Non-parametric Learning

CE-477: Machine Learning - CS-828: Theory of Machine Learning
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References of the lecture are mentioned in the last slide

Outline

- Non-parametric approach
  - Non-parametric density estimation
    - Parzen Windows
    - Kn-Nearest Neighbor Density Estimation
  - 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., Estimating a multi-modal distribution with a unimodal parametric density
  - Non-parametric methods don't assume that the model (from) of underlying densities is known in advance

Parametric vs. nonparametric methods

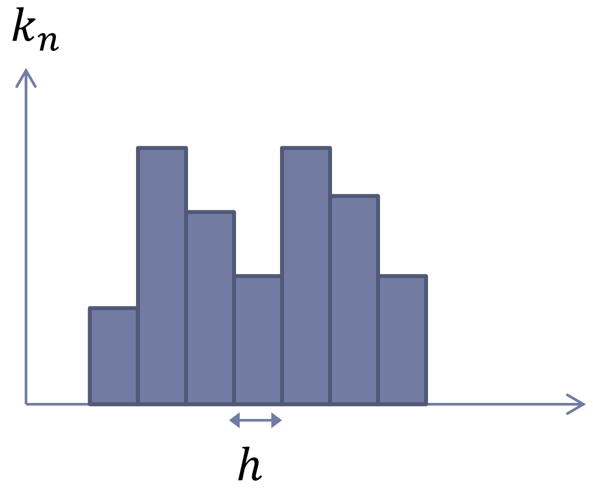
- Parametric methods need to find parameters from data and then use the inferred parameters to decide on new data points
  - Learning: finding parameters from data

- 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
  - $P(b_l) \approx k_n(b_l)/n \quad l = 1, \dots, L$
    - $k_n(b_l)$: number of samples (among n ones) lied in the bin b_l



- The corresponding estimated pdf:
  - $\hat{p}(x) = \frac{P(b_l)}{h} \qquad \left|x - \bar{x}_{b_l}\right| \leq \frac{h}{2}$

Mid-point of the bin b_l

Non-parametric density estimation

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

- $\mathcal{D} = \{\boldsymbol{x}^{(i)}\}_{i=1}^{n}$: a set of samples drawn i.i.d. according to $p(\boldsymbol{x})$
  - The probability that k of the n samples fall in $\mathcal{R}$:
    - $P_k = \binom{n}{k} P^k (1-P)^{n-k}$
    - $E[k] = nP$
    - $k \approx nP \Rightarrow \frac{k}{n}$ as an estimate for P

Non-parametric density estimation

- We can estimate smoothed $p(\boldsymbol{x})$ by estimating P:

- Assumptions: $p(\boldsymbol{x})$ is continuous and the region $\mathcal{R}$ enclosing $\boldsymbol{x}$ is so small that p is near constant in it:

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

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

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

- Let V approach zero if we want to find $p(\boldsymbol{x})$ instead of the averaged version.

Necessary conditions for converge

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

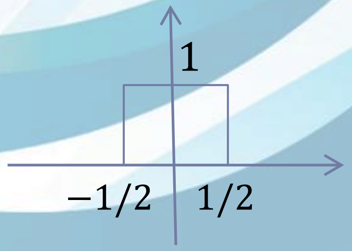
$$p_n(\boldsymbol{x}) = \frac{k_n/n}{V_n}$$

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

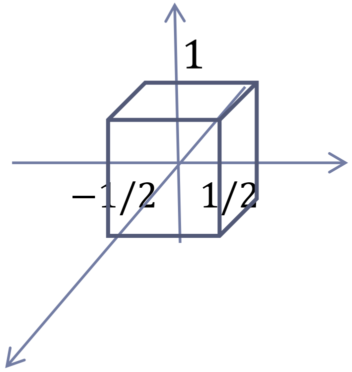
Non-parametric density estimation: Main approaches

- 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
  - k-nearest neighbor density estimator: fix k and determine the value of V from the data
    - Volume grows until it contains k neighbors of $\boldsymbol{x}$

Parzen window



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

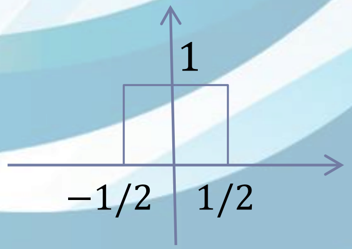


- Hypercube as a simple window function:

$$\varphi(\boldsymbol{u}) = \begin{cases} 1 & (|u_1| \leq \frac{1}{2} \wedge \ldots \wedge |u_d| \leq \frac{1}{2}) \\ 0 & o.w. \end{cases}$$

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

Parzen window



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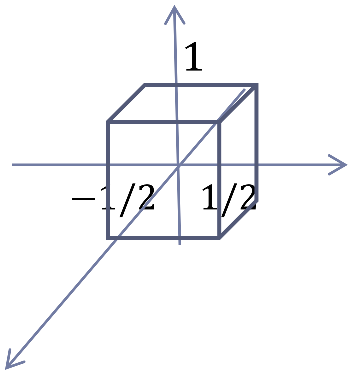

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- $p_n(\boldsymbol{x}) = \frac{k_n}{nV_n}$
  - $k_n = \sum_{i=1}^{n} \varphi\left(\frac{\boldsymbol{x}-\boldsymbol{x}^{(i)}}{h_n}\right) \longrightarrow$ number of samples in the hypercube around $\boldsymbol{x}$
  - $V_n = (h_n)^d$

