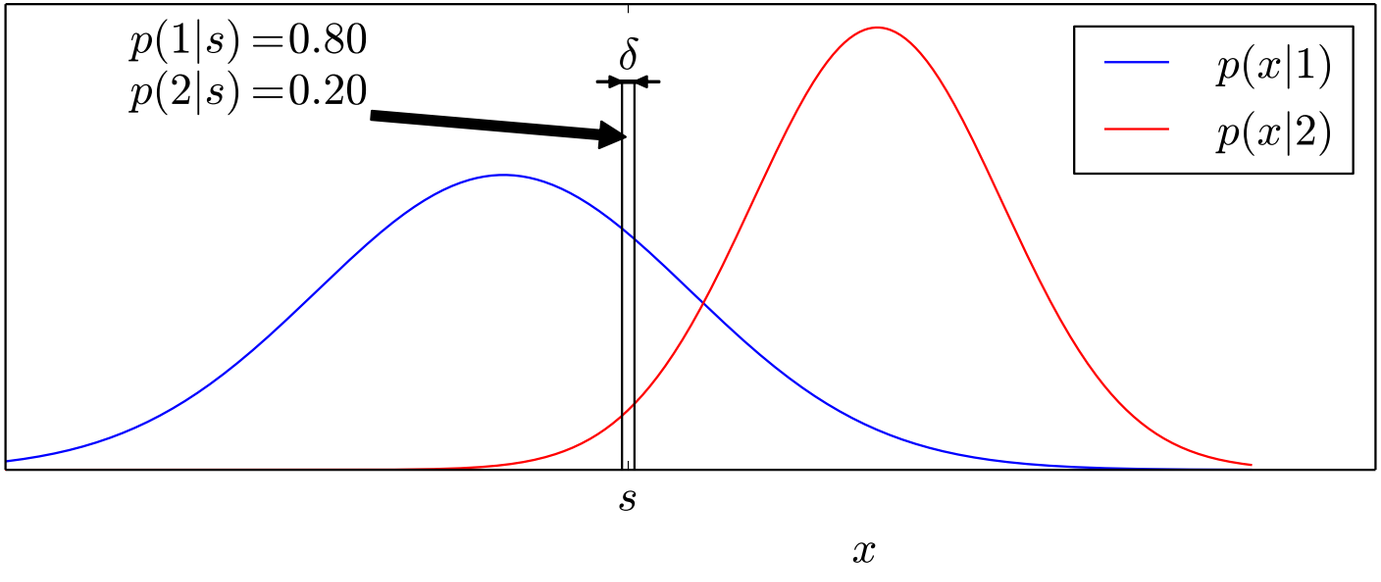
Assume the asymptotic case. We will show that the following bounds hold for the partial error $\epsilon_{NN}(x)$ and classification error $\bar{\epsilon}_{NN}$ in the 1-NN classification,

$$\epsilon_B(x) \leq \epsilon_{NN}(x) \leq 2\epsilon_B(x) - \tfrac{R}{R-1}\epsilon_B^2(x)\,, \tag{23}$$

$$\bar{\epsilon}_B \leq \bar{\epsilon}_{NN} \leq 2\bar{\epsilon}_B - \tfrac{R}{R-1}\bar{\epsilon}_B^2\,, \tag{24}$$

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 $N \to \infty$.

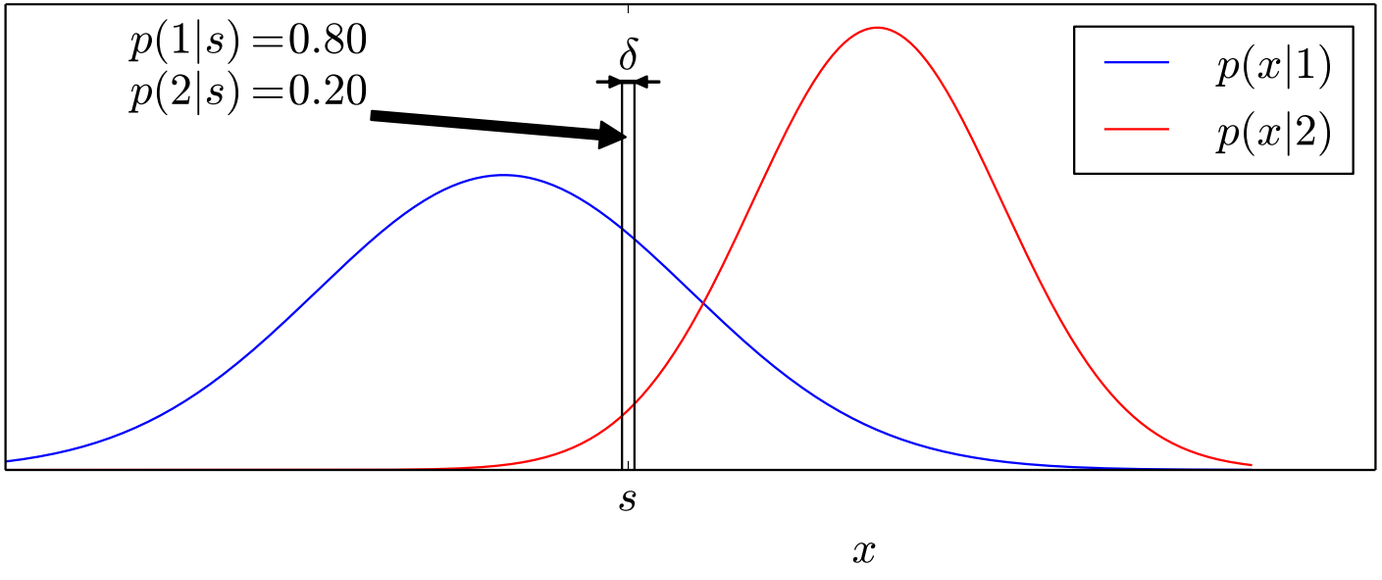
Observe the following:

