CHAPTER 8:

NONPARAMETRİC METHODS

Nonparametric Estimation

- Parametric (single global model), semiparametric (small number of local models)
- Nonparametric: Similar inputs have similar outputs
- Functions (pdf, discriminant, regression) change smoothly
- Keep the training data;“let the data speak for itself”
- Given x, find a small number of closest training instances and interpolate from these
- Aka lazy/memory-based/case-based/instance-based learning

Density Estimation

- Given the training set $\boldsymbol{X}=\{x^t\}_t$ drawn iid from $p(x)$
- Divide data into bins of size h
- Histogram:

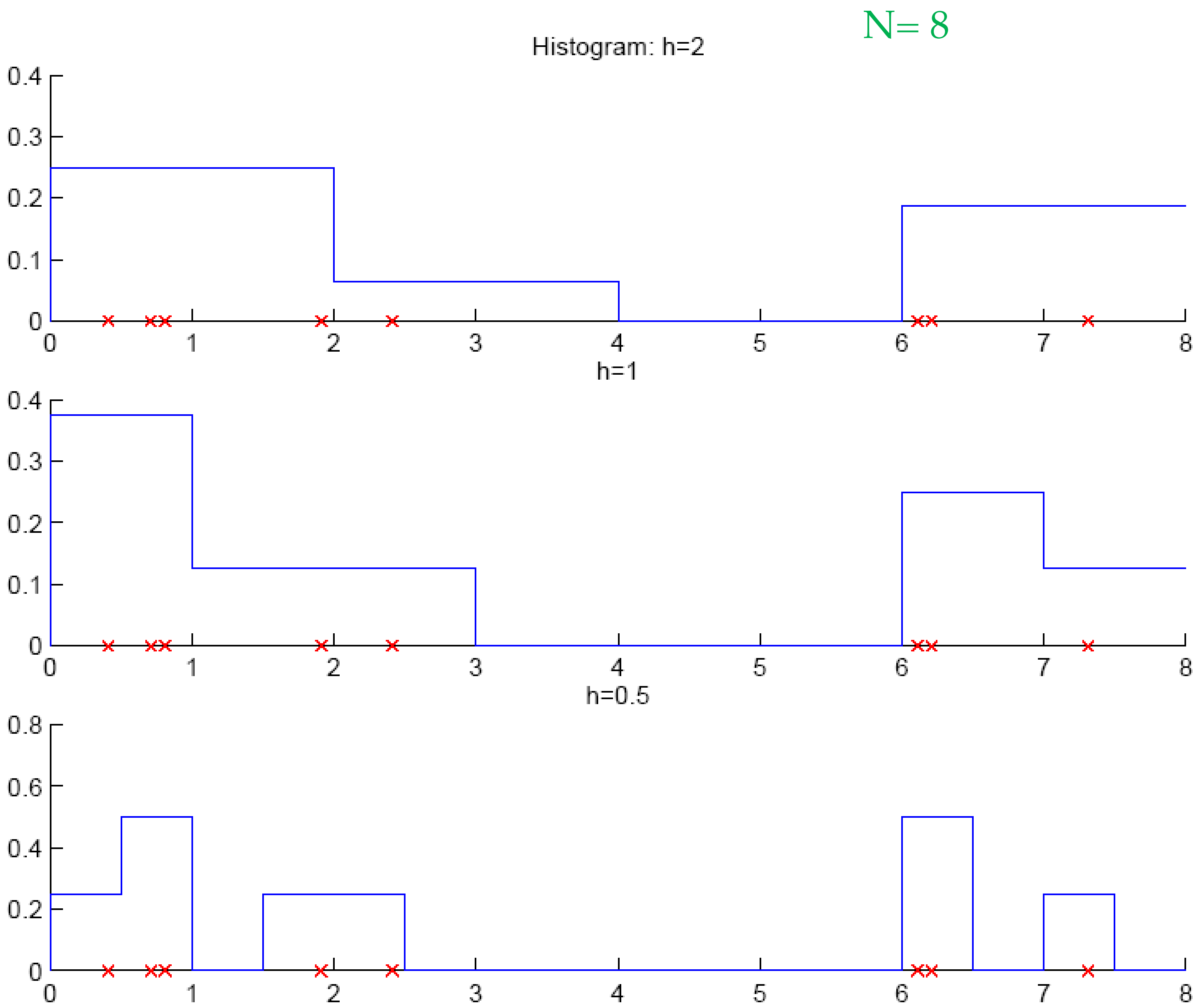
$$\hat{p}(x) = \frac{\#\{x^t \text{ in the same bin as } x\}}{Nh}$$

- Naive estimator:

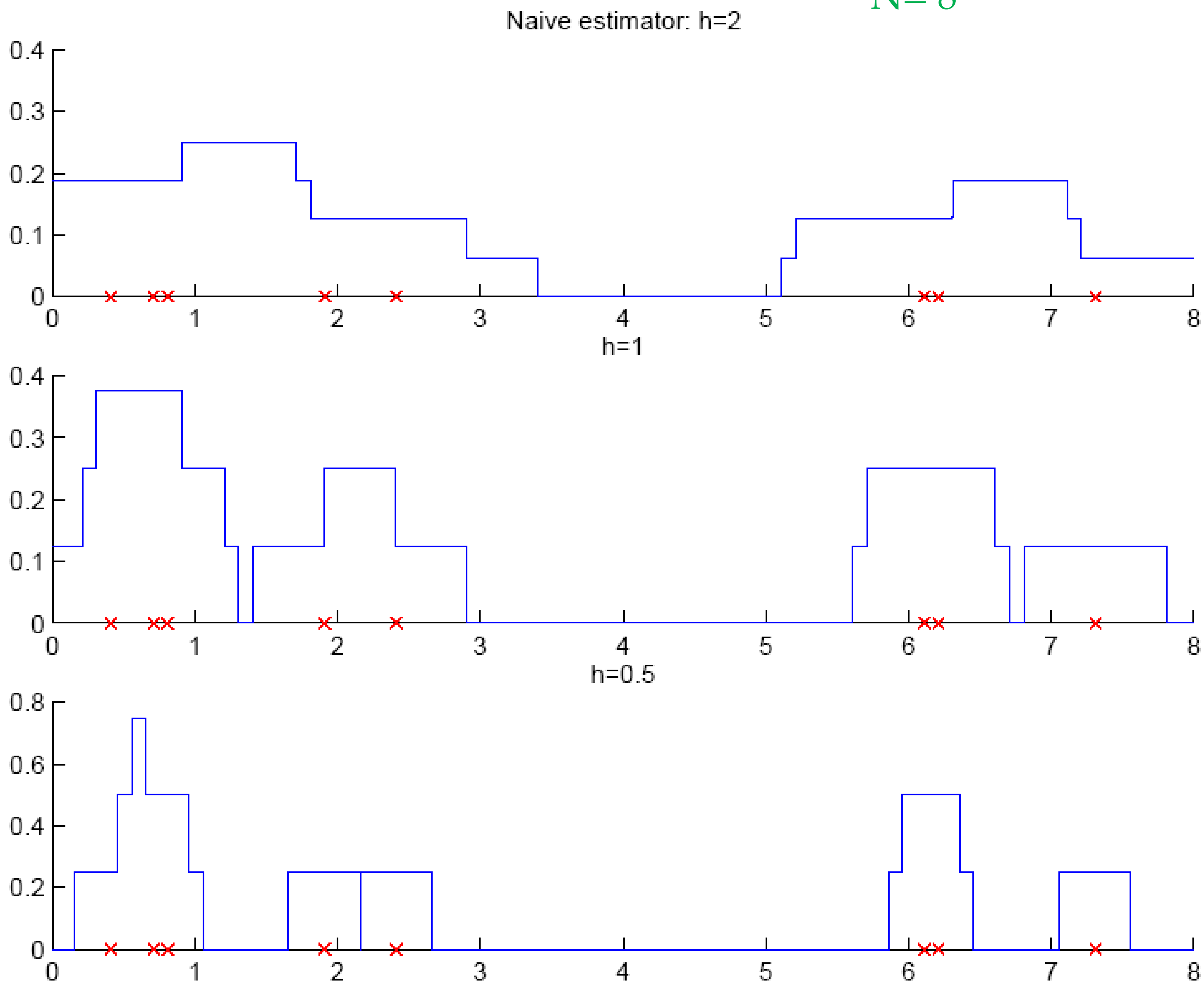
$$\hat{p}(x) = \frac{\#\{x - h/2 < x^t \leq x + h/2\}}{Nh}$$