Window function

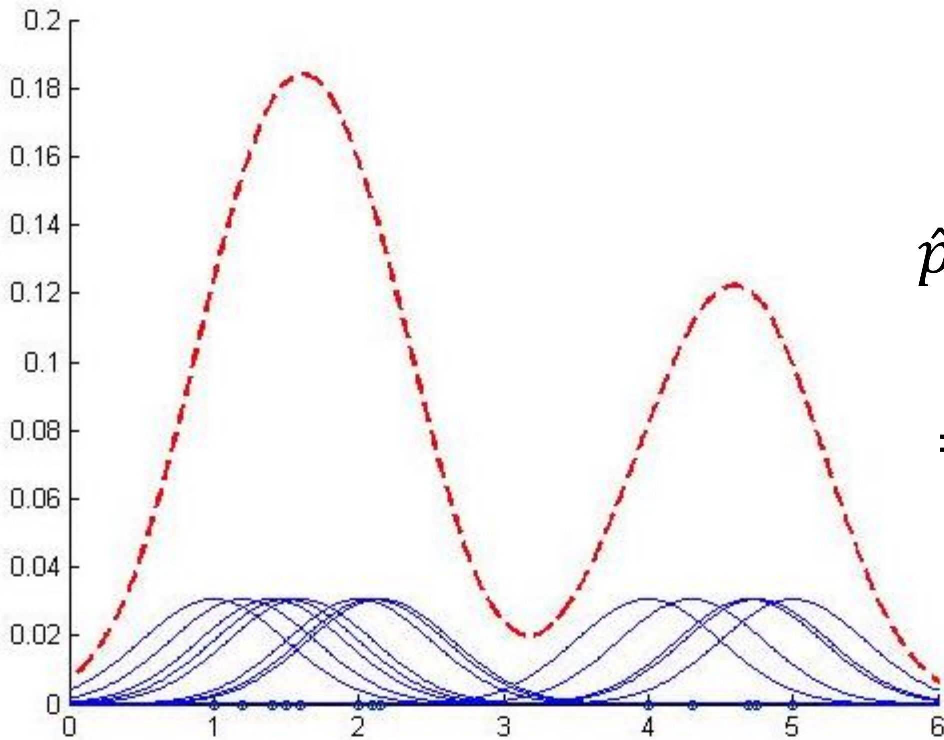
- Necessary conditions for window function to find legitimate density function:
  - $\varphi(\boldsymbol{x}) \geq 0$
  - $\int \varphi(\boldsymbol{x}) d\boldsymbol{x} = 1$

- Windows are also called **kernels** or potential functions.

Density estimation: non-parametric

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

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



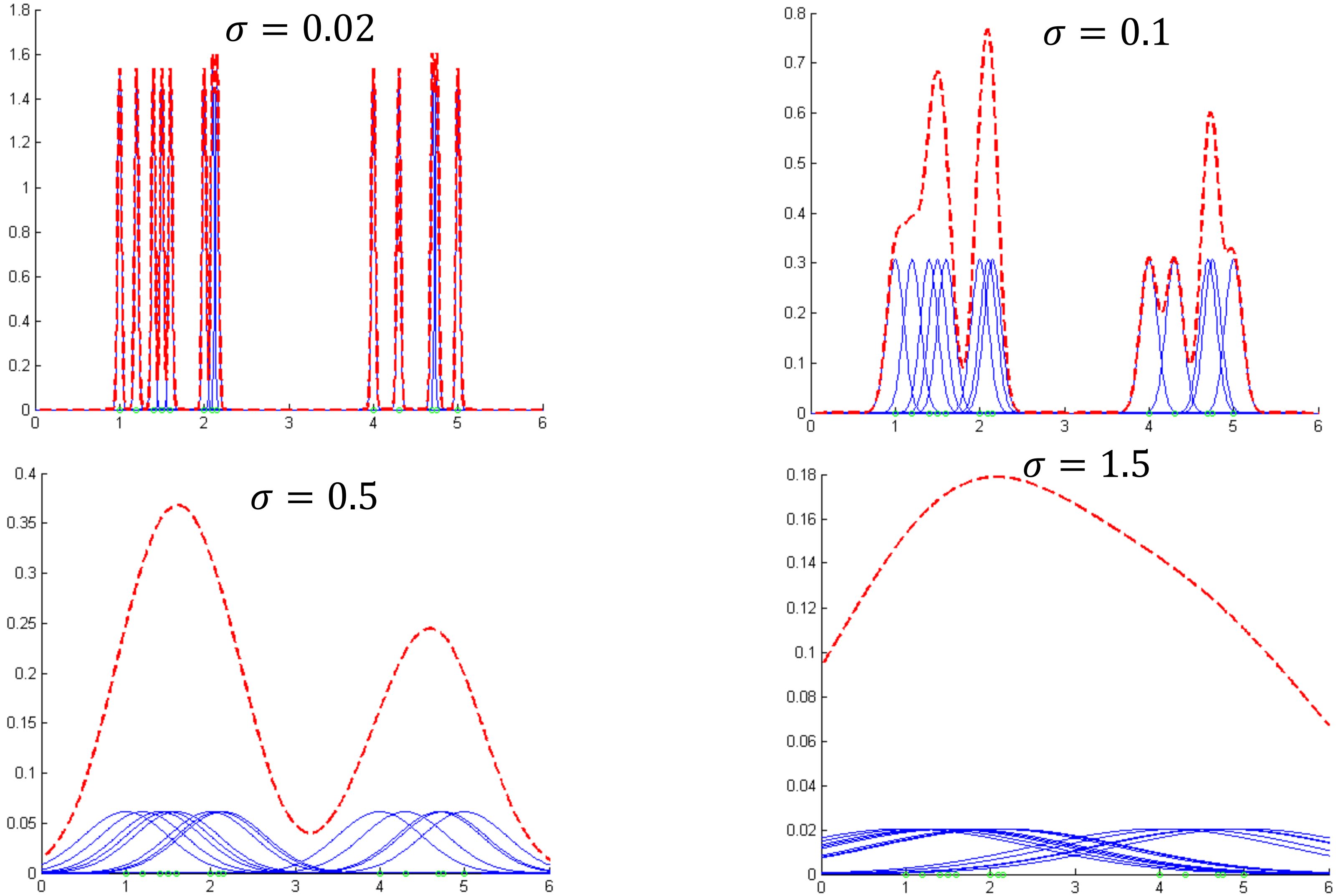
$\sigma = h$

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

$$= \frac{1}{n}\sum_{i=1}^{n} \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{\left(x-x^{(i)}\right)^2}{2\sigma^2}}$$

Choice of σ is crucial.