$$p(1|s) = 0.8\,, \quad p(2|s) = 0.2\,, \tag{25}$$

$$p(NN=1|s) = p(1|s) = 0.8\,, \quad p(NN=2|s) = p(2|s) = 0.2\,, \tag{26}$$

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

$$\epsilon_{NN}(s) = p(1|s)\, p(NN=2|s) + p(2|s)\, p(NN=1|s) \tag{27}$$

$$= 1 - p(1|s)\, p(NN=1|s) - p(2|s)\, p(NN=2|s) \tag{28}$$

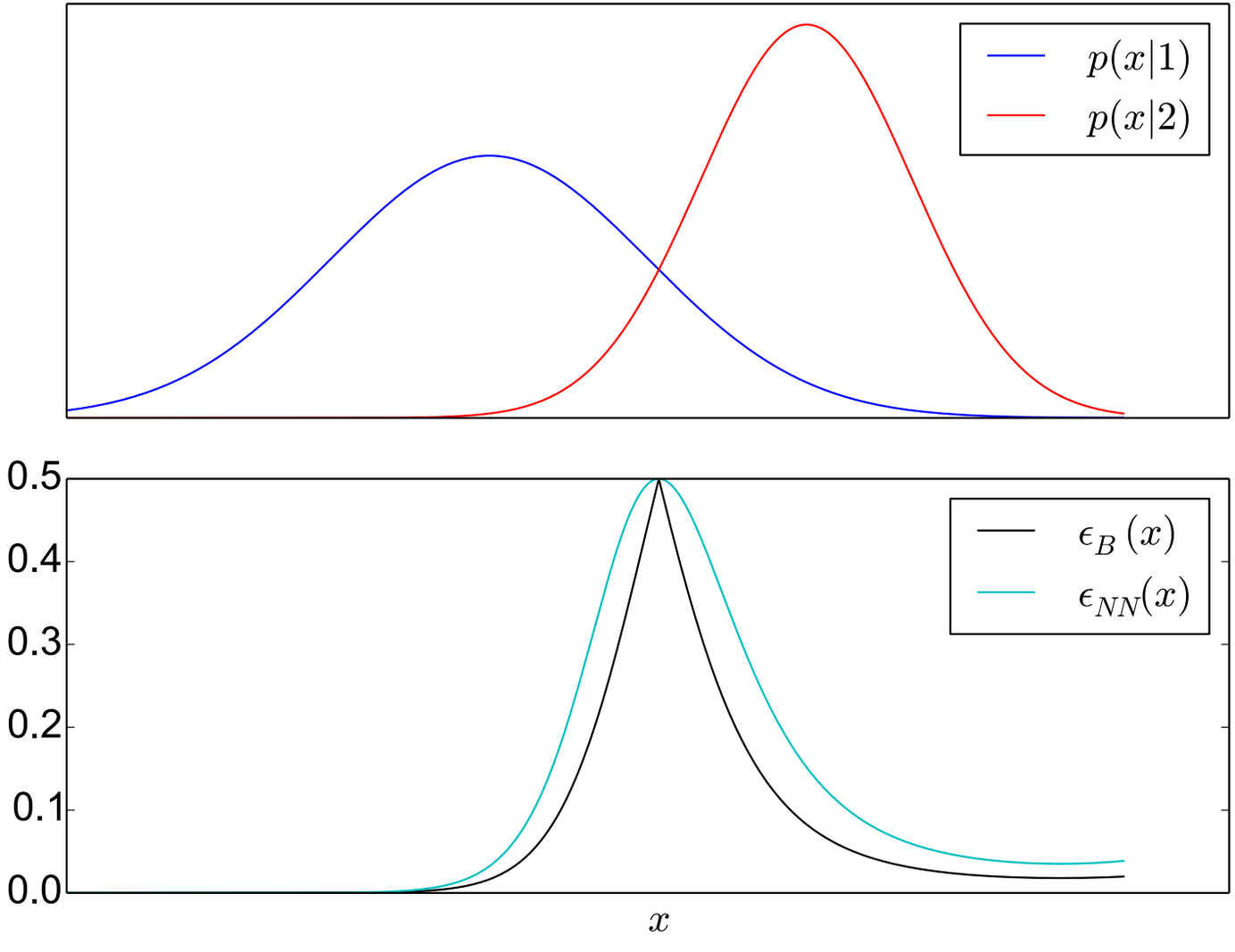
$$= 1 - p^2(1|s) - p^2(2|s)\,. \tag{29}$$

