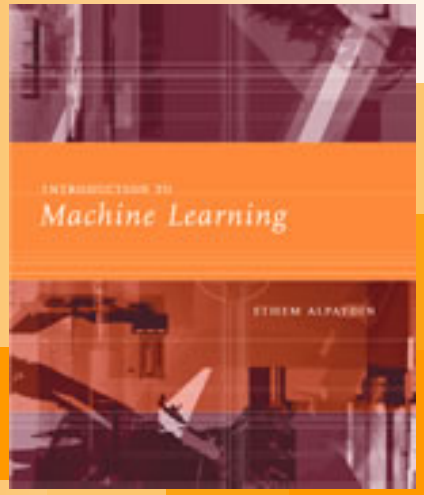

Lecture Slides for

INTRODUCTION TO

Machine Learning

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CHAPTER 8:

Nonparametric 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 $\mathcal{X}=\{x^t\}_t$ drawn iid from $p(x)$
- Divide data into bins of size h
- Histogram:

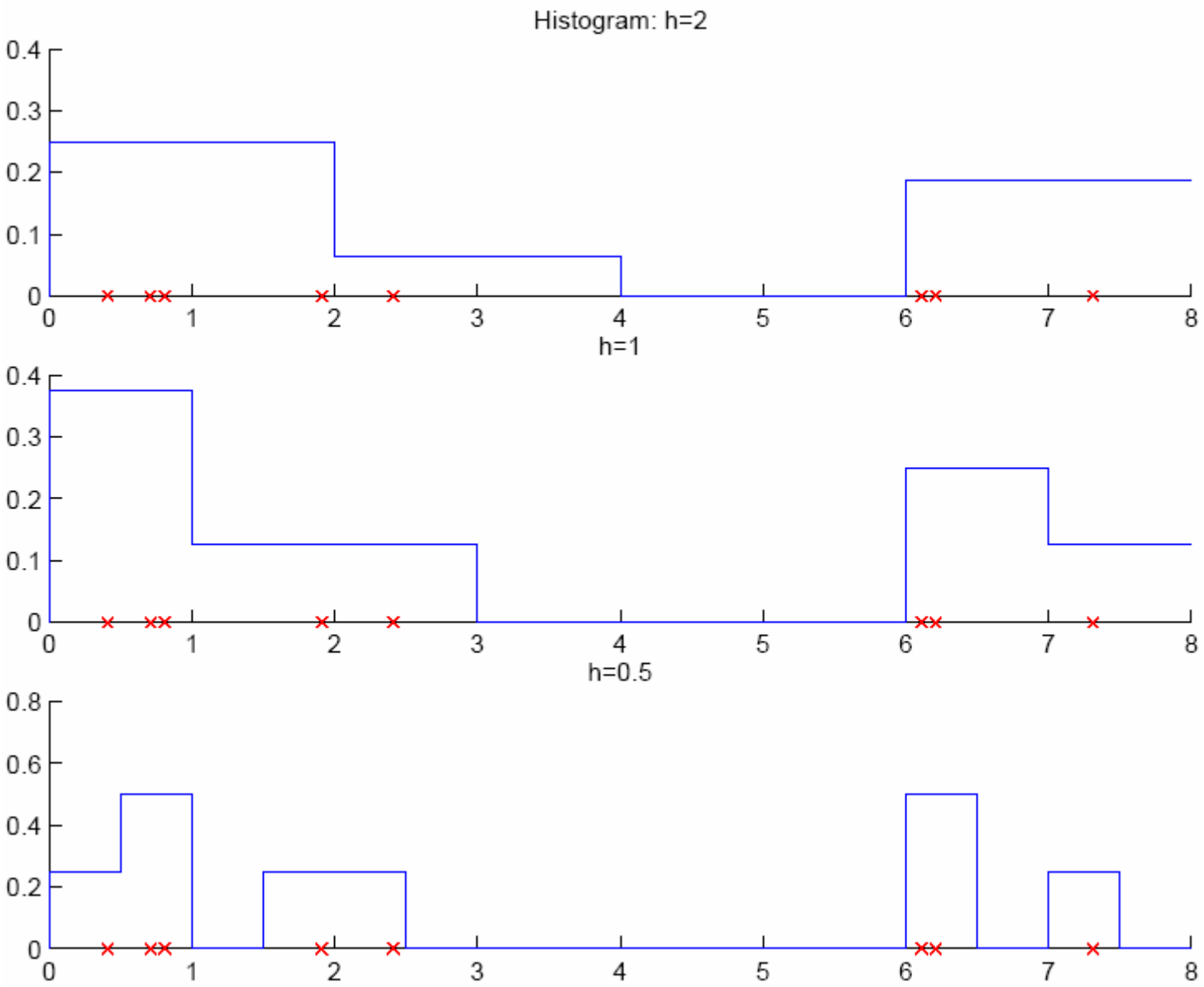
$$\hat{p}(x)=\frac{\#\left\{x^t \text{ in the same bin as } x\right\}}{Nh}$$