or equivalently,

$$\hat{p}(x) = \frac{1}{Nh}\sum_{t=1}^{N} w\left(\frac{x - x^t}{h}\right) \quad \text{where } w(u) = \begin{cases} 1 & \text{if } |u| < 1/2 \\ 0 & \text{otherwise} \end{cases}$$


N= 8
Histogram: h=2
h=1
h=0.5
0.4
0.3
0.2
0.1
0
0.8
0.6
0 1 2 3 4 5 6 7 8

N= 8



the kernel estimate is a sum of “boxes”

Kernel Estimator to get a smooth estimate

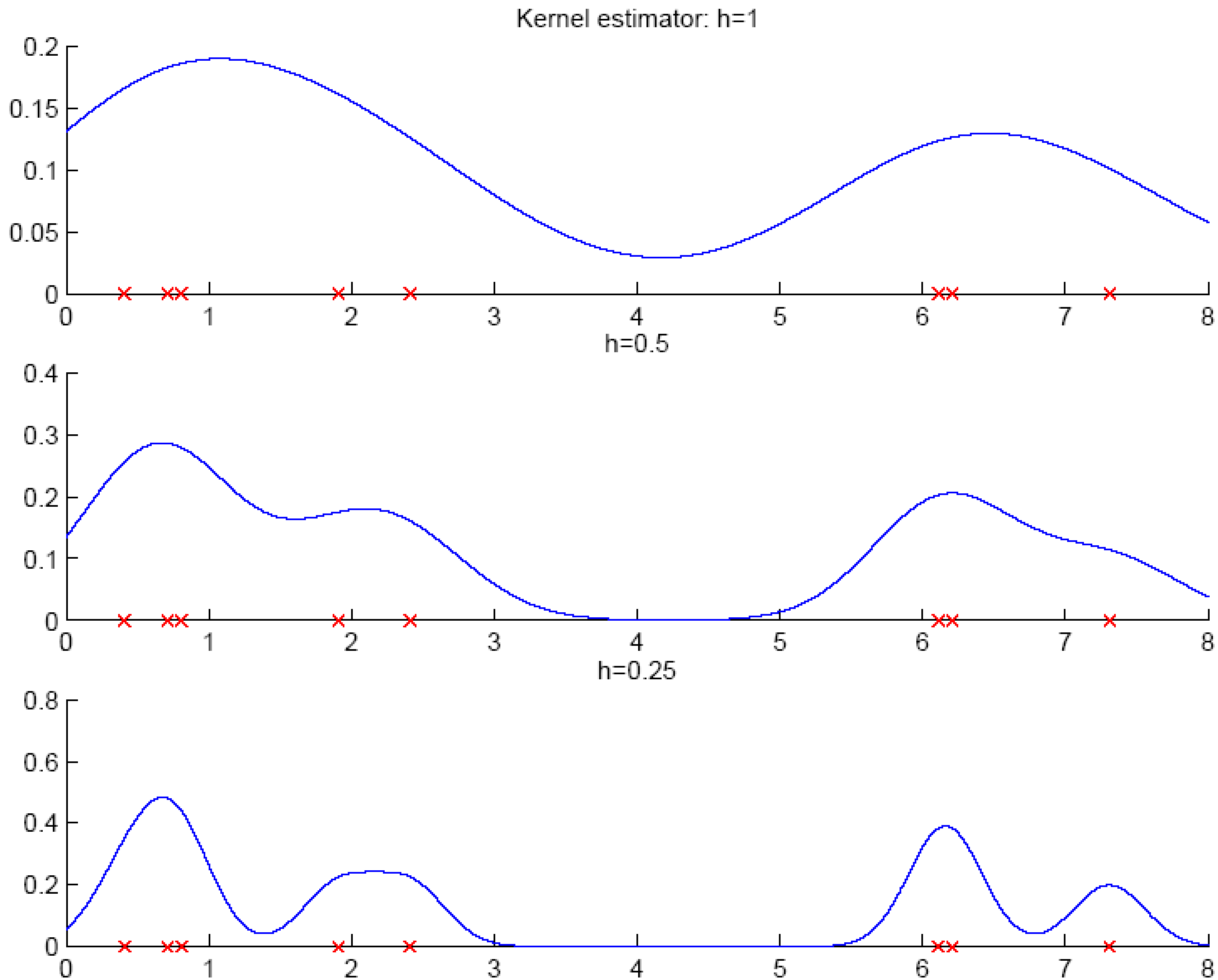
- Kernel function, e.g., Gaussian kernel:

$$K(u) = \frac{1}{\sqrt{2\pi}} \exp\left[-\frac{u^2}{2}\right]$$

- Kernel estimator (Parzen windows)

$$\hat{p}(x) = \frac{1}{Nh} \sum_{t=1}^{N} K\left(\frac{x - x^t}{h}\right)$$

- the kernel function K(.) determines the shape of the "influence"
- h determines the width of the "influence"
- the kernel estimate is the sum of "bumps"


Kernel estimator: h=1
0.2
0.15
0.1
0.05
0
0 1 2 3 4 5 6 7 8
h=0.5
0.4
0.3
0.2
0.1
0
0 1 2 3 4 5 6 7 8
h=0.25
0.8
0.6
0.4
0.2
0
0 1 2 3 4 5 6 7 8