Density estimation: non-parametric

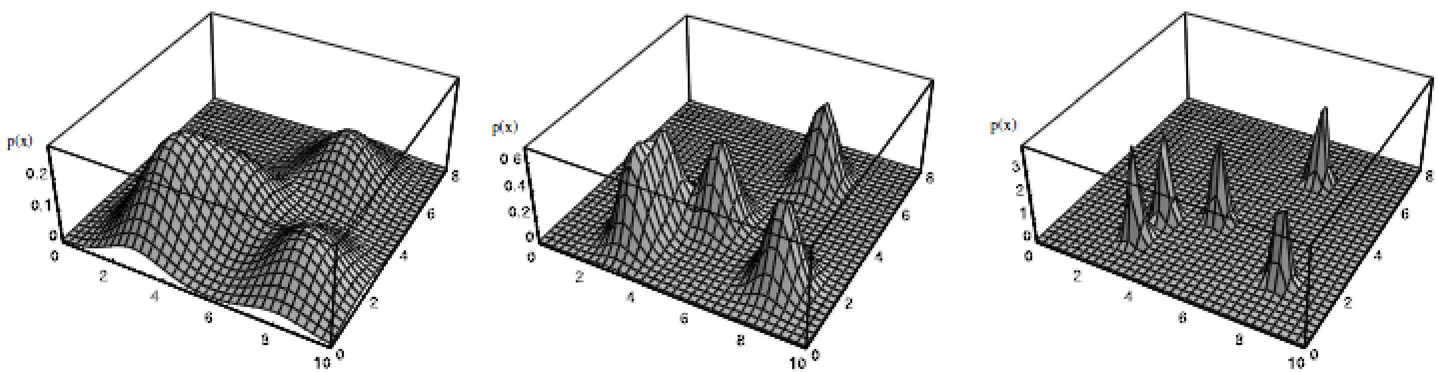


Window (or kernel) function: Width parameter

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

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

[Duda, Hurt, and Stork]



- For unlimited n, by letting V_n slowly approach zero as n increases $p_n(\boldsymbol{x})$ converges to $p(\boldsymbol{x})$

Width parameter

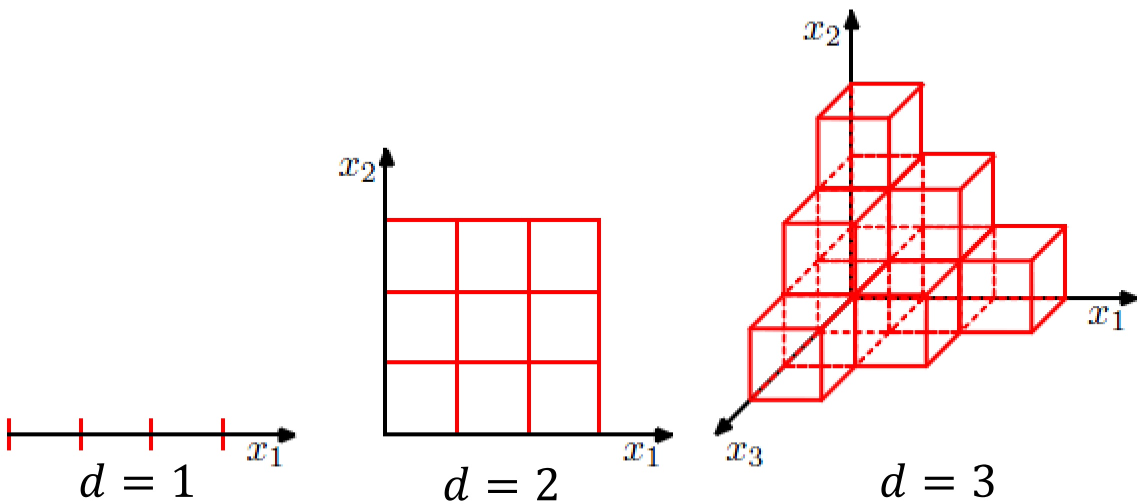
- For fixed n, a smaller h results in higher variance while a larger h leads to higher bias.

- For a fixed h, the variance decreases as the number of sample points n tends to infinity
  - 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.
  - 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
  - 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