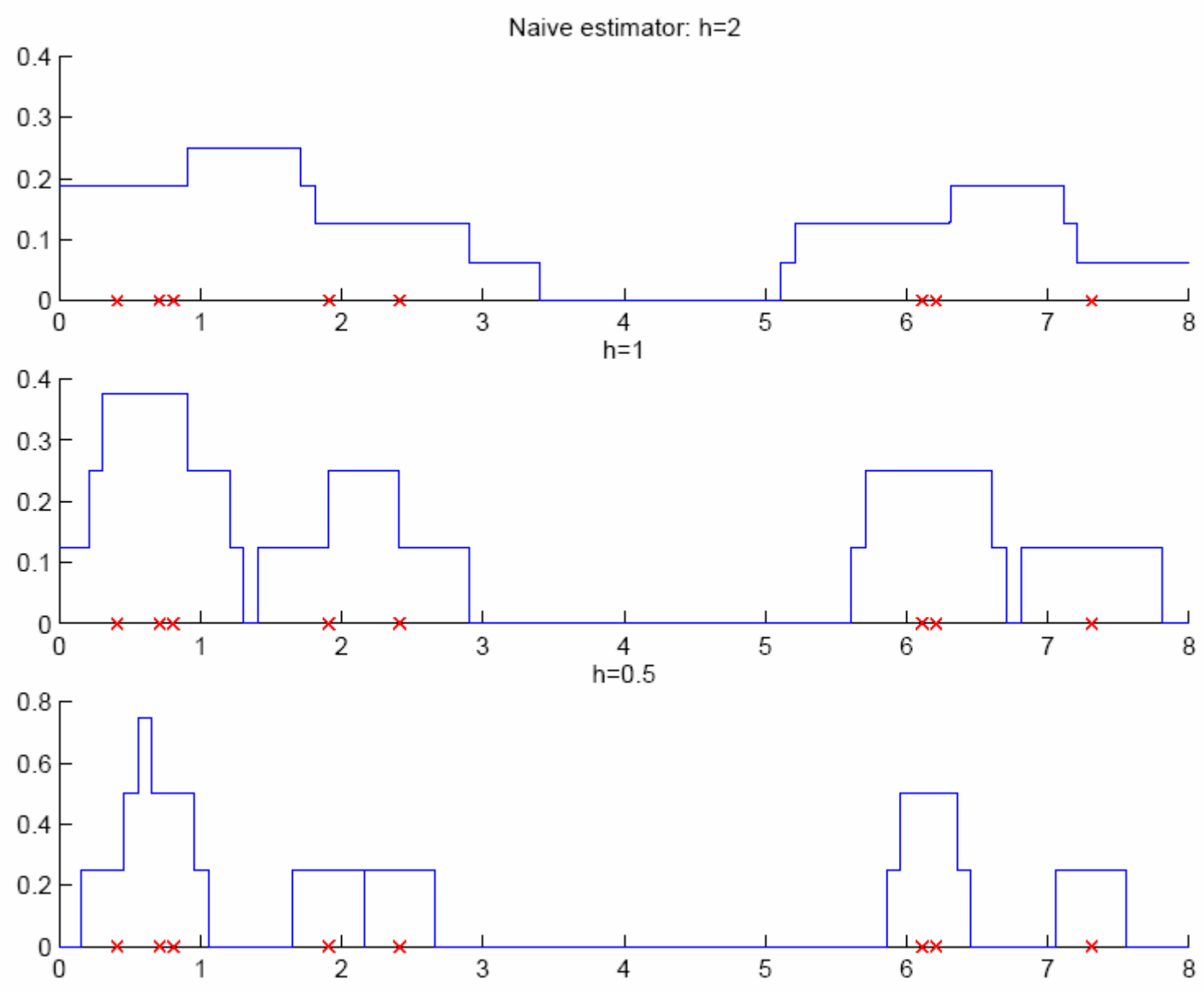
- Naive estimator:

