### Instance-based Learning

Machine Learning

Hamid R Rabiee – Zahra Dehghanian Spring 2025



#### Outline

- Non-parametric approach
  - Unsupervised: Non-parametric density estimation
    - Parzen Windows
    - Kn-Nearest Neighbor Density Estimation
  - Supervised: Instance-based learners
    - Classification
      - kNN classification
      - Weighted (or kernel) kNN
    - Regression
      - kNN regression
      - Locally linear weighted regression



#### Introduction

- Estimation of arbitrary density functions
  - Parametric density functions cannot usually fit the densities we encounter in practical problems
    - e.g., parametric densities are unimodal
  - Non-parametric methods don't assume that the model (from) of underlying densities is known in advance
- Non-parametric methods (for classification) can be categorized into
  - Generative
    - Estimate  $p(x|\mathcal{C}_i)$  from  $\mathcal{D}_i$  using non-parametric density estimation
  - Discriminative
    - Estimate  $p(C_i|x)$  from  $\mathcal{D}$



## Parametric vs. nonparametric methods

- Parametric methods need to find parameters from data and then use the inferred parameters to decide on new data points
  - Learning: finding parameters from data
- Nonparametric methods
  - Training examples are explicitly used
    - Training phase is not required
- Both supervised and unsupervised learning methods can be categorized into parametric and non-parametric methods.



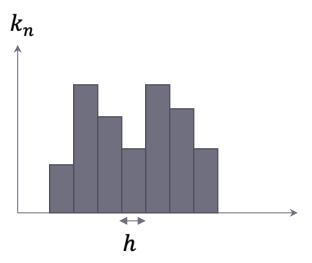
## Histogram approximation idea

- Histogram approximation of an unknown pdf
  - $P(b_l) \approx k_n(b_l)/n$  l = 1, ..., L
    - $k_n(b_l)$ : number of samples (among n ones) lied in the bin  $b_l$



• 
$$\hat{p}(x) = \frac{P(b_l)}{h} \left| x - \bar{x}_{b_l} \right| \le \frac{h}{2}$$

Mid-point of the bin  $b_l$ 





## Non-parametric density estimation

- Probability of falling in a region  $\mathcal{R}$ :
  - $P = \int_{\mathcal{R}} p(x')dx'$  (smoothed version of p(x))

- $\mathcal{D} = \{x^{(i)}\}_{i=1}^n$ : a set of samples drawn i.i.d. according to p(x)
  - ▶ The probability that k of the n samples fall in  $\mathcal{R}$ :

$$P_k = \binom{n}{k} P^k (1 - P)^{n-k}$$

$$E[k] = nP$$



## Non-parametric density estimation

- Probability of falling in a region  $\mathcal{R}$ :
  - $P = \int_{\mathcal{R}} p(x')dx'$  (smoothed version of p(x))
- $\mathcal{D} = \{x^{(i)}\}_{i=1}^n$ : a set of samples drawn i.i.d. according to p(x)
  - ▶ The probability that k of the n samples fall in  $\mathcal{R}$ :

$$P_k = \binom{n}{k} P^k (1 - P)^{n-k}$$

- $\triangleright E[k] = nP$
- ▶ This binomial distribution peaks sharply around the mean:
  - $k \approx nP \Rightarrow \frac{k}{n}$  as an estimate for P
  - $\blacktriangleright$  More accurate for larger n



## Non-parametric density estimation

- We can estimate smoothed p(x) by estimating P:
- Assumptions: p(x) is continuous and the region  $\mathcal R$  enclosing x is so small that p is near constant in it:

$$P = \int_{\mathcal{R}} p(\mathbf{x}')d\mathbf{x}' = p(\mathbf{x}) \times V$$

$$V = Vol(\mathcal{R})$$

$$\mathbf{x} \in \mathcal{R} \Rightarrow p(\mathbf{x}) = \frac{P}{V} \approx \frac{k/n}{V}$$

• Let V approach zero if we want to find p(x) instead of the averaged version.



## Necessary conditions for converge

- $p_n(x)$  is the estimate of p(x) using n samples:
  - $V_n$ : the volume of region around x
  - $k_n$ : the number of samples falling in the region

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

- Necessary conditions for converge of  $p_n(x)$  to p(x):
  - $\lim_{n\to\infty} V_n = 0$
  - $\lim_{n\to\infty} k_n = \infty$
  - $\lim_{n\to\infty} k_n/n = 0$



# Non-parametric density estimation: Main approaches

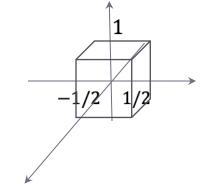
- Two approaches of satisfying conditions:
  - Kernel density estimator (Parzen window): fix V and determine K from the data
    - Number of points falling inside the volume can vary from point to point
    - converges to the true probability density in the limit  $n \to \infty$  when V shrinks suitably with n (e.g.,  $V_n = V_1/\sqrt{n}$ )
  - k-nearest neighbor density estimator: fix k and determine the value of V from the data
    - Volume grows until it contains k neighbors of x
    - converges to the true probability density in the limit  $n \to \infty$  when k grows with n (e.g.,  $k_n = k_1 \sqrt{n}$ )