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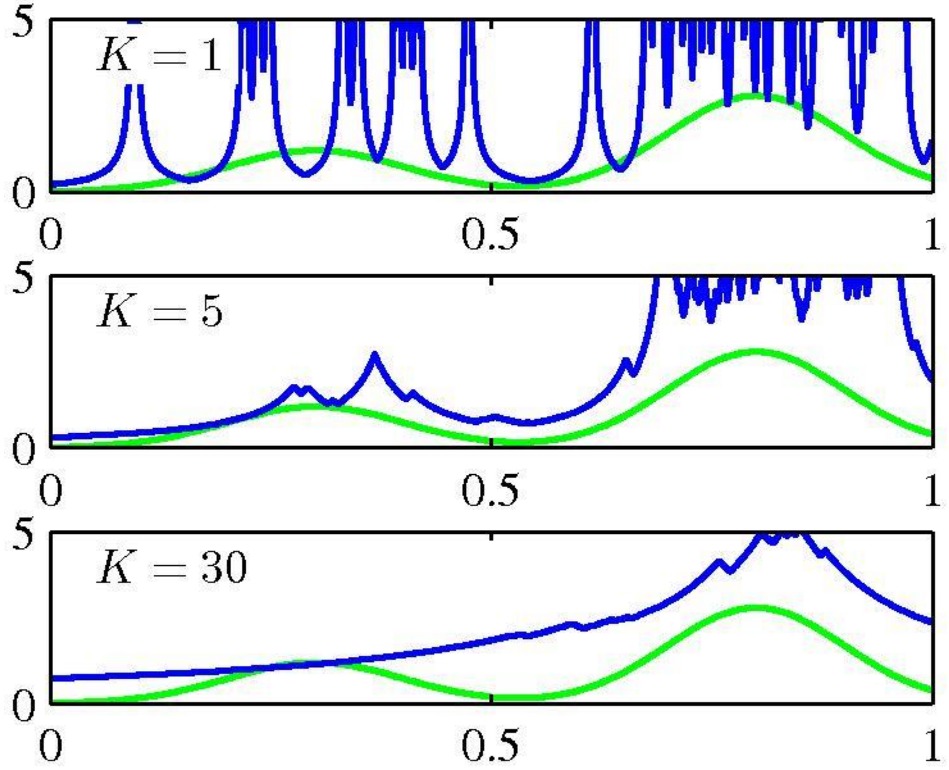
k_n-nearest neighbor estimation

- Cell volume is a function of the point location
  - To estimate $p(\boldsymbol{x})$, let the cell around $\boldsymbol{x}$ grow until it captures k_n samples called k_n nearest neighbors of $\boldsymbol{x}$.

- Two possibilities can occur:
  - high density near $\boldsymbol{x} \Rightarrow$ cell will be small which provides a good resolution
  - low density near $\boldsymbol{x} \Rightarrow$ cell will grow large and stop until higher density regions are reached

k_n-Nearest Neighbor Estimation: Example

- Different estimated distributions for different values of k



[Bishop]

Non-parametric density estimation: Summary

- 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 $p(\boldsymbol{x})$ 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 $(\boldsymbol{x}^{(1)}, y^{(1)}), \dots, (\boldsymbol{x}^{(n)}, y^{(n)})$.
  - Given test $\boldsymbol{x}$ predict: $\hat{y} = f(\boldsymbol{x}; \boldsymbol{x}^{(1)}, y^{(1)}, \dots, \boldsymbol{x}^{(n)}, y^{(n)})$.

- f is typically expressed in terms of the similarity of the test sample $\boldsymbol{x}$ to the training samples $\boldsymbol{x}^{(1)}, \dots, \boldsymbol{x}^{(n)}$

Parzen window & generative classification

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

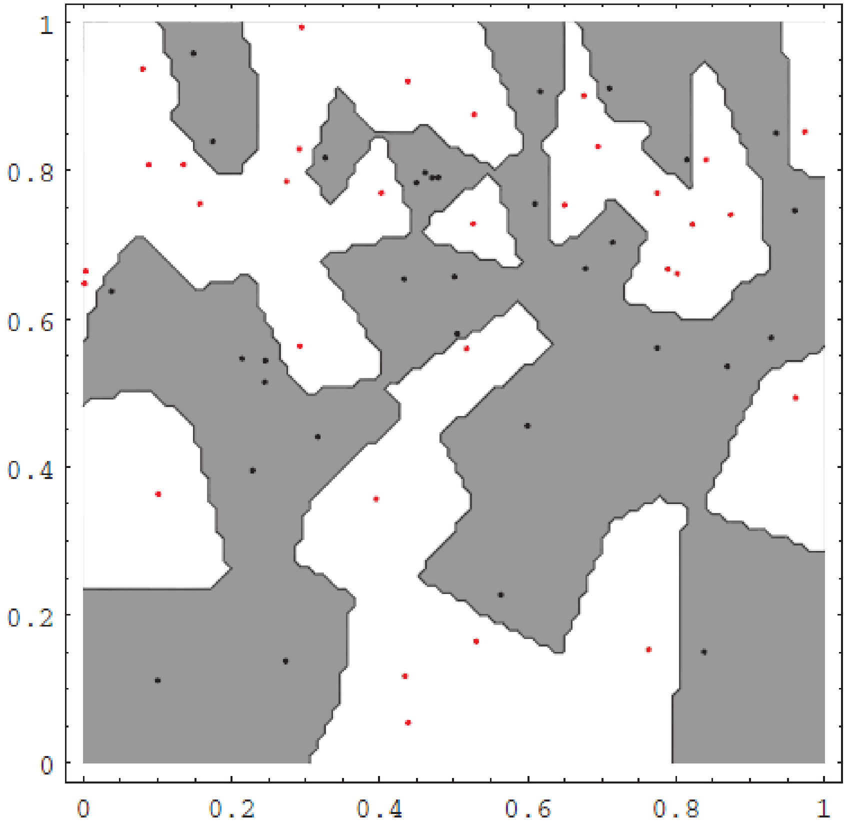
  otherwise decide $\mathcal{C}_2$

  - $n_j = |\mathcal{D}_j|$ $(j = 1,2)$: number of training samples in class $\mathcal{C}_j$
    - $\mathcal{D}_j$: set of training samples labels as $\mathcal{C}_j$