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

or

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


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



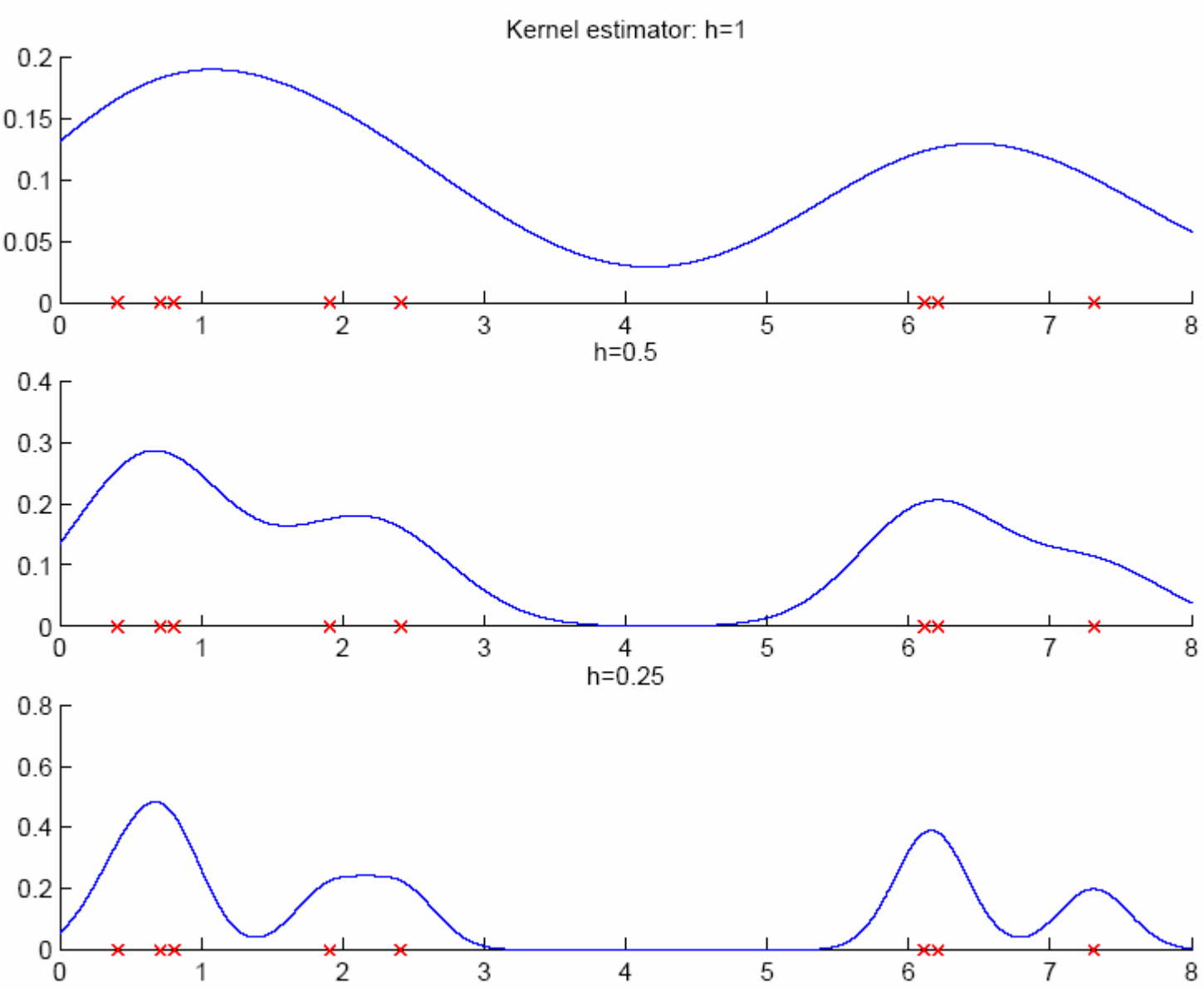
Kernel Estimator

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

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

- Kernel estimator (Parzen windows)