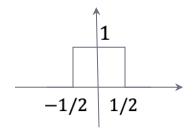


#### Parzen window

- Extension of histogram idea:
  - Hyper-cubes with length of side h (i.e., volume  $h^d$ ) are located on the samples
- Hypercube as a simple window function:

$$\varphi(\mathbf{u}) = \begin{cases} 1 & (|u_1| \le \frac{1}{2} \land \dots \land |u_d| \le \frac{1}{2}) \\ 0 & o.w. \end{cases}$$
$$p_n(\mathbf{x}) = \frac{1}{n} \times \frac{1}{h_n^d} \sum_{i=1}^n \varphi\left(\frac{\mathbf{x} - \mathbf{x}^{(i)}}{h_n}\right)$$





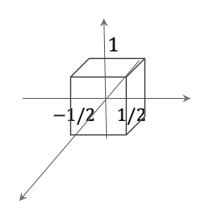
#### Parzen window

Extension of histogram idea:

Hyper-cubes with length of side h (i.e., volume  $h^d$ ) are located on the samples

Hypercube as a simple window function:

$$\varphi(\boldsymbol{u}) = \begin{cases} 1 & (|u_1| \le \frac{1}{2} \land \dots \land |u_d| \le \frac{1}{2}) \\ 0 & o.w. \end{cases}$$
$$p_n(\boldsymbol{x}) = \frac{1}{n} \times \frac{1}{h_n^d} \sum_{i=1}^n \varphi\left(\frac{\boldsymbol{x} - \boldsymbol{x}^{(i)}}{h_n}\right)$$



• 
$$p_n(\mathbf{x}) = \frac{k_n}{nV_n}$$

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

number of samples in the hypercube around x

• 
$$V_n = (h_n)^d$$



#### Window function

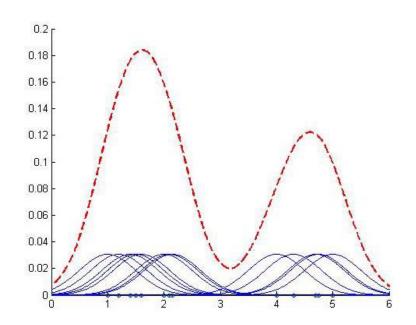
- Necessary conditions for window function to find legitimate density function:
  - $\varphi(x) \geq 0$
  - $\int \varphi(\mathbf{x})d\mathbf{x} = 1$
- Windows are also called **kernels** or potential functions.



## Density estimation: non-parametric

$$\hat{p}_n(x) = \frac{1}{n} \sum_{i=1}^n N(x|x^{(i)}, h^2) \longrightarrow \frac{1}{\sqrt{2\pi}h} e^{-\frac{(x-x^{(i)})^2}{2h^2}}$$

1 1.2 1.4 1.5 1.6 2 2.1 2.15 4 4.3 4.7 4.75 5



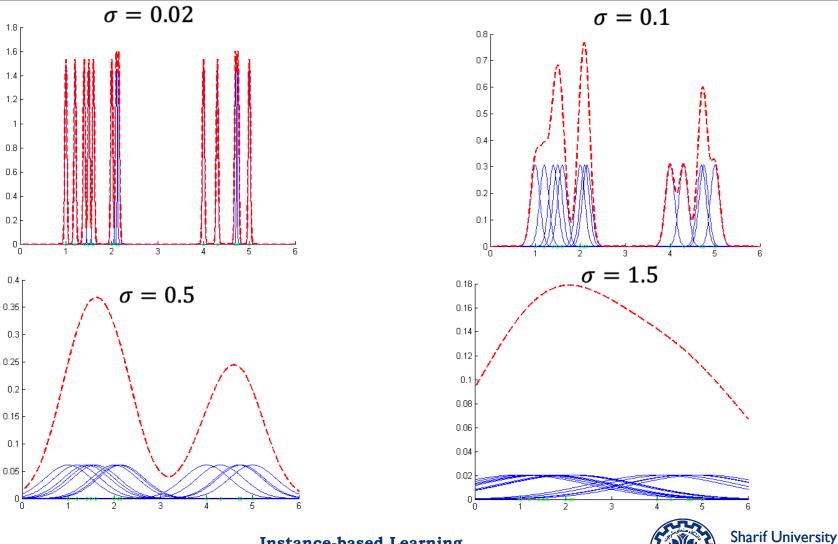
$$\sigma = h$$

$$\hat{p}(x) = \frac{1}{n} \sum_{i=1}^{n} N(x|x^{(i)}, \sigma^2)$$
$$= \frac{1}{n} \sum_{i=1}^{n} \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{(x-x^{(i)})^2}{2\sigma^2}}$$

Choice of  $\sigma$  is crucial.