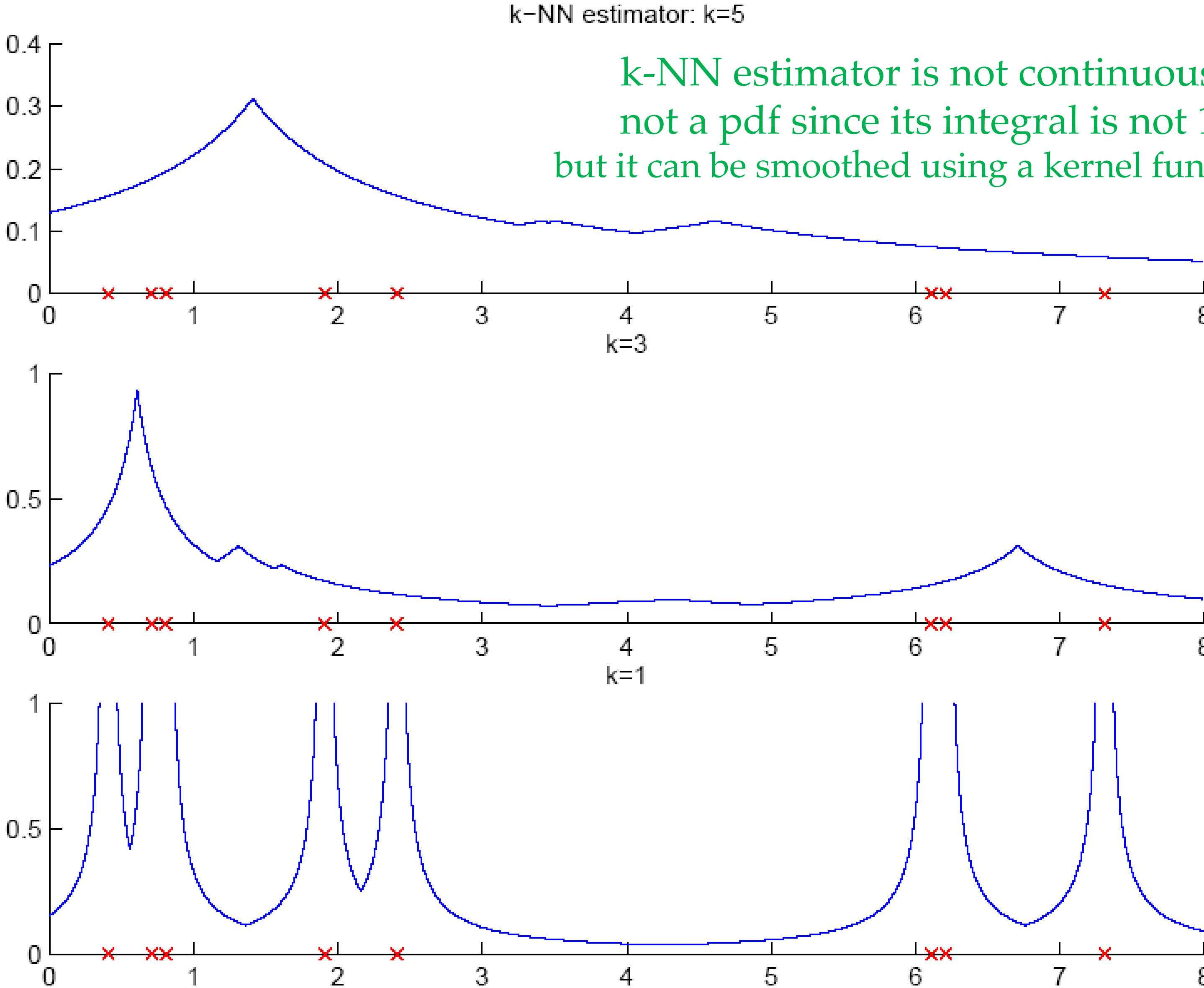
k-Nearest Neighbor Estimator

- Instead of fixing bin width h and counting the number of instances, fix the instances (neighbors) k and check bin width

$$\hat{p}(x) = \frac{k}{2Nd_k(x)}$$

$d_k(x)$, distance to kth closest instance to x

this is like a naïve estimator with $h = d_k(x)$



k-NN estimator is not continuous

not a pdf since its integral is not 1

but it can be smoothed using a kernel function

where density is high, bins are small and so $\hat{p}(x)$ is high

where density is low, bins are large and so $\hat{p}(x)$ is low

Multivariate Data (d dimensions)

- Kernel density estimator

$$\hat{p}(\mathbf{x}) = \frac{1}{Nh^d} \sum_{t=1}^{N} K\left(\frac{\mathbf{x} - \mathbf{x}^t}{h} \right)$$

Multivariate Gaussian kernel

spheric

$$K(\mathbf{u}) = \left(\frac{1}{\sqrt{2\pi}} \right)^d \exp\left[-\frac{\|\mathbf{u}\|^2}{2} \right]$$

Euclidean distance

inputs should be normalized to have the same variance

ellipsoid

$$K(\mathbf{u}) = \frac{1}{(2\pi)^{d/2} |\mathbf{S}|^{1/2}} \exp\left[-\frac{1}{2} \mathbf{u}^T \mathbf{S}^{-1} \mathbf{u} \right]$$

Mahalanobis distance

Nonparametric Classification

- Estimate $p(x|C_i)$ and use Bayes' rule
- Kernel estimator

$$\hat{p}(\mathbf{x}|C_i) = \frac{1}{N_i h^d} \sum_{t=1}^{N} K\left(\frac{\mathbf{x}-\mathbf{x}^t}{h}\right) r_i^t \quad \hat{P}(C_i) = \frac{N_i}{N}$$

$$g_i(\mathbf{x}) = \hat{p}(\mathbf{x}|C_i)\hat{P}(C_i) = \frac{1}{Nh^d} \sum_{t=1}^{N} K\left(\frac{\mathbf{x}-\mathbf{x}^t}{h}\right) r_i^t$$

- *particular case:* k-NN estimator

k_i : # of k-nn in class C_i
$V^k(\mathbf{x})$: volume of hypersphere centered at x with radius $||x-x_{(k)}||$

$$\hat{p}(\mathbf{x}|C_i) = \frac{k_i}{N_i V^k(\mathbf{x})} \quad \text{then } \hat{P}(C_i|\mathbf{x}) = \frac{\hat{p}(\mathbf{x}|C_i)\hat{P}(C_i)}{\hat{p}(\mathbf{x})} = \frac{k_i}{k}$$

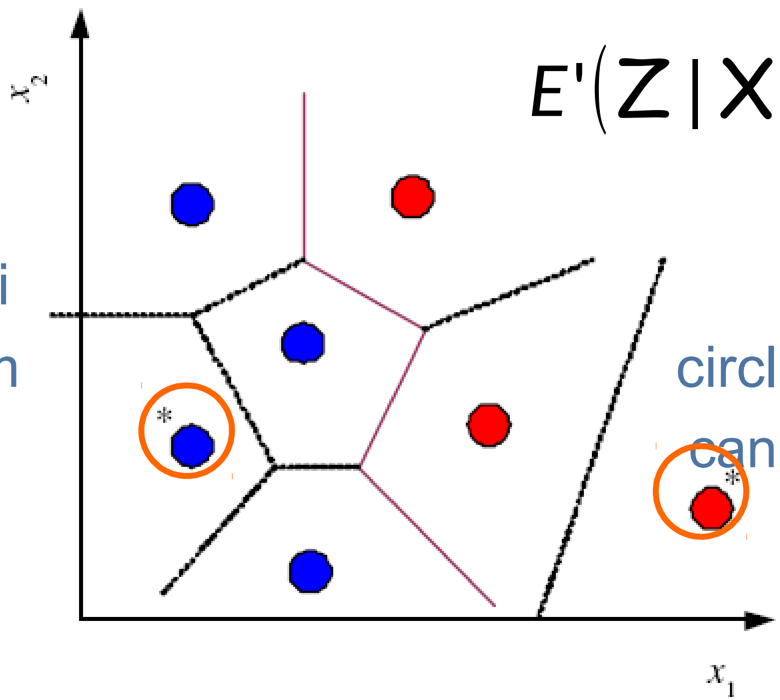
assigns x to the class having more examples among the k-NN of x