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

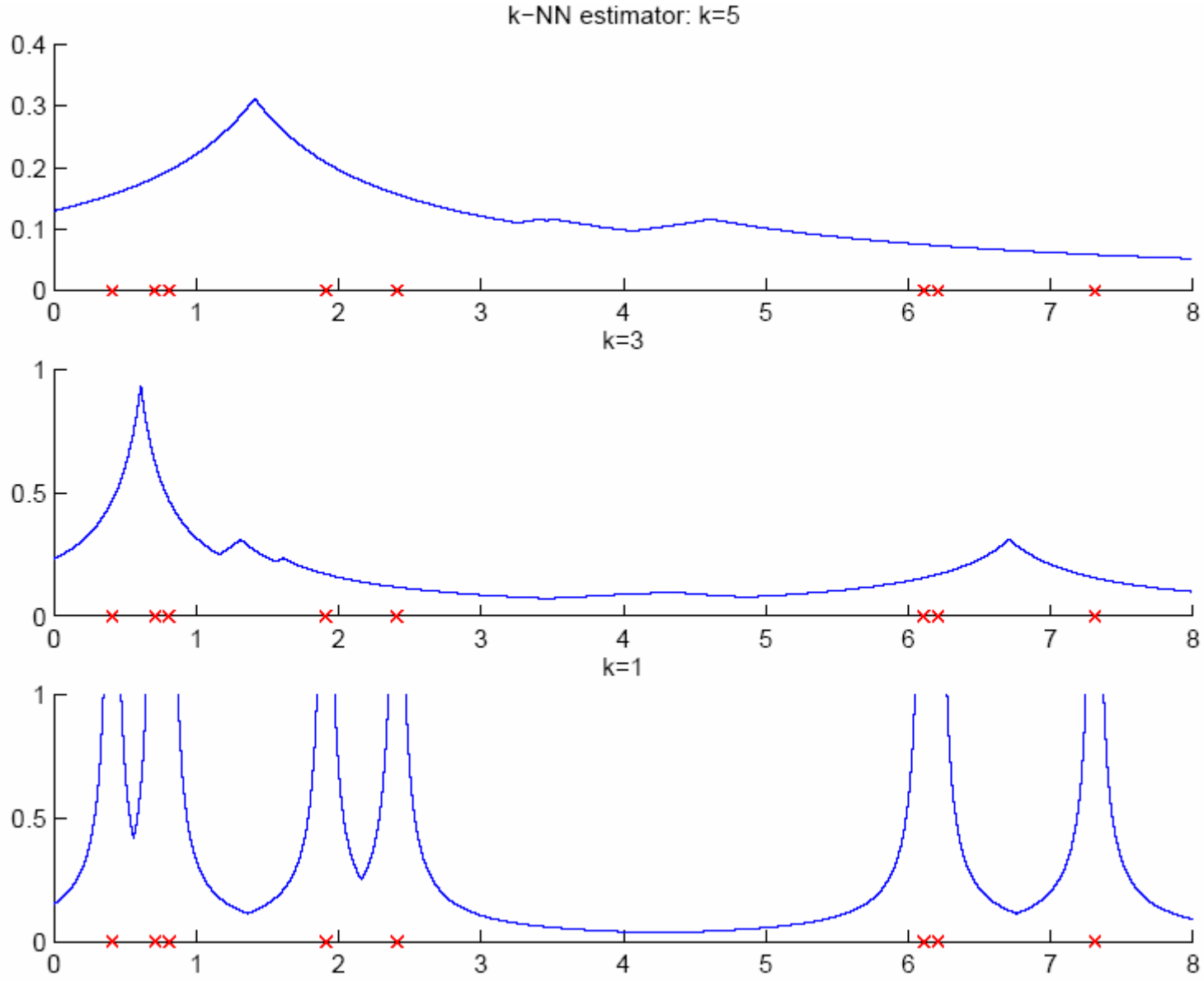

Kernel estimator: h=1
0.2
0.15
0.1
0.05
0
0 1 2 3 4 5 6 7 8
h=0.5
0.4
0.3
0.2
0.1
0
0 1 2 3 4 5 6 7 8
h=0.25
0.8
0.6
0.4
0.2
0
0 1 2 3 4 5 6 7 8

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


k−NN estimator: k=5
0.4
0.3
0.2
0.1
0
0 1 2 3 4 5 6 7 8
k=3
1
0.5
0
0 1 2 3 4 5 6 7 8
k=1
1
0.5
0
0 1 2 3 4 5 6 7 8

Multivariate Data

- Kernel density estimator

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

Multivariate Gaussian kernel

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

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

Nonparametric Classification

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

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

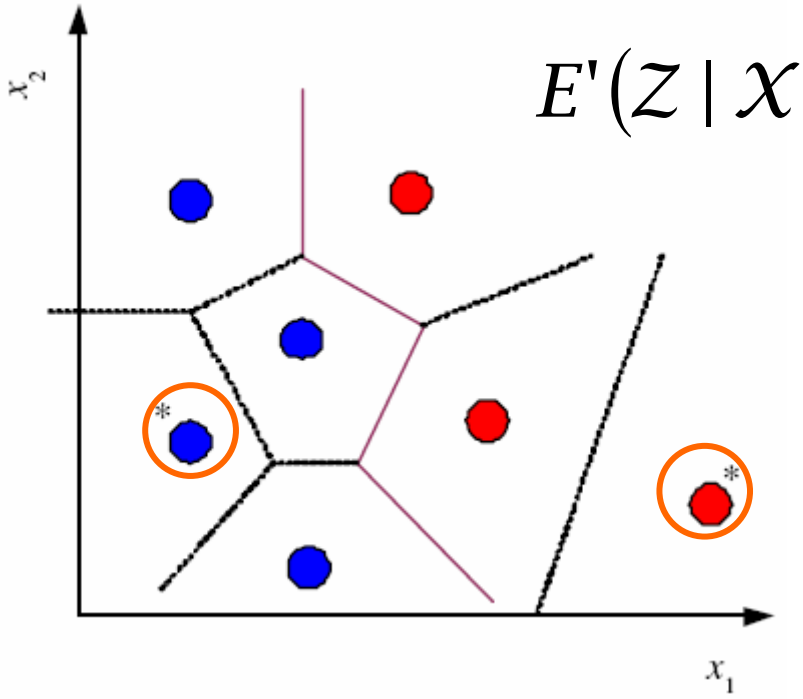
$$g_i(\mathbf{x})=\hat{p}(\mathbf{x}\mid C_i)\hat{P}(C_i)=\frac{1}{Nh^d}\sum_{t=1}^{N} K\left(\frac{\mathbf{x}-\mathbf{x}^t}{h}\right) r_i^t$$

- k-NN estimator

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

Condensed Nearest Neighbor

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



$$E'(\mathcal{Z} \mid \mathcal{X}) = E(\mathcal{X} \mid \mathcal{Z}) + \lambda|\mathcal{Z}|$$