## Density estimation: non-parametric

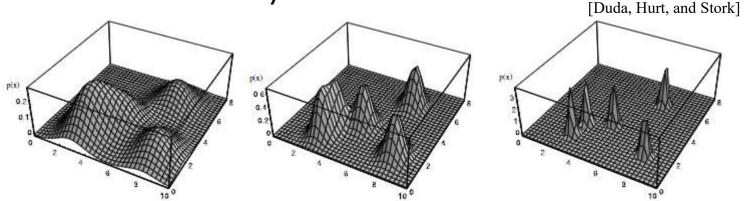


of Technology

## Window (or kernel) function: Width parameter

$$p_n(x) = \frac{1}{n} \times \frac{1}{h_n^d} \sum_{i=1}^n \varphi\left(\frac{x - x^{(i)}}{h_n}\right)$$

- Choosing  $h_n$ :
  - Too large: low resolution
  - Too small: much variability



• For unlimited n, by letting  $V_n$  slowly approach zero as n increases  $p_n(x)$  converges to p(x)



## Width parameter

- For fixed n, a smaller h results in higher variance while a larger h leads to higher bias.
- For a fixed h, the variance decreases as the number of sample points n tends to infinity
  - lacktriangleright for a large enough number of samples, the smaller h the better the accuracy of the resulting estimate
- In practice, where only a finite number of samples is possible, a compromise between h and n must be made.
  - lacktriangledown h can be set using techniques like cross-validation where the density estimation used for learning tasks such as classification

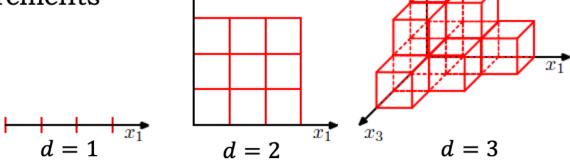


## Practical issues: Curse of dimensionality

- Large n is necessary to find an acceptable density estimation in high dimensional feature spaces
  - $\triangleright$  n must grow exponentially with the dimensionality d.
    - If n equidistant points are required to densely fill a one-dim interval,  $n^d$  points are needed to fill the corresponding d-dim hypercube.

□ We need an exponentially large quantity of training data to ensure that the cells are not empty  $x_2$ 

Also complexity requirements





## Non-parametric density estimation: Main approaches

#### Two approaches of satisfying conditions:

- Kernel density estimator (Parzen window): fix V and determine K from the data
  - Number of points falling inside the volume can vary from point to point
  - ▶ converges to the true probability density in the limit  $n \to \infty$  when  $\forall$  shrinks suitably with n (e.g.,  $V_n = V_1/\sqrt{n}$ )
- k-nearest neighbor density estimator: fix k and determine the value of V from the data
  - ightharpoonup Volume grows until it contains k neighbors of x
  - > converges to the true probability density in the limit  $n \to \infty$  when k grows with n (e.g.,  $k_n = k_1 \sqrt{n}$ )



#### $k_n$ -nearest neighbor estimation

- Cell volume is a function of the point location
  - To estimate p(x), let the cell around x grow until it captures  $k_n$  samples called  $k_n$  nearest neighbors of x.
- ▶ Two possibilities can occur:
  - high density near  $x \Rightarrow$  cell will be small which provides a good resolution
  - Iow density near  $x \Rightarrow$  cell will grow large and stop until higher density regions are reached



#### $k_n$ -nearest neighbor estimation

$$p_n(\mathbf{x}) = \frac{k_n/n}{V_n} \Rightarrow V_n \approx \frac{1}{p(\mathbf{x})} \times k_n/n$$

• A family of estimates by setting  $k_n=k_1\sqrt{n}$  and choosing different values for  $k_1$ :

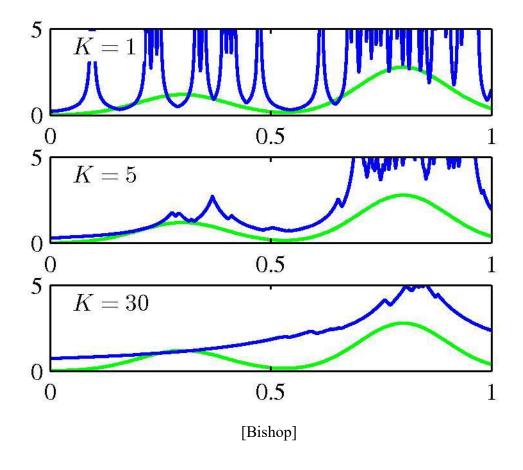
$$p_n(\mathbf{x}) = \frac{k_n/n}{V_n} \Rightarrow V_n \approx \frac{1/p(\mathbf{x})}{\sqrt{n}}$$

$$V_n \text{ is a function of } \mathbf{x}$$

$$k_1 = 1$$

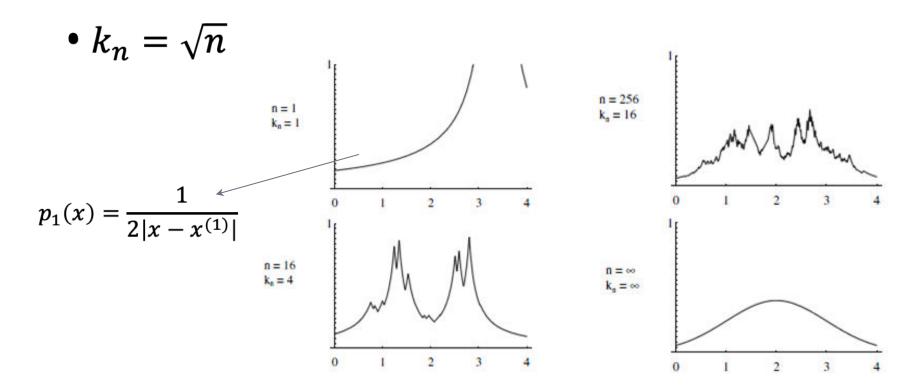
## $k_n$ -Nearest Neighbor Estimation: Example