Condensed Nearest Neighbor

- Time/space complexity of k-NN is O (N)
- Find a subset Z of X that is small and is accurate in classifying X (Hart, 1968)

$$E'(Z|X) = E(X|Z) + \lambda|Z|$$

Voronoi diagram



circled data points can be discarded

Condensed Nearest Neighbor

- Incremental algorithm: Add instance if needed

$\mathcal{Z} \leftarrow \emptyset$

Repeat

For all $\boldsymbol{x} \in \mathcal{X}$ (in random order)

Find $\boldsymbol{x}' \in \mathcal{Z}$ s.t. $\|\boldsymbol{x} - \boldsymbol{x}'\| = \min_{\boldsymbol{x}^j \in \mathcal{Z}} \|\boldsymbol{x} - \boldsymbol{x}^j\|$

If class($\boldsymbol{x}$)$\neq$class($\boldsymbol{x}'$) add $\boldsymbol{x}$ to $\mathcal{Z}$

Until $\mathcal{Z}$ does not change

Distance-based Classification

- Find a distance function $D(\boldsymbol{x}^r, \boldsymbol{x}^s)$ such that

  if $\boldsymbol{x}^r$ and $\boldsymbol{x}^s$ belong to the same class, distance is small and if they belong to different classes, distance is large
- Assume a parametric model and learn its parameters using data, e.g.,

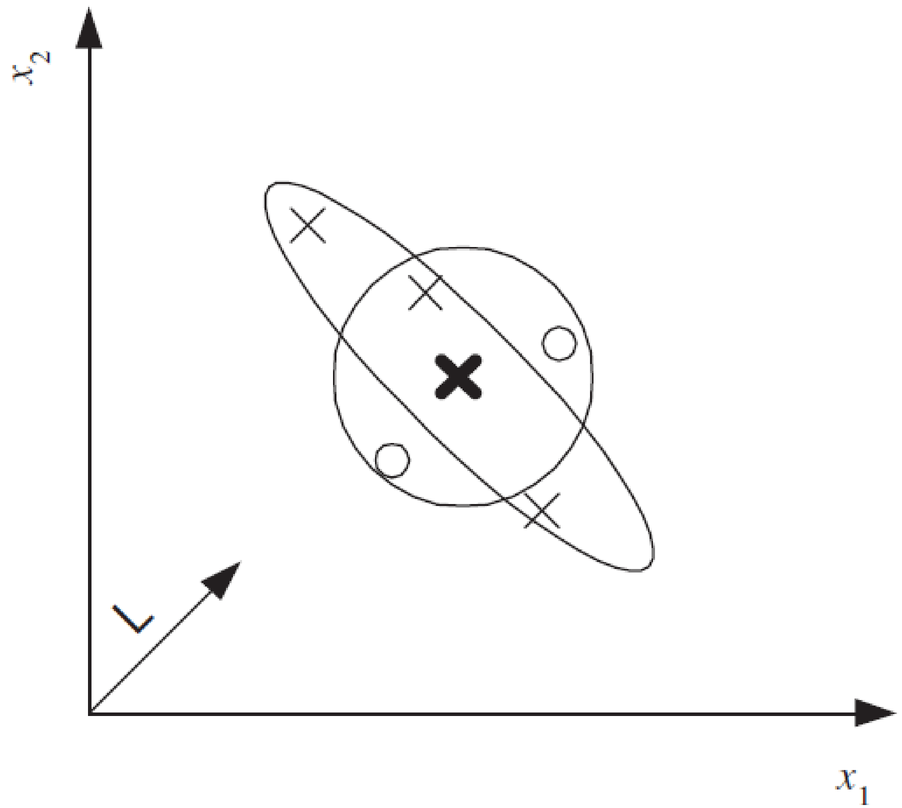
$$\mathcal{D}(\mathbf{x}, \mathbf{x}^t | \mathbf{M}) = (\mathbf{x} - \mathbf{x}^t)^T \mathbf{M} (\mathbf{x} - \mathbf{x}^t)$$

Learning a Distance Function

- The three-way relationship between distances, dimensionality reduction, and feature extraction.
- $\mathbf{M}=\mathbf{L}^T\mathbf{L}$ is dxd and $\mathbf{L}$ is kxd

$$\begin{aligned}
\mathcal{D}(\mathbf{x},\mathbf{x}^t|\mathbf{M}) &= (\mathbf{x}-\mathbf{x}^t)^T\mathbf{M}(\mathbf{x}-\mathbf{x}^t) = (\mathbf{x}-\mathbf{x}^t)^T\mathbf{L}^T\mathbf{L}(\mathbf{x}-\mathbf{x}^t) \\
&= (\mathbf{L}(\mathbf{x}-\mathbf{x}^t))^T(\mathbf{L}(\mathbf{x}-\mathbf{x}^t)) = (\mathbf{L}\mathbf{x}-\mathbf{L}\mathbf{x}^t)^T(\mathbf{L}\mathbf{x}-\mathbf{L}\mathbf{x}^t)) \\
&= (\mathbf{z}-\mathbf{z}^t)^T(\mathbf{z}-\mathbf{z}^t) = \|\mathbf{z}-\mathbf{z}^t\|^2
\end{aligned}$$

- Similarity-based representation using similarity scores
- Large-margin nearest neighbor (chapter 13)



Euclidean distance (circle) is not suitable,
Mahalanobis distance using an **M** (ellipse) is suitable.
After the data is projected along **L**, Euclidean distance can be used

