Pattern Classification

05. Density Estimation

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Recap: Gaussian Densities

- Assume a multi dimensional Gaussian density for each $P(\underline{X}|C_i)$

- Features may be independent (or conditionally independent), i.e., independent Gaussians

- Features may be dependent in other cases

Recap: Applying Bayes Rule

- One way on how to apply Bayes rule in practical situations:
  - Obtain the training set $\underline{X}(1), \underline{X}(2) \cdots \underline{X}(M)$
  - Assume a multi-dimensional Gaussian density for each class, i.e., $P(\underline{X}|C_i)$
  - To obtain the form of each density we need $\underline{\mu}_i$ and Σ_i for each class i → estimate from training set
  - Estimate the a priori probabilities $P(C_i)$ from the training set, i.e., according to the frequencies of each class
  - Using the obtained estimates, plug in Bayes rule to obtain the classification rule

Density Estimation

- In Bayes rule, the probability densities have to be estimated
- One way is to assume that they are multivariate Gaussian and estimate μ & Σ of these distributions
- Estimate the densities from data

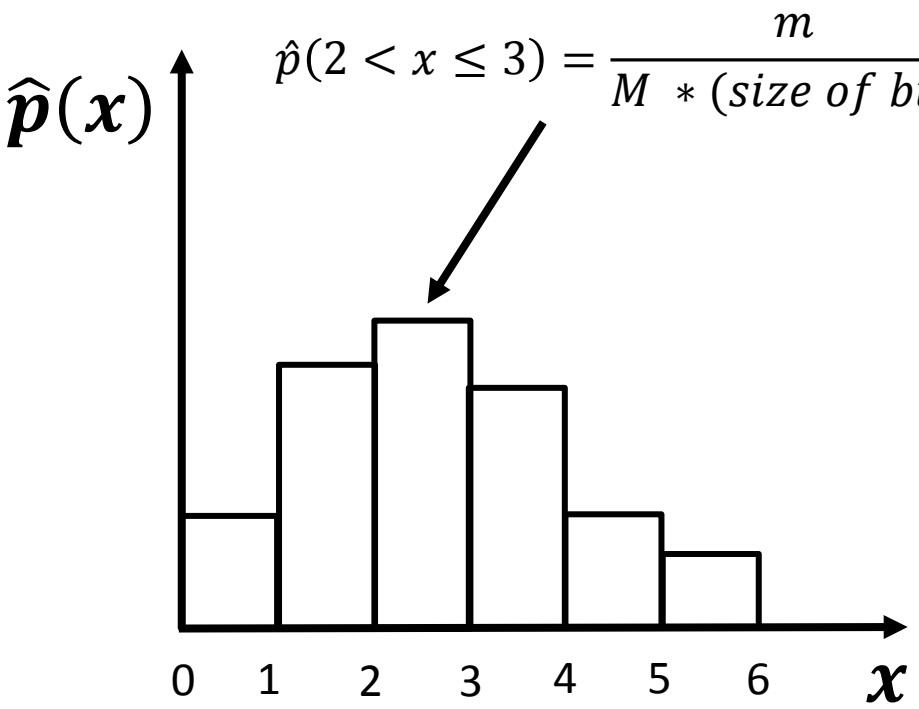
Histogram Analysis

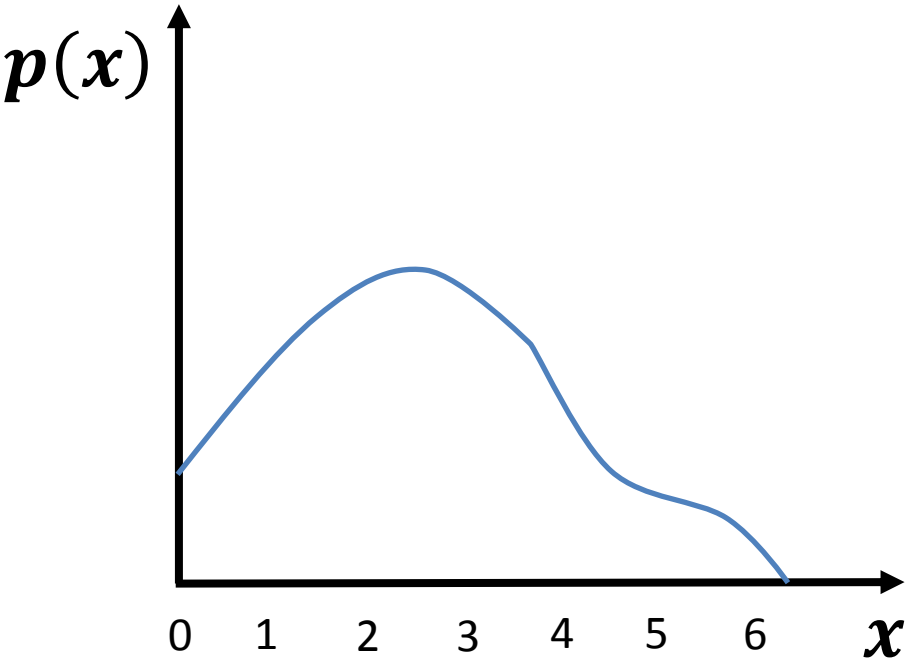
$$\hat{p}(x) = \frac{m}{M \ * (size\ of\ bin)}$$