• Discontinuities in the slopes





#### $k_n$ -Nearest Neighbor Estimation: Example



[Duda, Hurt, and Stork]



## Non-parametric density estimation: Summary

- Generality of distributions
  - With enough samples, convergence to an arbitrarily complicated target density can be obtained.
- The number of required samples must be very large to assure convergence
  - grows exponentially with the dimensionality of the feature space
- These methods are very sensitive to the choice of window width or number of nearest neighbors
- There may be severe requirements for computation time and storage (needed to save all training samples).
  - 'training' phase simply requires storage of the training set
  - computational cost of evaluating p(x) grows linearly with the size of the data set



## Nonparametric learners

- Memory-based or instance-based learners
  - lazy learning: (almost) all the work is done at the test time.
- Generic description:
  - Memorize training  $(x^{(1)}, y^{(1)}), ..., (x^{(n)}, y^{(n)})$ .
  - Given test x predict:  $\hat{y} = f(x; x^{(1)}, y^{(1)}, ..., x^{(n)}, y^{(n)})$ .
- f is typically expressed in terms of the similarity of the test sample x to the training samples  $x^{(1)}, \ldots, x^{(n)}$



## Parzen window & generative classification

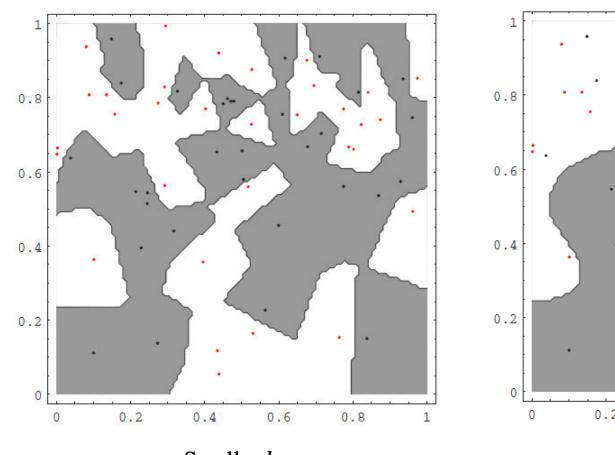
$$\text{If} \ \frac{\frac{1}{n_1} \times \frac{1}{h^d} \sum_{x^{(i)} \in \mathcal{D}_1} \phi \Big( \frac{x - x^{(i)}}{h} \Big)}{\frac{1}{n_2} \times \frac{1}{h^d} \sum_{x^{(i)} \in \mathcal{D}_2} \phi \Big( \frac{x - x^{(i)}}{h} \Big)} \times \frac{P(\mathcal{C}_1)}{P(\mathcal{C}_2)} > 1 \ \text{decide} \ \mathcal{C}_1$$

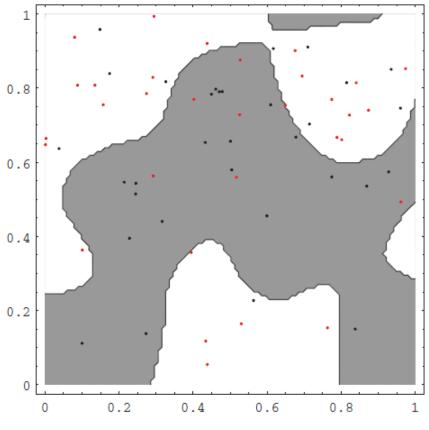
otherwise decide  $C_2$ 

- $n_j = \left|\mathcal{D}_j\right| \ (j=1,2)$ : number of training samples in class  $\mathcal{C}_j$ 
  - $\triangleright \mathcal{D}_i$ : set of training samples labels as  $\mathcal{C}_i$
- $\blacktriangleright$  For large n, it needs both high time and memory requirements



## Parzen window & generative classification: Example





Smaller h

[Duda, Hurt, and Stork]

**Instance-based Learning** 



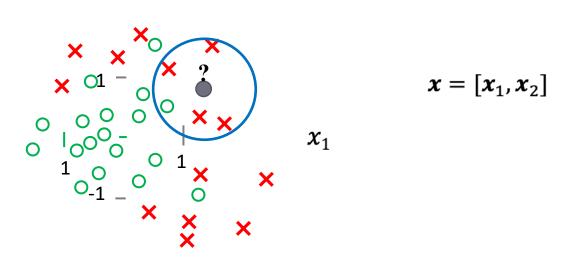
## Classification: k-Nearest-Neighbor (kNN)

**8** k-NN classifier: k > 1 nearest neighbors

 $\boldsymbol{x}_2$ 

• Label for x predicted by majority voting among its k-NN.