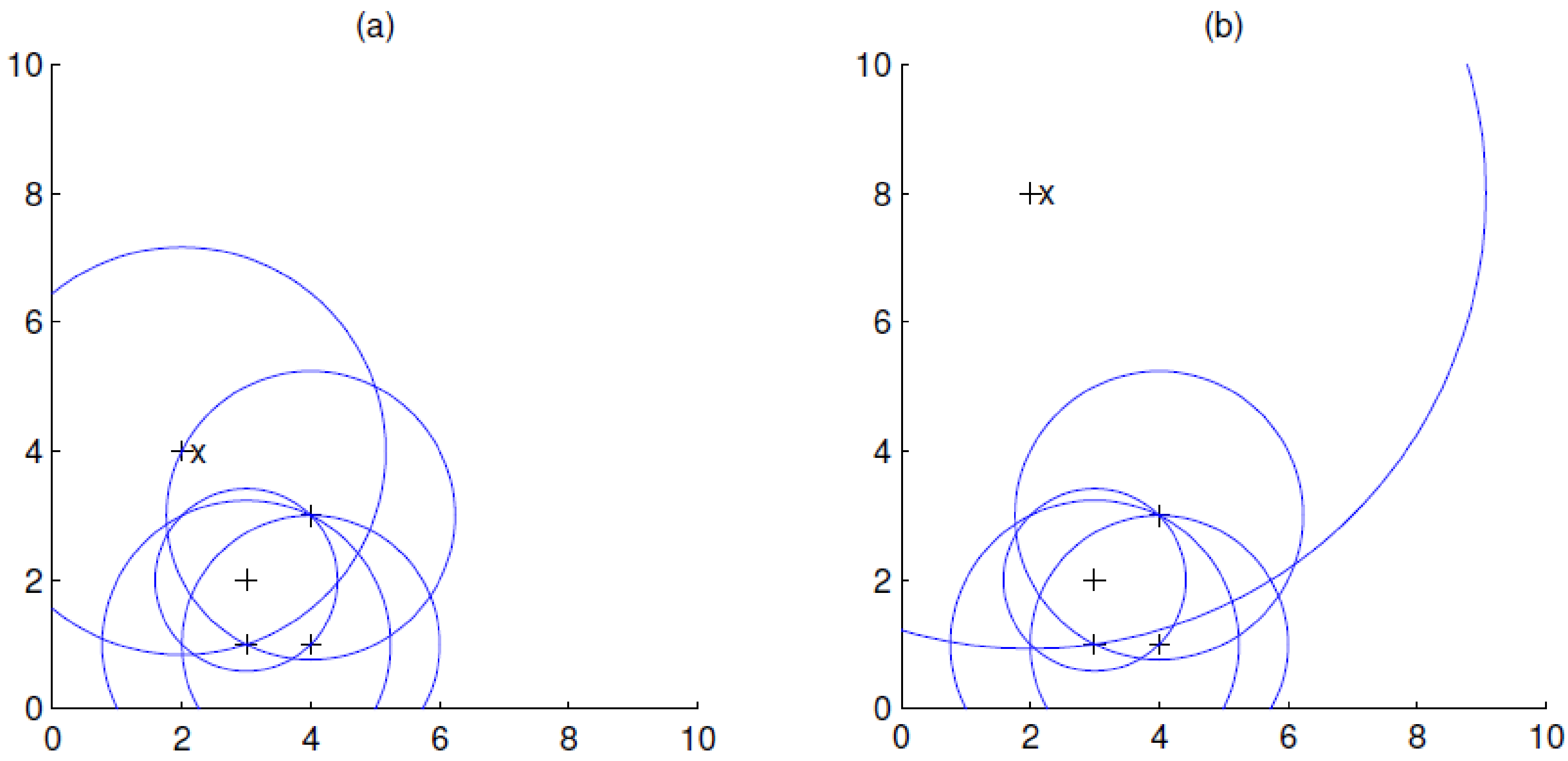
Outlier Detection

- Find outlier/novelty points
- Not a two-class problem because outliers are very few, of many types, and seldom labeled
- Instead, one-class classification problem: Find instances that have low probability
- In nonparametric case: Find instances far away from other instances

Local Outlier Factor

$$\mathrm{LOF}(\boldsymbol{x}) = \frac{d_k(\boldsymbol{x})}{\sum_{\boldsymbol{s}\in\mathcal{N}(\boldsymbol{x})} d_k(\boldsymbol{s}) / |\mathcal{N}(\boldsymbol{x})|}$$