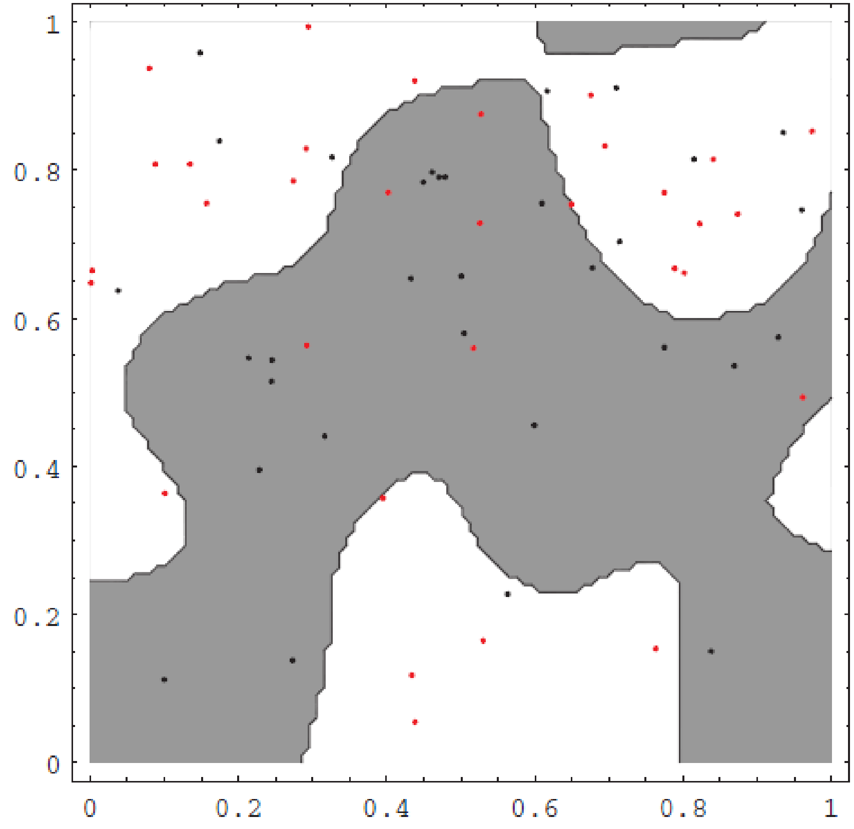
- For large n, it needs both high time and memory requirements

- We can also use k_n-nearest neighbor density estimation technique for this generative classification approach. How?

Parzen window & generative classification: Example



Smaller h



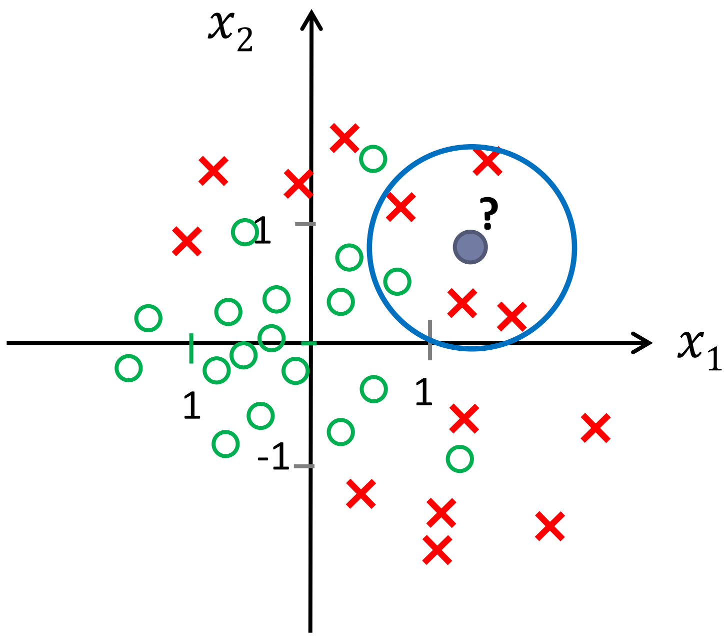
larger h

[Duda, Hurt, and Stork]

Classification: k-Nearest-Neighbor (kNN)

- k-NN classifier: $k > 1$ nearest neighbors
  - Label for $\boldsymbol{x}$ predicted by majority voting among its k-NN.

- $k = 5$



$\boldsymbol{x} = [\boldsymbol{x}_1, \boldsymbol{x}_2]$

- What is the effect of k?

kNN classifier

- Given
  - Training data $\{(\boldsymbol{x}^{(1)}, y^{(1)}), \dots, (\boldsymbol{x}^{(n)}, y^{(n)})\}$ are simply stored.
  - Test sample: $\boldsymbol{x}$

- To classify $\boldsymbol{x}$:
  - Find k nearest training samples to $\boldsymbol{x}$
  - Out of these k samples, identify the number of samples k_j belonging to class $\mathcal{C}_j$ ($j = 1, \dots, C$).
  - Assign $\boldsymbol{x}$ to the class $\mathcal{C}_{j^*}$ where $j^* = \underset{j=1,\dots,c}{\operatorname{argmax}} k_j$

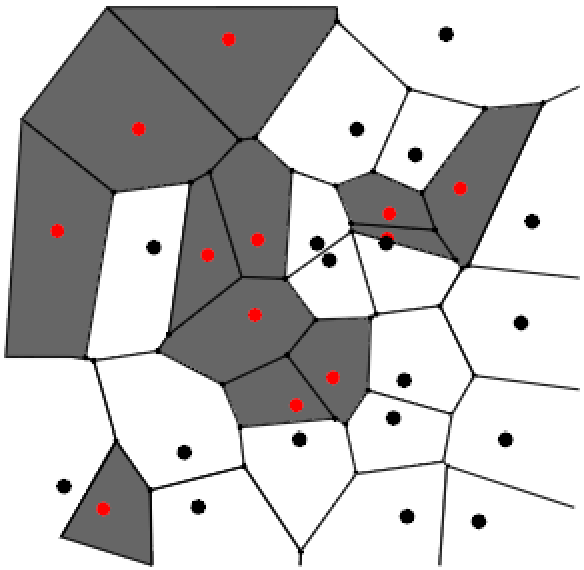
- It can be considered as a discriminative method.