• 
$$k = 5$$



What is the effect of k?



#### kNN classifier

#### Given

- Training data  $\{(x^{(1)}, y^{(1)}), \dots, (x^{(n)}, y^{(n)})\}$  are simply stored.
- Test sample: x
- To classify x:
  - Find k nearest training samples to x
  - Out of these k samples, identify the number of samples  $k_j$  belonging to class  $C_i$  (j = 1, ..., C).
  - Assign x to the class  $C_{j^*}$  where  $j^* = \underset{j=1,...,c}{\operatorname{argmax}} k_j$
- It can be considered as a discriminative method.



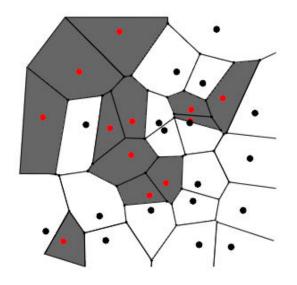
### Probabilistic perspective of kNN

- kNN as a discriminative nonparametric classifier
  - Non-parametric density estimation for  $P(C_i|x)$ 
    - ▶  $P(C_j|x) \approx \frac{k_j}{k}$  where  $k_j$  shows the number of training samples among k nearest neighbors of x that are labeled  $C_j$
  - Bayes decision rule for assigning labels



## Nearest-neighbor classifier: Example

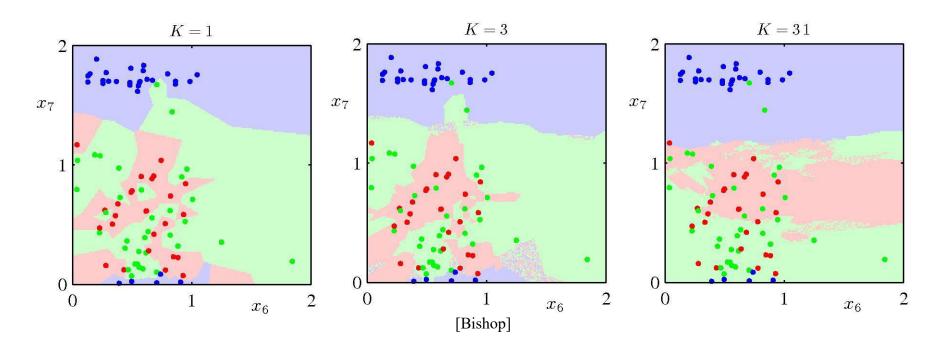
- Voronoi tessellation:
  - Each cell consists of all points closer to a given training point than to any other training points
    - All points in a cell are labeled by the category of the corresponding training point.



[Duda, Hurt, and Strok's Book]



## kNN classifier: Effect of k



Need to determine an appropriate value for k (e.g., by crossvalidation)



## Nearest neighbor classifier: error bound

- Nearest-Neighbor: kNN with k=1
  - Decision rule:  $\hat{y} = y^{NN(x)}$  where  $NN(x) = \underset{i=1,...,N}{\operatorname{argmin}} \|x x^{(i)}\|$
- Cover & Hart 67: asymptotic risk of NN classifier satisfies:

$$R^* \le R_{\infty}^{NN} \le 2R^*(1 - R^*) \le 2R^*$$

 $R_n$ : expected risk of NN classifier with n training examples drawn from p(x, y)

$$R_{\infty}^{NN} = \lim_{n \to \infty} R_n^{NN}$$

 $R^*$ : the optimal Bayes risk



#### k-NN classifier: error bound

•

• Devr 96: the asymptotic risk of the kNN classifier  $R_{\infty} = \lim_{n \to \infty} R_n$  satisfies

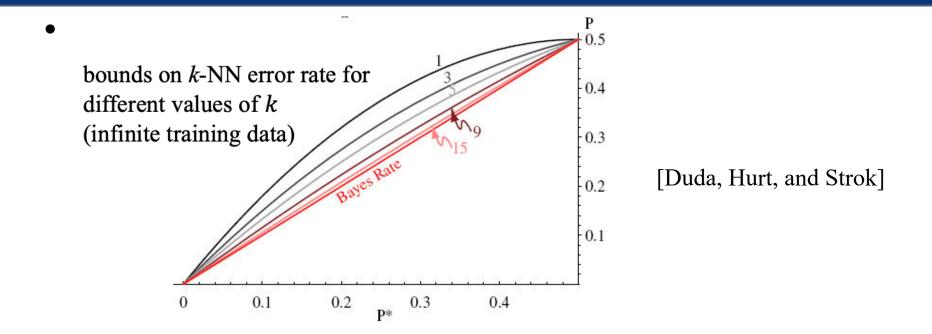
$$R^* \le R_{\infty}^{kNN} \le R^* + \sqrt{\frac{2R_{\infty}^{NN}}{k}}$$

where  $R^*$  is the optimal Bayes risk.