the larger LOF(x), the most likely x is an outlier



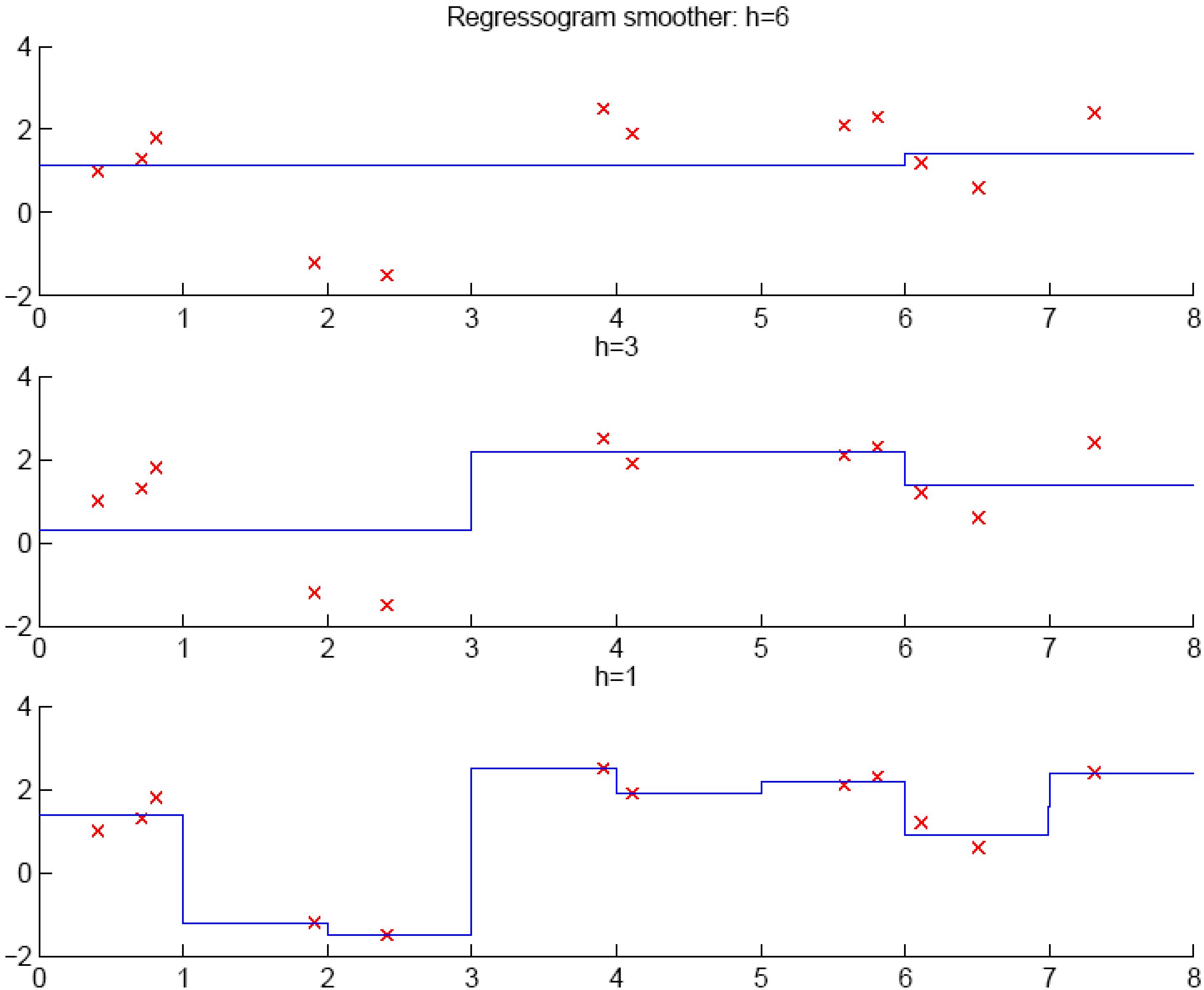
Nonparametric Regression

- Aka smoothing models
- Regressogram

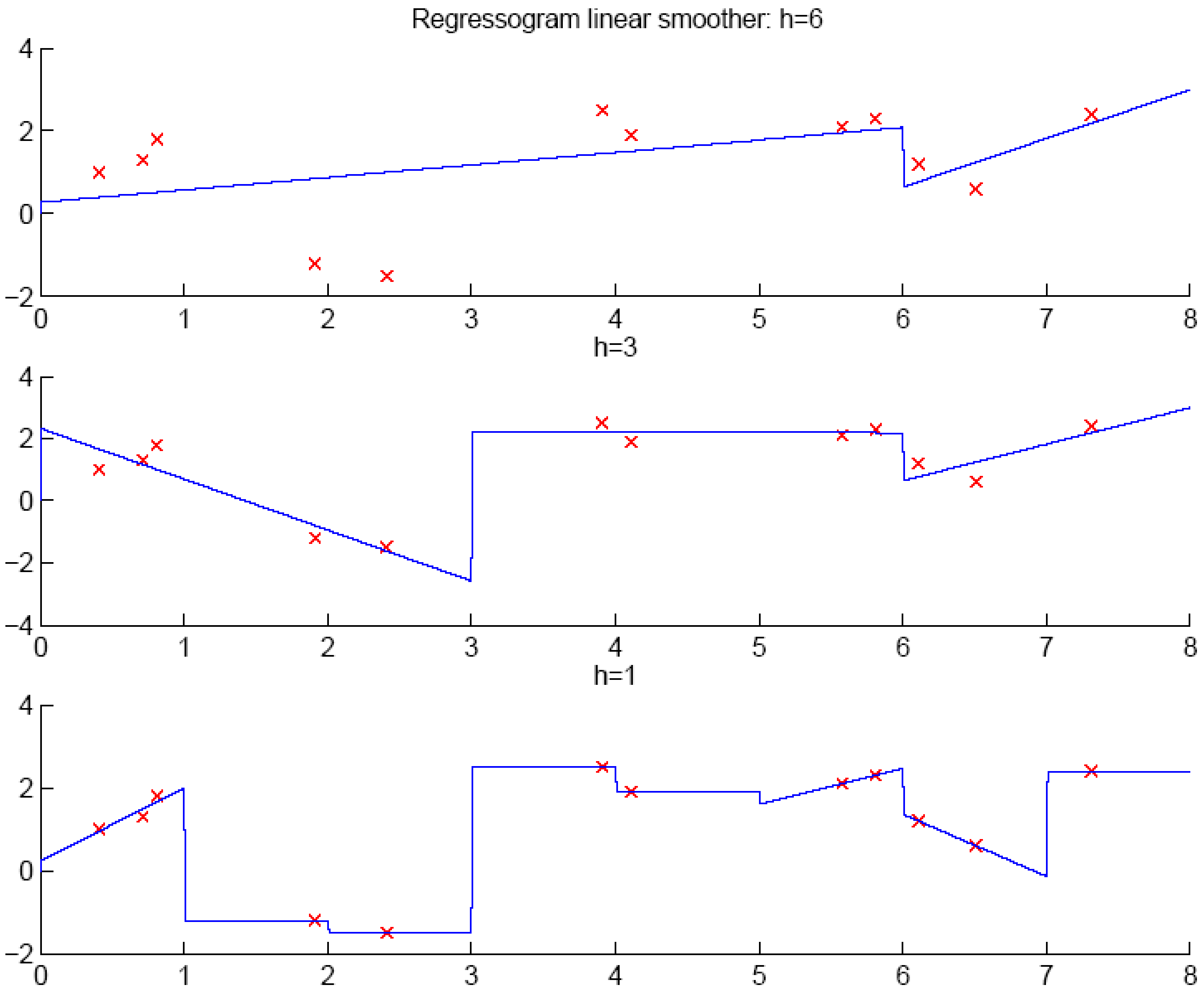
$$\hat{g}(x) = \frac{\sum_{t=1}^{N} b(x, x^t)\, r^t}{\sum_{t=1}^{N} b(x, x^t)}$$

where

$$b(x, x^t) = \begin{cases} 1 & \text{if } x^t \text{ is in the same bin with } x \\ 0 & \text{otherwise} \end{cases}$$



Regressogram smoother: h=6
h=3
h=1
4
2
0
−2
0
1
2
3
4
5
6
7
8


Regressogram linear smoother: h=6
h=3
h=1
4
2
0
−2
−4
0
1
2
3
4
5
6
7
8

Running Mean/Kernel Smoother

- Running mean smoother

$$\hat{g}(x) = \frac{\sum_{t=1}^{N} w\left(\frac{x - x^t}{h}\right) r^t}{\sum_{t=1}^{N} w\left(\frac{x - x^t}{h}\right)}$$

where

$$w(u) = \begin{cases} 1 & \text{if } |u| < 1 \\ 0 & \text{otherwise} \end{cases}$$