Probabilistic perspective of kNN

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

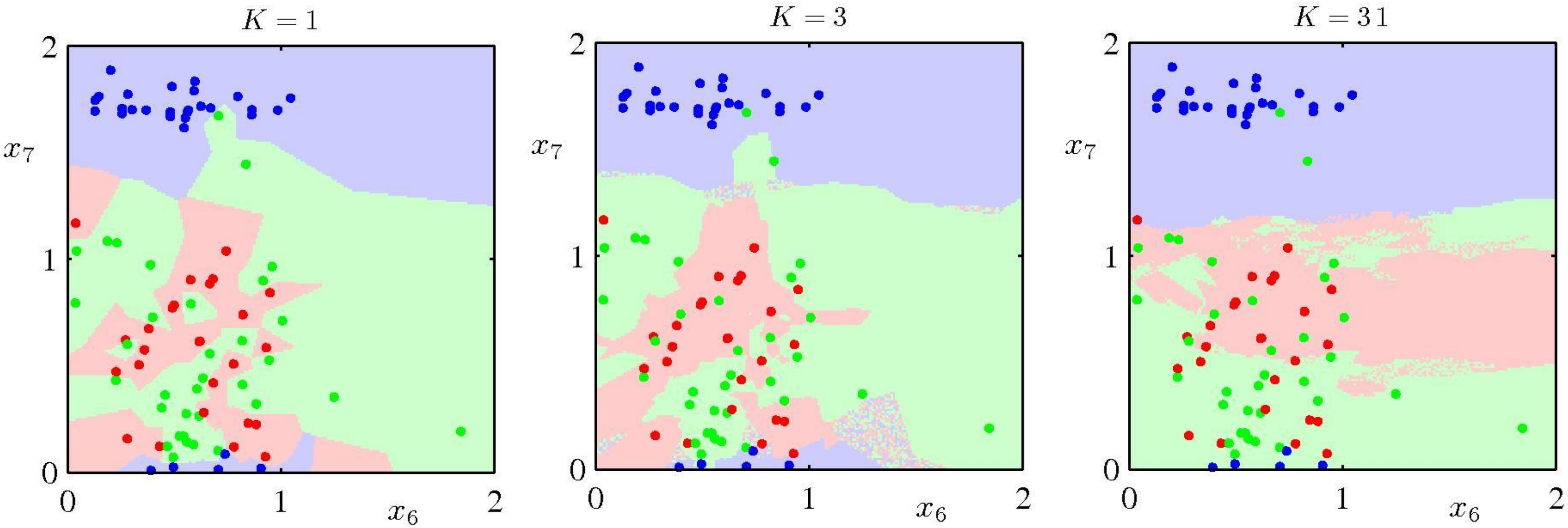
Nearest-neighbor classifier: Example

- 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



[Bishop]

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

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

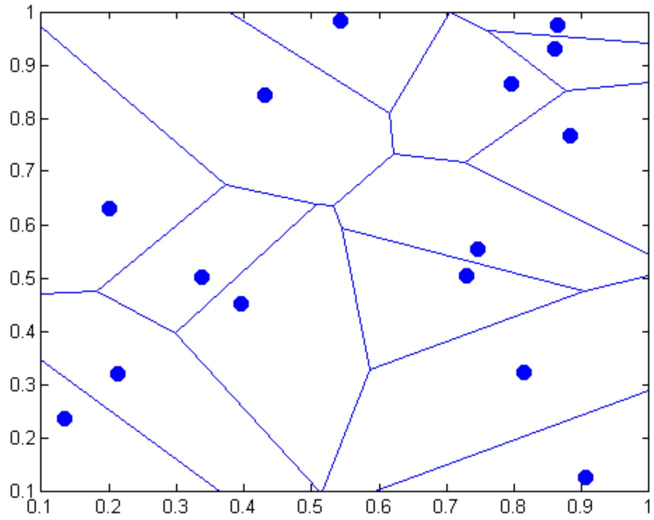
$$d(\boldsymbol{x},\boldsymbol{x}') = \sqrt{\|\boldsymbol{x}-\boldsymbol{x}'\|_2^2} = \sqrt{(x_1-x_1')^2+\dots+(x_d-x_d')^2}$$

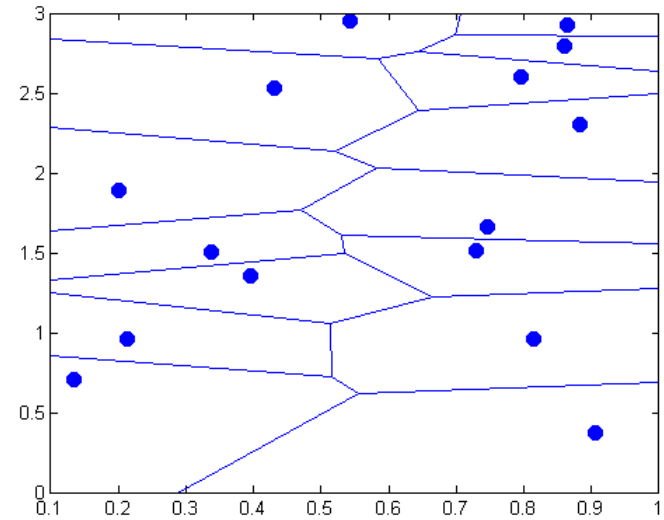
Sensitive to irrelevant features

- Distance learning methods for this purpose
  - Weighted Euclidean distance
    - $d_{\boldsymbol{w}}(\boldsymbol{x},\boldsymbol{x}') = \sqrt{w_1(x_1-x_1')^2+\dots+w_d(x_d-x_d')^2}$
  - Mahalanobis distance
    - $d_{\boldsymbol{A}}(\boldsymbol{x},\boldsymbol{x}') = \sqrt{(\boldsymbol{x}-\boldsymbol{x}')^T\boldsymbol{A}(\boldsymbol{x}-\boldsymbol{x}')}$

- Other distances:
  - Hamming, angle, …
  - $L_p(\boldsymbol{x},\boldsymbol{x}') = \sqrt[p]{\sum_{i=1}^{d}\left(x_i-x_i'\right)^p}$