- As k increases, the upper bounds get closer to the lower bound (the Bayes Error rate).
  - When  $k \to \infty$ , the two bounds meet and k-NN rule becomes optimal.



#### Bound on the k-Nearest Neighbor Error Rate



- As k increases, the upper bounds get closer to the lower bound (the Bayes Error rate).
  - When  $k \to \infty$ , the two bounds meet and k-NN rule becomes optimal.



#### Instance-based learner

- Main things to construct an instance-based learner:
  - A distance metric
  - Number of nearest neighbors of the test data that we look at
  - A weighting function (optional)
  - How to find the output based on neighbors?



#### Distance measures

Euclidean distance

$$d(\mathbf{x}, \mathbf{x}') = \sqrt{\|\mathbf{x} - \mathbf{x}'\|_2^2} = \sqrt{(x_1 - x_1')^2 + \dots + (x_d - x_d')^2}$$

Sensitive to irrelevant features

- Distance learning methods for this purpose
  - Weighted Euclidean distance

• 
$$d_{\mathbf{w}}(\mathbf{x}, \mathbf{x}') = \sqrt{w_1(x_1 - x_1')^2 + \dots + w_d(x_d - x_d')^2}$$

Mahalanobis distance

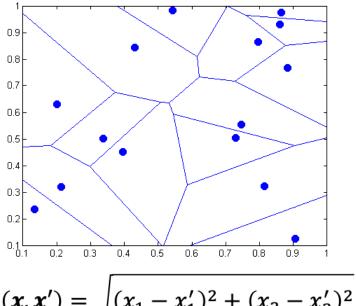
• 
$$d_A(\mathbf{x}, \mathbf{x}') = \sqrt{(\mathbf{x} - \mathbf{x}')^T A(\mathbf{x} - \mathbf{x}')}$$

- Other distances:
  - Hamming, angle, ...

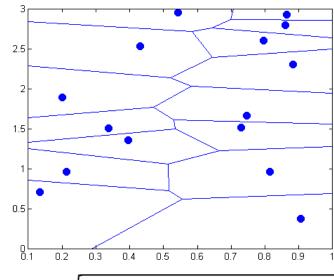
• 
$$L_p(\mathbf{x}, \mathbf{x}') = \sqrt[p]{\sum_{i=1}^d (x_i - x_i')^p}$$



#### Distance measure: example



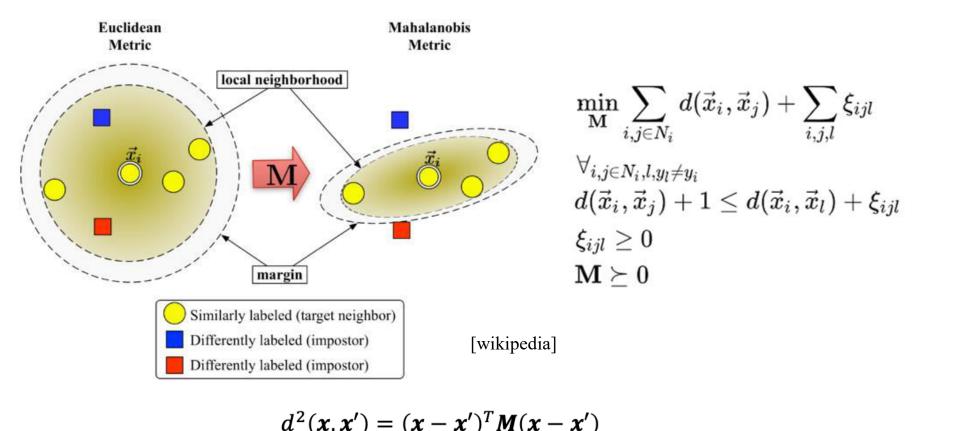
$$d(\mathbf{x}, \mathbf{x}') = \sqrt{(x_1 - x_1')^2 + (x_2 - x_2')^2}$$



$$d(\mathbf{x}, \mathbf{x}') = \sqrt{(x_1 - x_1')^2 + 3(x_2 - x_2')^2}$$



## Metric Learning Example: LMNN





## Weighted kNN classification

Weight nearer neighbors more heavily:

$$\hat{y} = f(\mathbf{x}) = \underset{c=1,\dots,C}{\operatorname{argmax}} \sum_{j \in N_k(\mathbf{x})} w_j(\mathbf{x}) \times I(c = y^{(j)})$$

$$w_j(\mathbf{x}) = \frac{1}{\|\mathbf{x} - \mathbf{x}^{(j)}\|^2}$$
An example of weighting function

• In the weighted kNN, we can use all training examples instead of just k (Stepard's method):