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

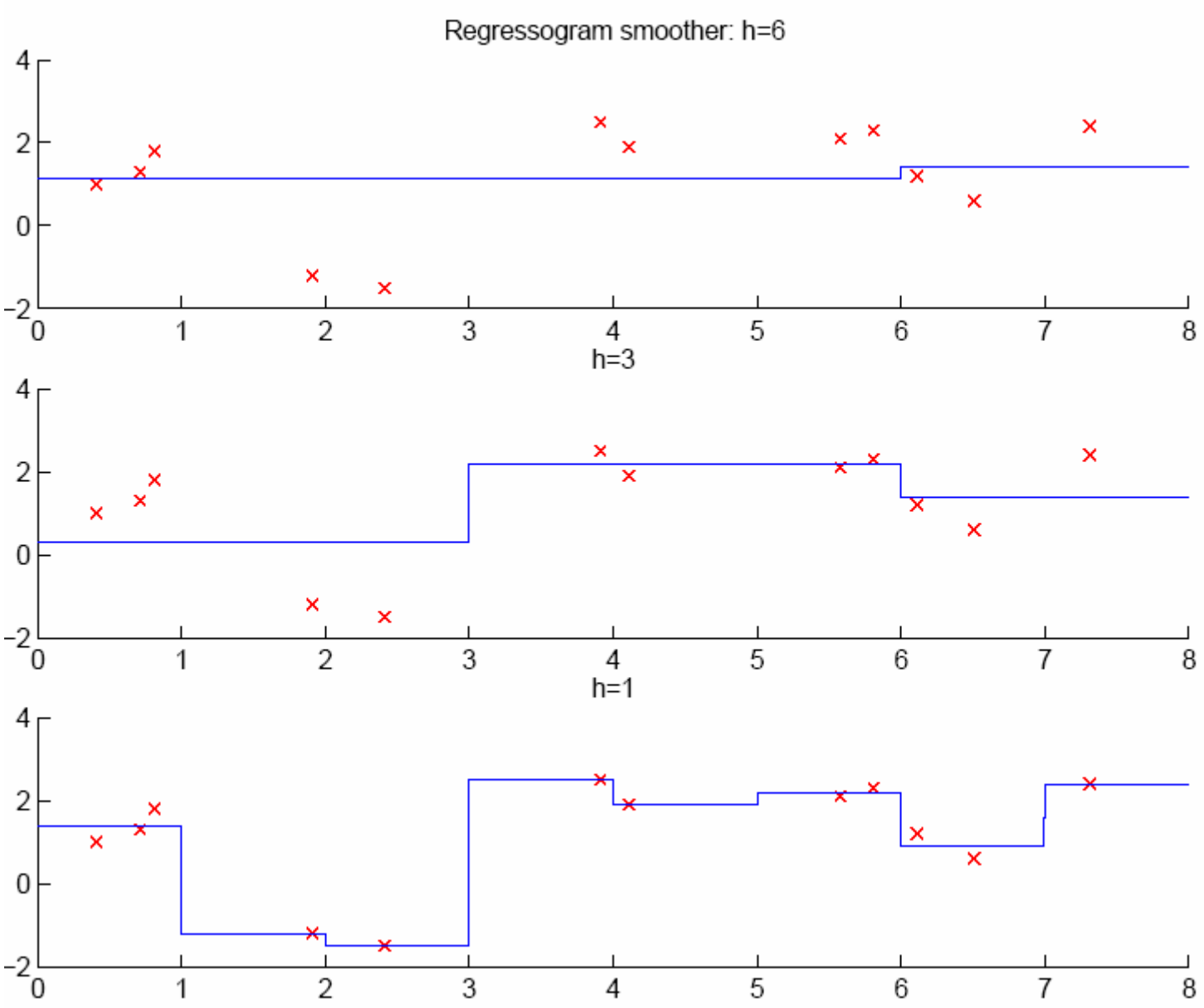
Nonparametric Regression

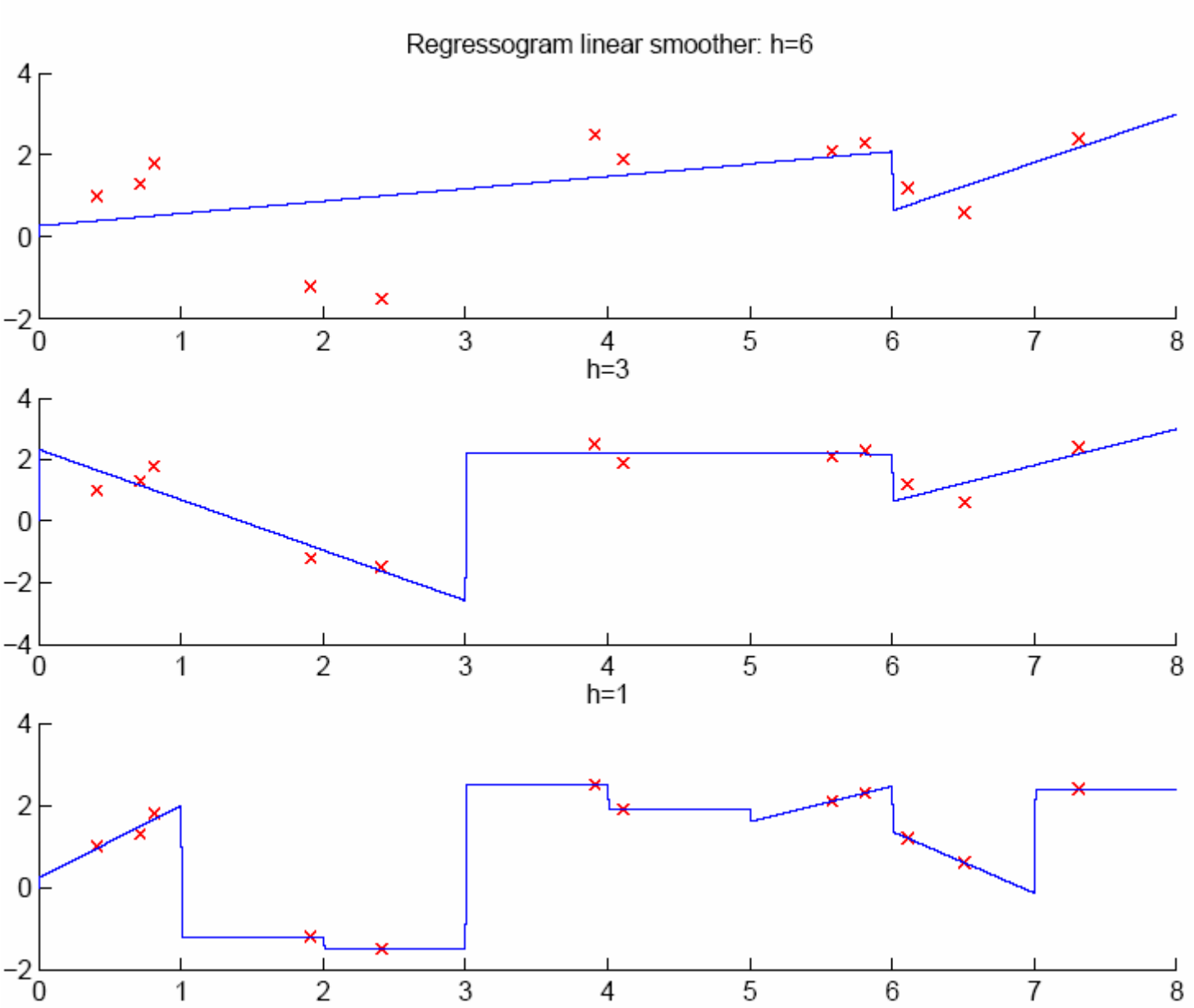
- Aka smoothing models
- Regressogram