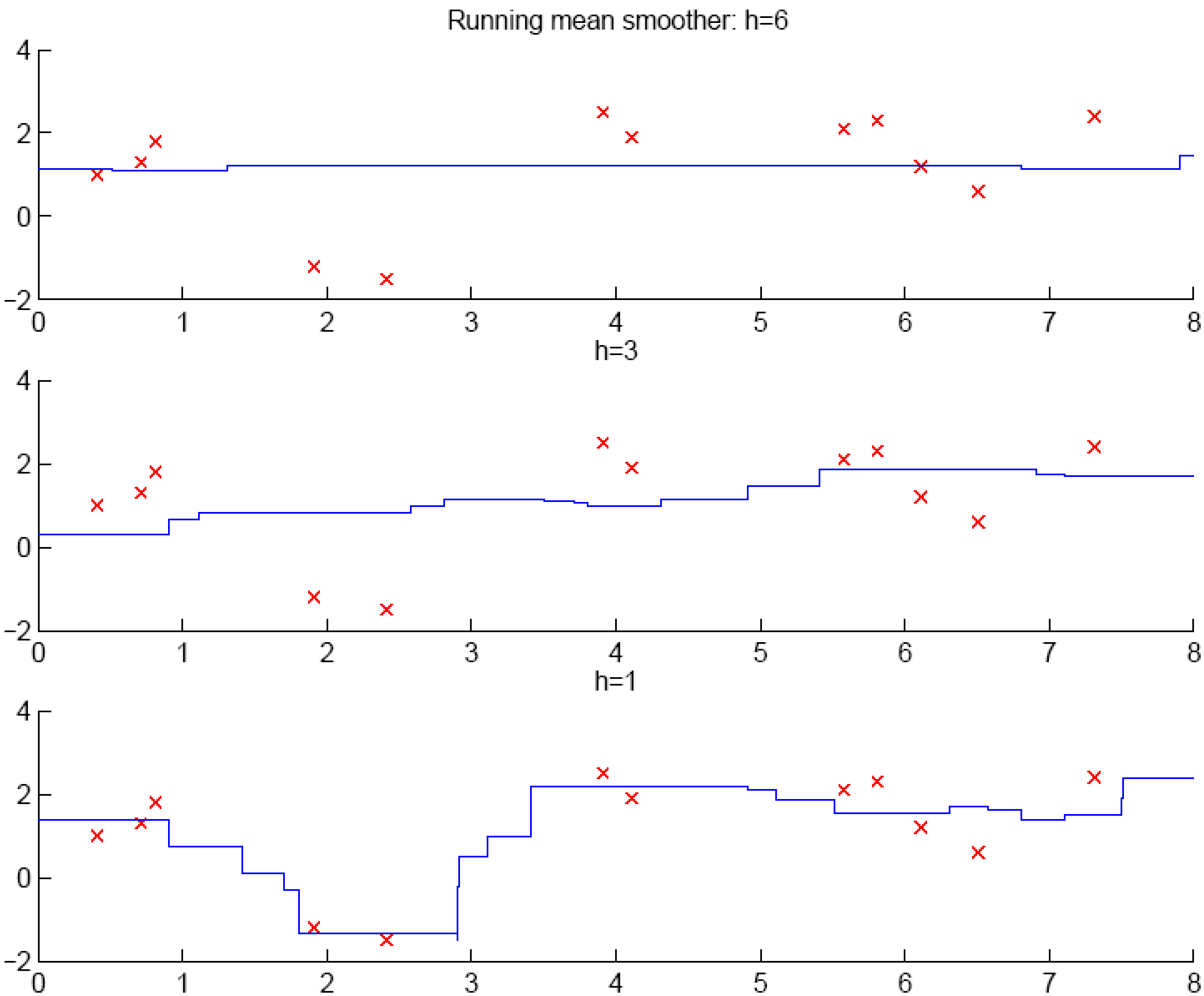
- Running line smoother

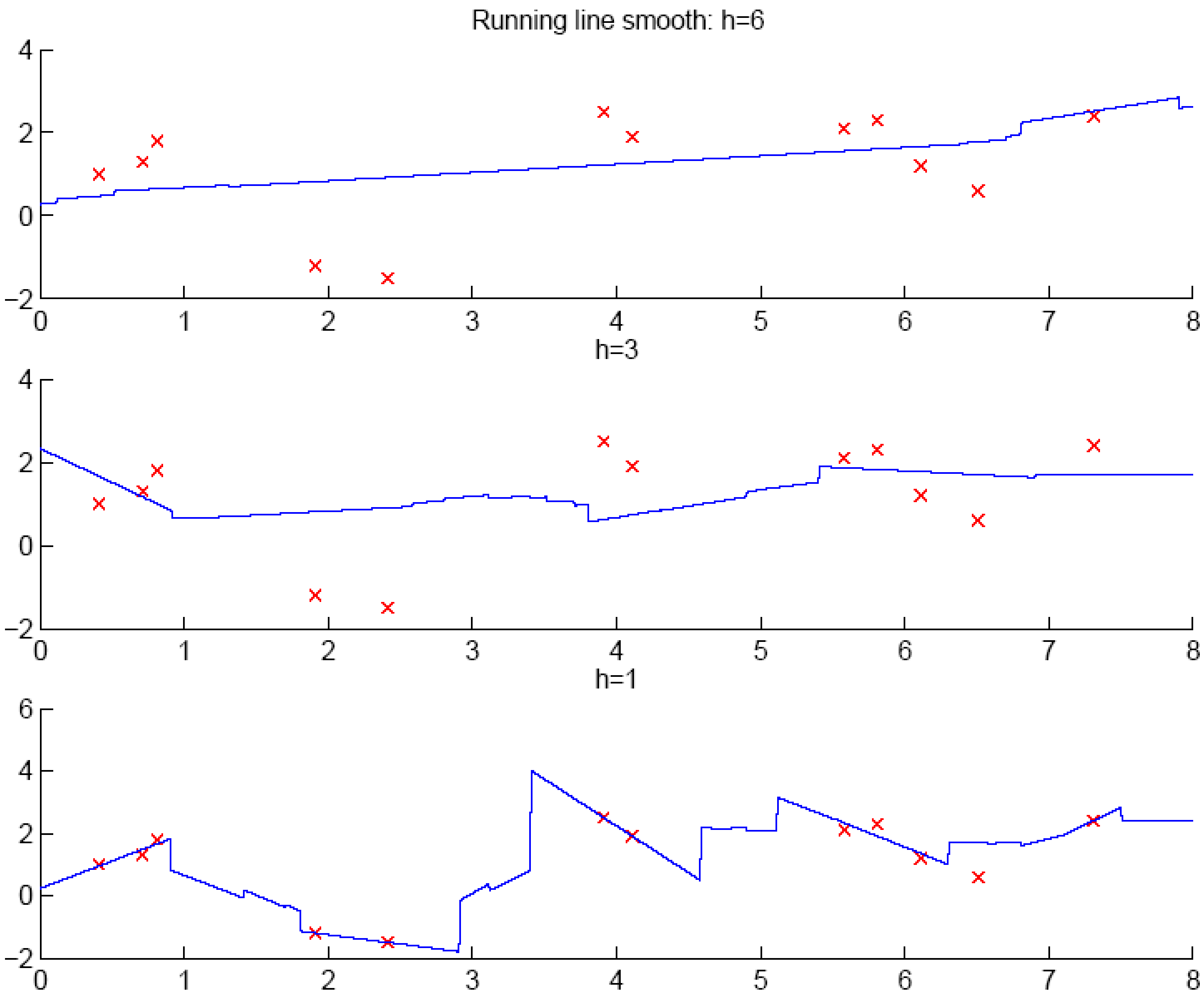
- Kernel smoother

$$\hat{g}(x) = \frac{\sum_{t=1}^{N} K\left(\frac{x - x^t}{h}\right) r^t}{\sum_{t=1}^{N} K\left(\frac{x - x^t}{h}\right)}$$