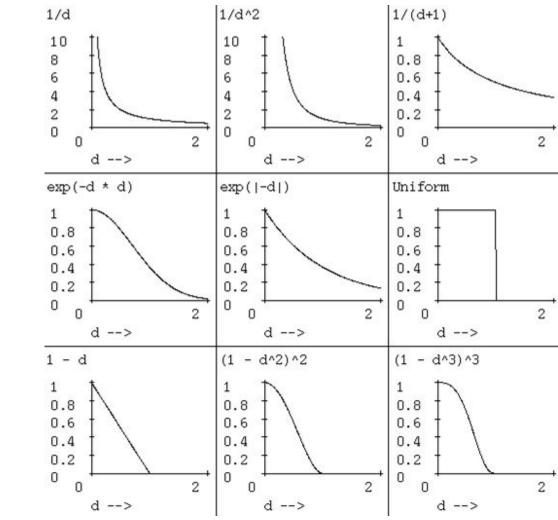
$$\hat{y} = f(\mathbf{x}) = \underset{c=1,...,C}{\operatorname{argmax}} \sum_{j=1}^{n} w_j(\mathbf{x}) \times I(c = y^{(j)})$$

• Weights can be found using a kernel function  $w_j(x) = K(x, x^{(j)})$ :

• e.g., 
$$K(x, x^{(j)}) = e^{-\frac{d(x, x^{(j)})}{\sigma^2}}$$



# Weighting functions



[Fig. has been adopted from Andrew Moore's tutorial on "Instance-based learning"]



 $d=d(\mathbf{x},\mathbf{x}')$ 

## kNN regression

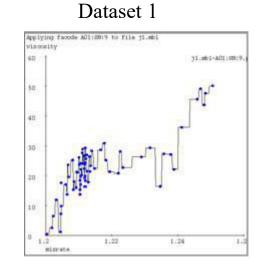
- Simplest k-NN regression:
  - Let  $x'^{(1)}$ , ...,  $x'^{(k)}$  be the k nearest neighbors of x and  $y'^{(1)}$ , ...,  $y'^{(k)}$  be their labels.

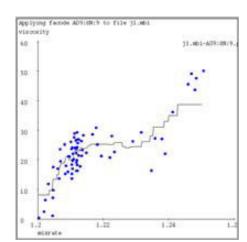
$$\hat{y} = \frac{1}{k} \sum_{j \in N_k(x)} y'^{(j)}$$

- Problems of kNN regression for fitting functions:
  - Problem 1: Discontinuities in the estimated function
    - Solution: Weighted (or kernel) regression
  - INN: noise-fitting problem
  - kNN (k > 1) smoothes away noise, but there are other deficiencies.
    - · flats the ends

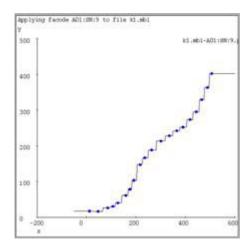


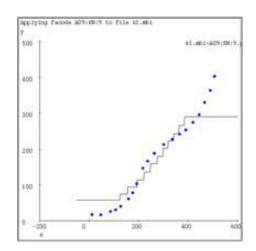
#### kNN regression: examples





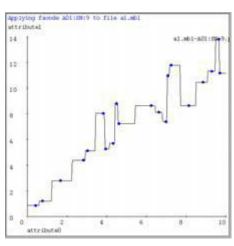


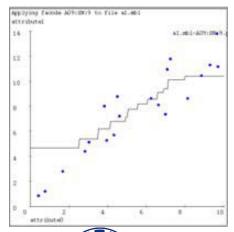




**Instance-based Learning** 

Dataset 3







k = 1

k = 9

#### Weighted (or kernel) kNN regression

Higher weights to nearer neighbors:

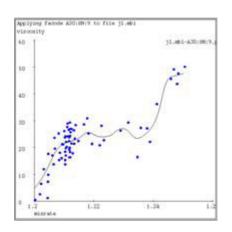
$$\hat{y} = f(\mathbf{x}) = \frac{\sum_{j \in N_k(\mathbf{x})} w_j(\mathbf{x}) \times y^{(j)}}{\sum_{j \in N_k(\mathbf{x})} w_j(\mathbf{x})}$$

In the weighted kNN regression, we can use all training examples instead of just k in the weighted form:

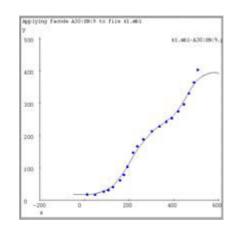
$$\hat{y} = f(x) = \frac{\sum_{j=1}^{n} w_j(x) \times y^{(j)}}{\sum_{j=1}^{n} w_j(x)}$$



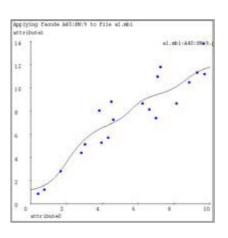
# Kernel kNN regression



$$\sigma = \frac{1}{32}$$
 of x-axis width



$$\sigma = \frac{1}{32}$$
 of x-axis width

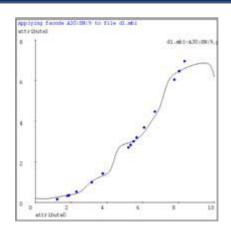


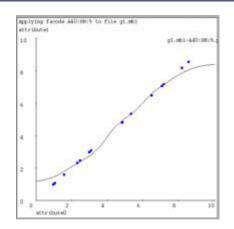
$$\sigma = \frac{1}{16}$$
 of x-axis width

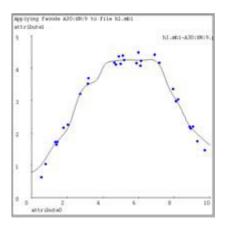
• Choosing a good parameter (kernel width) is important.