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

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


Regressogram linear smoother: h=6
h=3
h=1

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

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

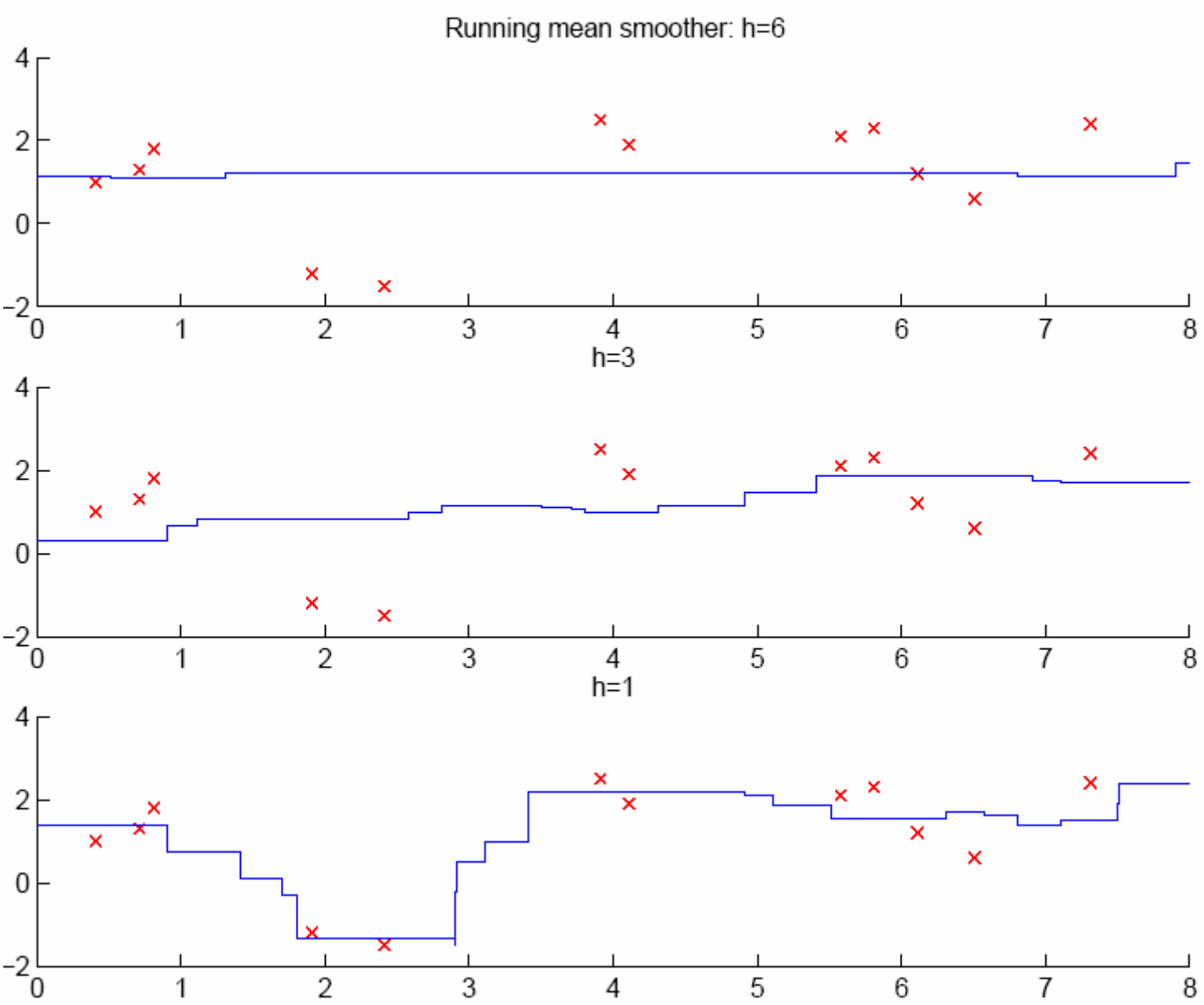
- Running line smoother

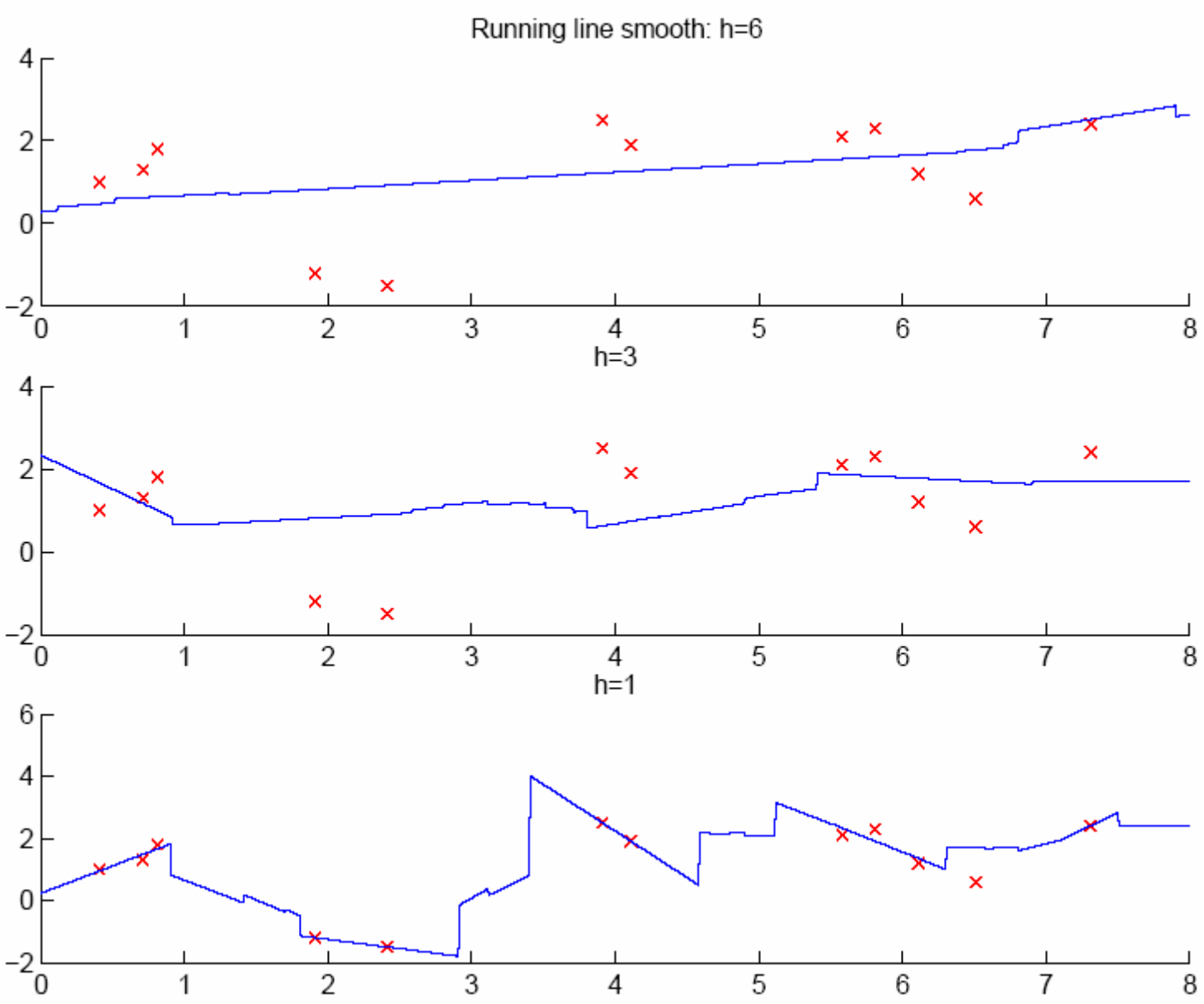
- Kernel smoother

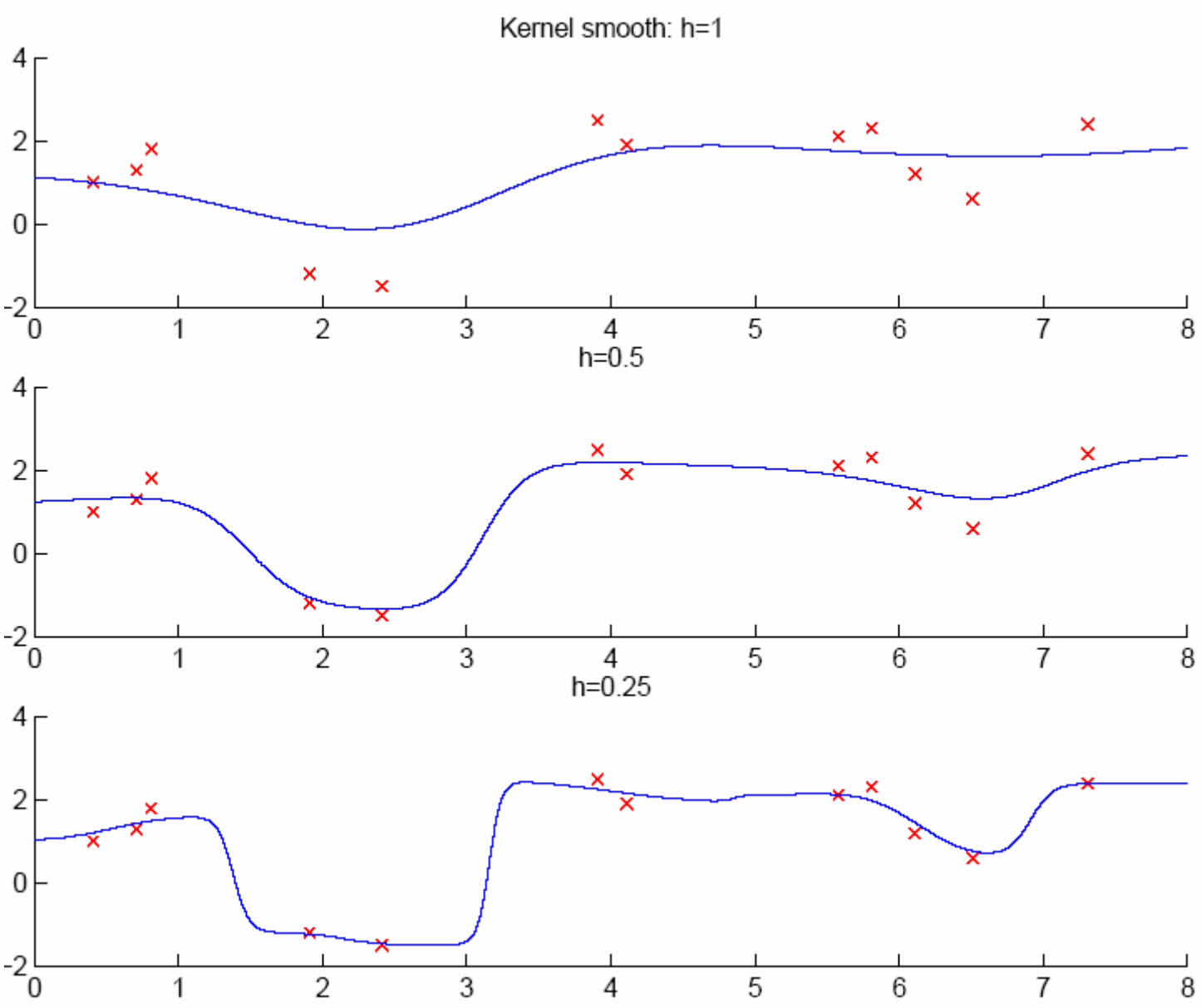
$$\hat{g}(x)=\frac{\sum_{t=1}^{N} K\left(\frac{x-x^t}{h}\right) r^t}{\sum_{t=1}^{N} K\left(\frac{x-x^t}{h}\right)}$$

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
h=3
h=1


Kernel smooth: h=1
h=0.5
h=0.25

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.