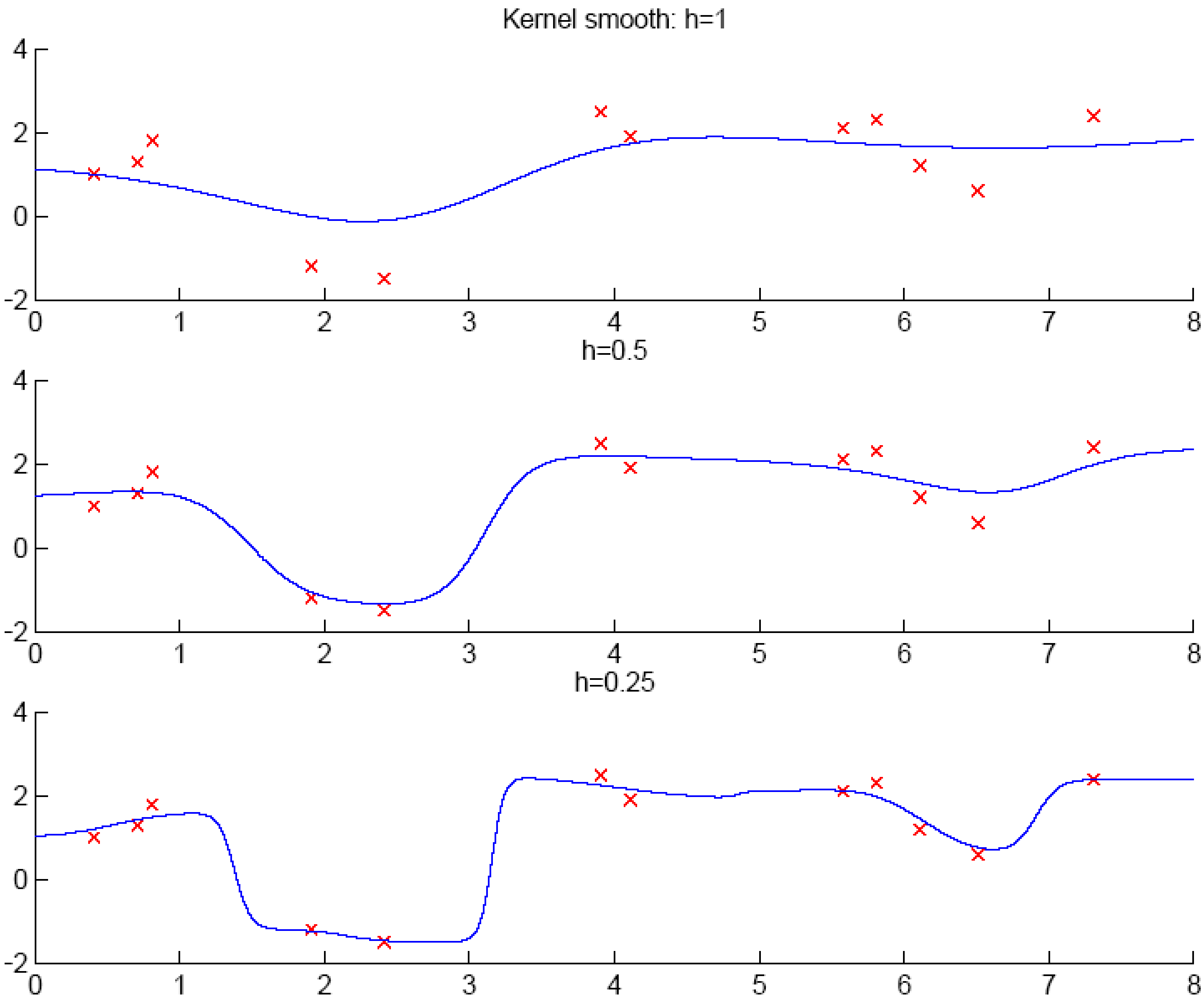
where $K(\ )$ is Gaussian

- Additive models (Hastie and Tibshirani, 1990)


Running mean smoother: h=6
h=3
h=1
4
2
0
−2
0
1
2
3
4
5
6
7
8

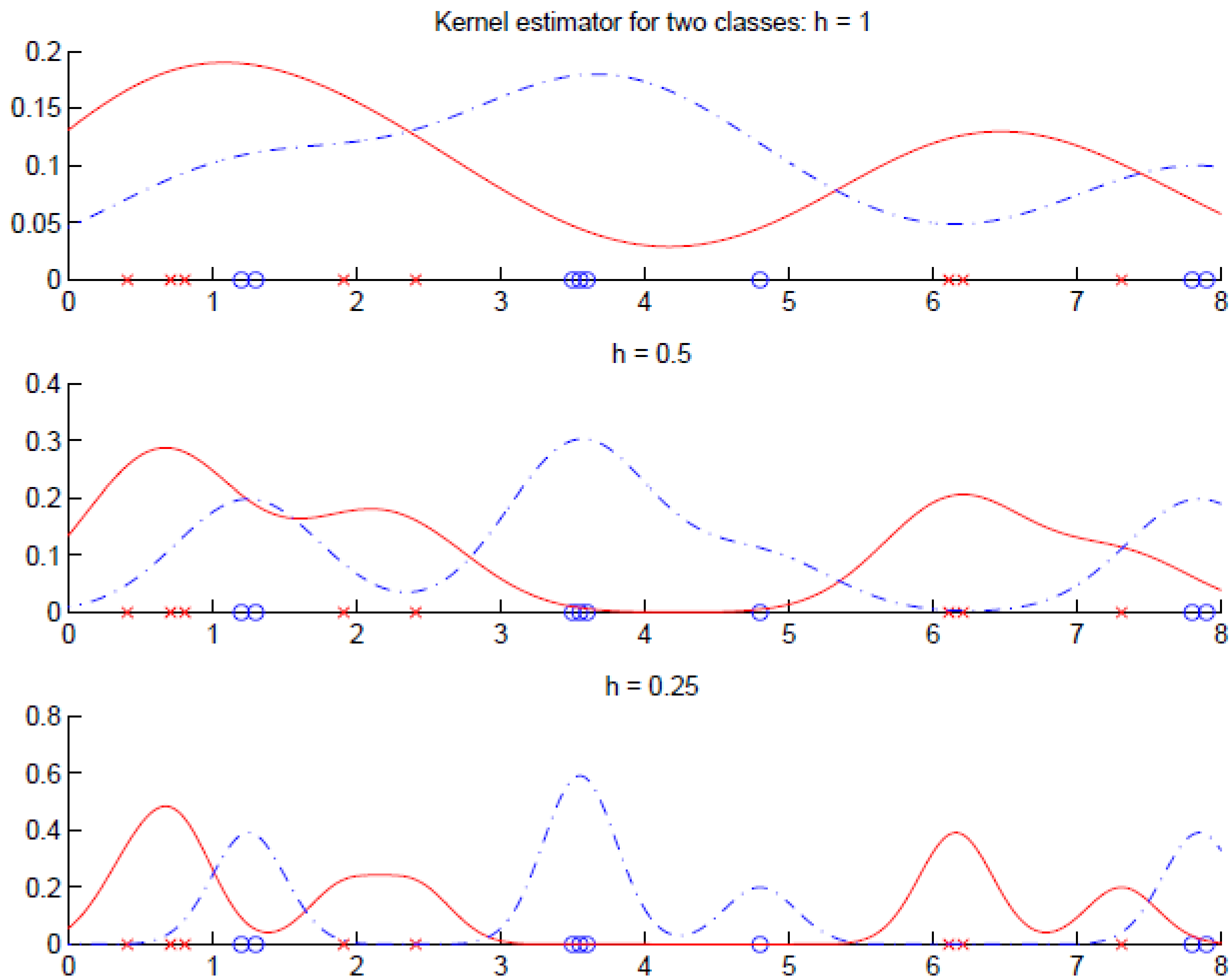


Running line smooth: h=6
4
2
0
−2
0
1
2
3
4
5
6
7
8
h=3
4
2
0
−2
0
1
2
3
4
5
6
7
8
h=1
6
4
2
0
−2
0
1
2
3
4
5
6
7
8


Kernel smooth: h=1
h=0.5
h=0.25
4
2
0
-2
0
1
2
3
4
5
6
7
8

How to Choose k or h ?

- When k or h is small, single instances matter; bias is small, variance is large (undersmoothing): High complexity
- As k or h increases, we average over more instances and variance decreases but bias increases (oversmoothing): Low complexity
- Cross-validation is used to finetune k or h.


Kernel estimator for two classes: h = 1
0.2
0.15
0.1
0.05
0
0 1 2 3 4 5 6 7 8
h = 0.5
0.4
0.3
0.2
0.1
0
0 1 2 3 4 5 6 7 8
h = 0.25
0.8
0.6
0.4
0.2
0
0 1 2 3 4 5 6 7 8