## Kernel kNN regression







In these datasets, some regions are without samples Best kernel widths have been used

- Disadvantages:
  - not capturing the simple structure of the data
  - failure to extrapolate at edges

[Figs. have been adopted from Andrew Moore's tutorial on "Instance-based learning"]



# Locally weighted linear regression

- For each test sample, it produces linear approximation to the target function in a local region
- Instead of finding the output using weighted averaging (as in the kernel regression), we fit a parametric function locally:

$$\hat{y} = f(\mathbf{x}, \mathbf{x}^{(1)}, y^{(1)}, \dots, \mathbf{x}^{(n)}, y^{(n)})$$
  
 $\hat{y} = f(\mathbf{x}; \mathbf{w}) = w_0 + w_1 x_1 + \dots + w_d x_d$ 

$$J(\mathbf{w}) = \sum_{i \in N_k(\mathbf{x})} (y^{(i)} - \mathbf{w}^T \mathbf{x}^{(i)})^2$$

w is found for each test sample

Unweighted linear



## Locally weighted linear regression

$$\hat{y} = f(x, x^{(1)}, y^{(1)}, \dots, x^{(n)}, y^{(n)})$$

$$J(\boldsymbol{w}(\boldsymbol{x})) = \sum_{i \in N_k(\boldsymbol{x})} (y^{(i)} - \boldsymbol{w}^T \boldsymbol{x}^{(i)})^2$$
 unweighted 
$$J(\boldsymbol{w}(\boldsymbol{x})) = \sum_{i \in N_k(\boldsymbol{x})} K(\boldsymbol{x}, \boldsymbol{x}^{(i)}) (y^{(i)} - \boldsymbol{w}^T \boldsymbol{x}^{(i)})^2$$
 weighted weighted

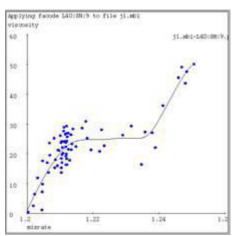
$$J(\boldsymbol{w}(\boldsymbol{x})) = \sum_{i=1}^{n} K(\boldsymbol{x}, \boldsymbol{x}^{(i)}) (y^{(i)} - \boldsymbol{w}^{T} \boldsymbol{x}^{(i)})^{2}$$

1

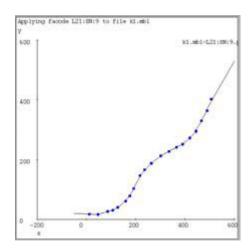
Weighted on all training examples



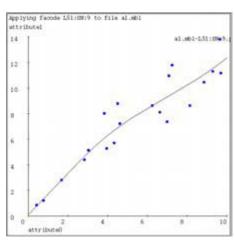
# Locally weighted linear regression: example



$$\sigma = \frac{1}{16}$$
 of x-axis width



 $\sigma = \frac{1}{32}$  of x-axis width



$$\sigma = \frac{1}{8}$$
 of x-axis width

More proper result than weighted kNN regression

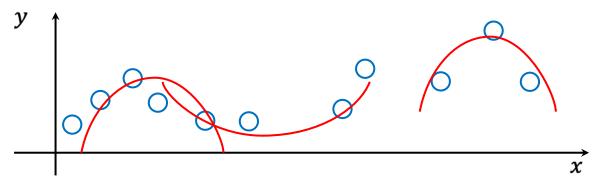


#### Locally weighted regression: summary

- Idea I: weighted kNN regression
  - using the weighted average on the output of x's neighbors (or on the outputs of all training data):

$$\hat{y} = \frac{\sum_{i=1}^{k} y'^{(i)} K(x, x'^{(i)})}{\sum_{j=1}^{k} K(x, x'^{(j)})}$$

- Idea 2: Locally weighted parametric regression
  - Fit a parametric model (e.g. linear function) to the neighbors of x (or on all training data).
  - Implicit assumption: the target function is reasonably smooth.



#### Parametric vs. nonparametric methods

• Is SVM classifier parametric?

$$\hat{y} = \operatorname{sign}(w_0 + \sum_{\alpha_i > 0} \alpha_i y^{(i)} K(\boldsymbol{x}, \boldsymbol{x}^{(i)}))$$

- In general, we can not summarize it in a simple parametric form.
  - Need to keep around support vectors (possibly all of the training data).
- However,  $\alpha_i$  are kind of parameters that are found in the training phase



# Instance-based learning: summary

- Learning is just storing the training data
  - prediction on a new data based on the training data themselves
- An instance-based learner does not rely on assumption concerning the structure of the underlying density function.
- With large datasets, instance-based methods are slow for prediction on the test data
  - kd-tree, Locally Sensitive Hashing (LSH), and other kNN approximations can help.



#### Reference

- T. Mitchell, "Machine Learning", 1998. [Chapter 8]
- C.M. Bishop, "Pattern Recognition and Machine Intelligence", Section 2.5.