Distance measure: example





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

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

Weighted kNN classification

- Weight nearer neighbors more heavily:

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

$$w_j(\boldsymbol{x}) = \frac{1}{\|\boldsymbol{x} - \boldsymbol{x}^{(j)}\|^2}$$

An example of weighting function

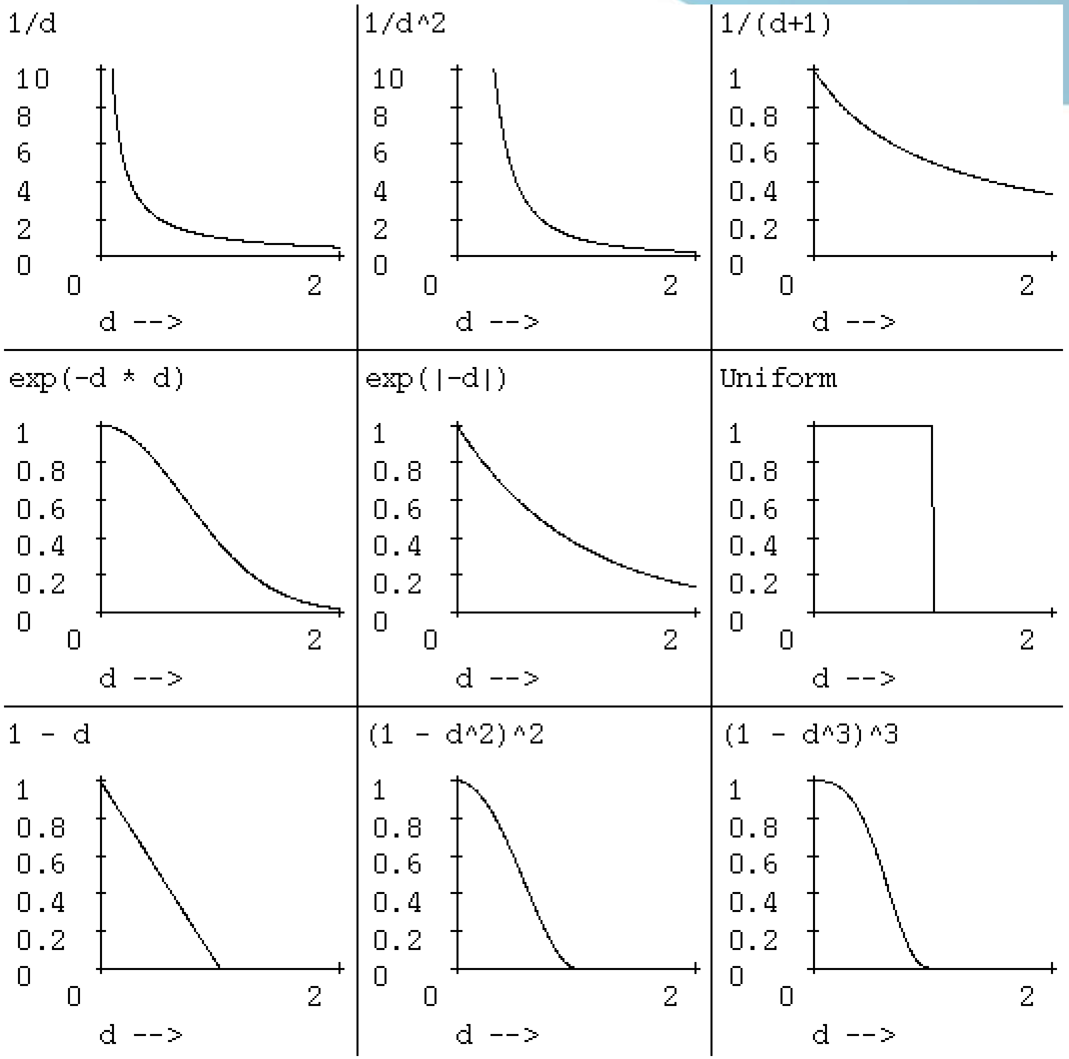
- In the weighted kNN, we can use all training examples instead of just k (Stepard's method):

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

- Weights can be found using a kernel function $w_j(\boldsymbol{x}) = K(\boldsymbol{x}, \boldsymbol{x}^{(j)})$:
  - e.g., $K(\boldsymbol{x}, \boldsymbol{x}^{(j)}) = e^{-\frac{d(\boldsymbol{x}, \boldsymbol{x}^{(j)})}{\sigma^2}}$