Generally, for R classes, the error will be

$$\epsilon_{NN}(s) = 1 - \sum_{k \in R} p^2(k|s)\,. \tag{30}$$

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:

$$\epsilon_B(x) \leq \epsilon_{NN}(x) \leq 2\epsilon_B(x) - \frac{R}{R-1}\epsilon_B^2(x)\,, \tag{31}$$

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:

$$P(x) = \max_k p(k|x) \tag{32}$$

$$\Rightarrow \quad \epsilon_B(x) = 1 - P(x)\,. \tag{33}$$

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

$$\epsilon_{NN}(x) = 1 - \sum_{k \in R} p^2(k|x) = 1 - P^2(x) - \sum_{k \neq q(x)} p^2(k|x)\,. \tag{34}$$

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. (34) is maximized. This will provide the upper bound.

1-NN Classification Error Bounds (2)

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

$$\sum_{k \neq q(x)} p(k|x) + P(x) = 1 \qquad \text{(posteriors sum to 1)} \tag{35}$$

$$\sum_{k \neq q(x)} p^2(k|x) \to \min \tag{36}$$

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

$$p(k|x) = \frac{1 - P(x)}{R - 1} = \frac{\epsilon_B(x)}{R - 1} \qquad (k \neq q(x)) \tag{37}$$

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

$$\epsilon_{NN}(x) \leq 1 - P^2(x) - \sum_{k \neq q(x)} p^2(k|x) = 1 - (1 - \epsilon_B(x))^2 - (R - 1)\frac{\epsilon_B^2(x)}{(R - 1)^2}\,. \tag{38}$$

1-NN Classification Error Bounds (3)

$$\epsilon_{NN}(x) \leq 1 - P^2(x) - \sum_{k \neq q(x)} p^2(k|x) \; = 1 - (1 - \epsilon_B(x))^2 - \frac{\epsilon_B^2(x)}{R-1}\,. \tag{39}$$

After expanding this, we get

$$\epsilon_{NN}(x) \leq 1 - (1 - \epsilon_B(x))^2 - \frac{\epsilon_B^2(x)}{(R-1)} \tag{40}$$

$$= 1 - 1 + 2\epsilon_B(x) - \epsilon_B^2(x) - \epsilon_B^2(x)\frac{R}{R-1} \tag{41}$$

$$= \; 2\epsilon_B(x) - \epsilon_B^2(x)\tfrac{R}{R-1} \tag{42}$$

Note that for $R = 2$, the bound is tight because using $\epsilon_B(x) = 1 - P(x)$ in Eq. (39) gives

$$\epsilon_{NN}(x) \leq 1 - P^2(x) - \frac{(1 - P(x))^2}{1} = \epsilon_{NN}(x)\,. \tag{43}$$

1-NN Classification Error Bounds (4)

The inequality for the local errors has been proven:

$$\epsilon_{NN}(x) \leq 2\epsilon_B(x) - \epsilon_B^2(x)\frac{R}{R-1} \tag{44}$$

Is there a similar upper 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. (45) by $p(x)$, and integrating, gives

$$\bar{\epsilon}_{NN} \leq 2\bar{\epsilon}_B(x) - \frac{R}{R-1}\int \epsilon_B^2(x)p(x)\mathrm{d}x \tag{45}$$

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

$$\mathrm{var}(x) = E\left(x^2\right) - E^2(x)\,,\ \mathrm{var}(x) \geq 0 \qquad \Rightarrow \qquad E(x^2) \geq E^2(x) \tag{46}$$

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

$$\bar{\epsilon}_{NN} \leq 2\bar{\epsilon}_B(x) - \frac{R}{R-1}\int \epsilon_B^2(x)p(x)\mathrm{d}x \leq \ 2\bar{\epsilon}_B(x) - \frac{R}{R-1}\bar{\epsilon}_B^2\ . \tag{47}$$

K-NN Classification Error Bound

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

$$\bar{\epsilon}_{KNN} \leq \bar{\epsilon}_B + \bar{\epsilon}_{1NN}/\sqrt{K \text{ const}} \tag{48}$$

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:

$$\bar{\epsilon}_{edit} = \bar{\epsilon}_B \frac{1 - \bar{\epsilon}_B}{1 - \bar{\epsilon}_{KNN}} \tag{49}$$

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