Weighting functions

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



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

kNN regression

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

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

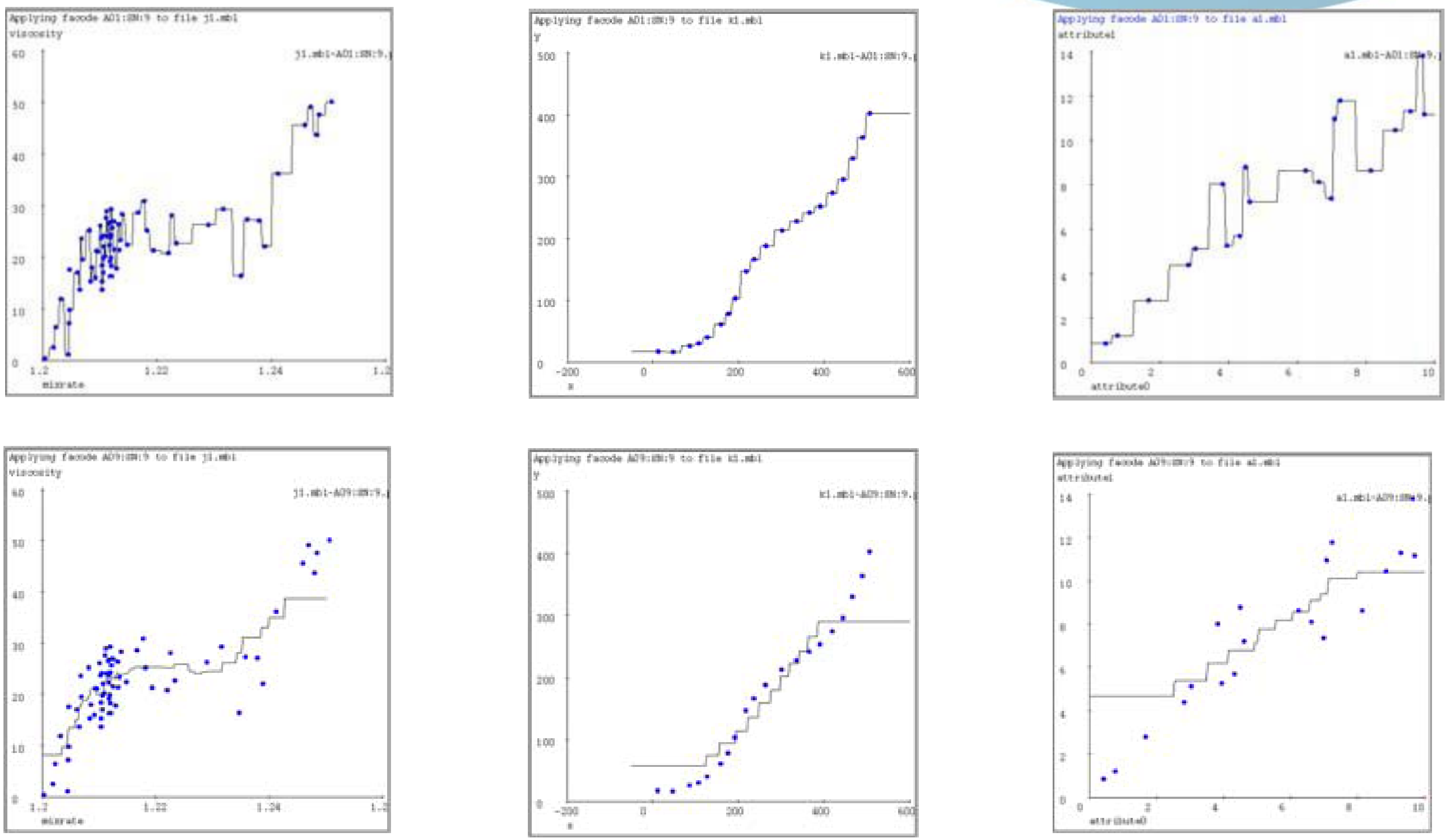
- Problems of kNN regression for fitting functions:
  - Problem 1: Discontinuities in the estimated function
    - Solution: Weighted (or kernel) regression
  - 1NN: noise-fitting problem
  - kNN ($k > 1$) smoothes away noise, but there are other deficiencies.
    - flats the ends

kNN regression: examples

Dataset 1 | Dataset 2 | Dataset 3

$k = 1$

$k = 9$



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

Weighted (or kernel) kNN regression

- Higher weights to nearer neighbors:

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

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

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

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:

$$\hat{y} = f\left(\boldsymbol{x}, \boldsymbol{x}^{(1)}, y^{(1)}, \ldots, \boldsymbol{x}^{(n)}, y^{(n)}\right)$$

$$\hat{y} = f(\boldsymbol{x}; \boldsymbol{w}) = w_0 + w_1 x_1 + \cdots + w_d x_d$$

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

Unweighted linear

$\boldsymbol{w}$ is found for each test sample

Locally weighted linear regression

$$\hat{y} = f\left(\boldsymbol{x}, \boldsymbol{x}^{(1)}, y^{(1)}, \ldots, \boldsymbol{x}^{(n)}, y^{(n)}\right)$$

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

unweighted

e.g, $K\left(\boldsymbol{x}, \boldsymbol{x}^{(i)}\right) = e^{-\frac{\left\|x - x^{(i)}\right\|^2}{2\sigma^2}}$

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

weighted

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

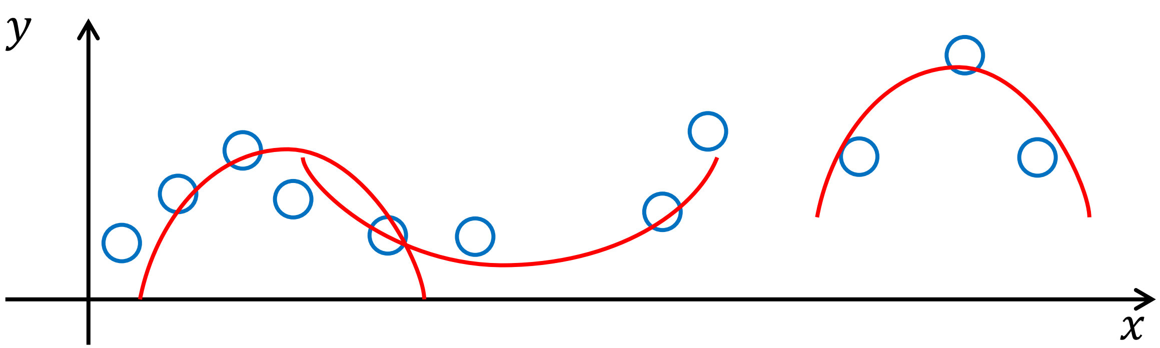
Weighted on all training examples

Locally weighted regression: summary

- Idea 1: weighted kNN regression
  - using the weighted average on the output of $\boldsymbol{x}$'s neighbors (or on the outputs of all training data):

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

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



Parametric vs. nonparametric methods

- Is SVM classifier parametric?

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

  - 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, α_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

- Mahdieh Soleymani, Machine learning, Sharif university