- m is the number of data points falling within a given range, i.e., histogram bin
- M is the total number of points (that belongs to the same class)
- Size of bin: size of the histogram bin

Histogram Analysis

- Consider 1-D example:
  - m is number of data points within the given range, e.g., $2 < x \leq 3$



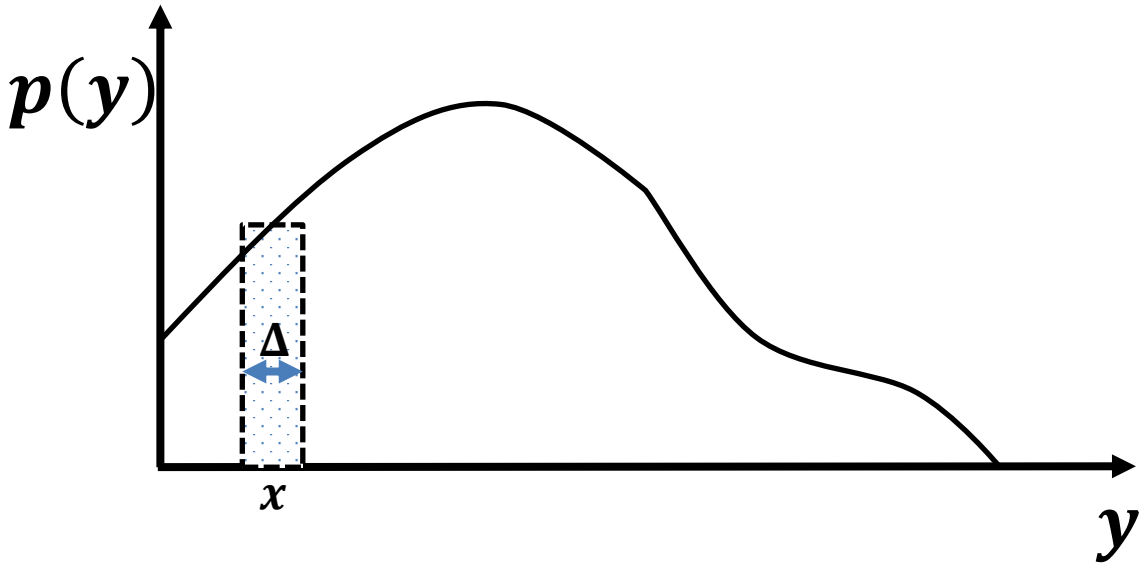


Data was originally generated from this density

Histogram Analysis

$$\int_{x-\frac{\Delta}{2}}^{x+\frac{\Delta}{2}} p(x)dx \approx \Delta \,.\, p(x)$$

- Probability (generated point $\epsilon \left[x - \frac{\Delta}{2}, x + \frac{\Delta}{2}\right]) \approx \Delta \,.\, p(x) \equiv z$



Bin size $\equiv \Delta$

Histogram Analysis

$$\int_{x-\frac{\Delta}{2}}^{x+\frac{\Delta}{2}} p(x)dx \approx \Delta \,.\, p(x)$$

- Probability (generated point $\epsilon \left[X - \frac{\Delta}{2}, \; X + \frac{\Delta}{2}\right)) \approx \Delta \,.\, p(x) \equiv z$

- Assume we draw a number M of points according to p(x) → binomial distribution

- Binomial distribution with probability z for number of points falling in BIN

Histogram Analysis

$$P(k\ points\ falling\ in\ BIN\ out\ of\ M\ points) = \binom{M}{k} z^k (1-z)^{M-k}$$

$$E(\#\ points\ in\ BIN) = M.z = M.p(x).\Delta$$

- Example: flip a coin 10 times

$$P(8\ Heads) = \binom{10}{8} p^8 (1-p)^{10-8}$$

$$E(\#\ Heads) = p.M = 0.5 * 10 = 5$$

$p \equiv probability\ of\ head$

Histogram Analysis

$$E(\#\ points\ in\ BIN) = M.z$$
$$= M.p(x).\Delta$$

- If k points fall in the histogram range then assuming:

$$k \approx M.p(x).\Delta$$

- Then, estimate of p(x) is:

$$p(x) = \frac{k}{M\Delta}$$

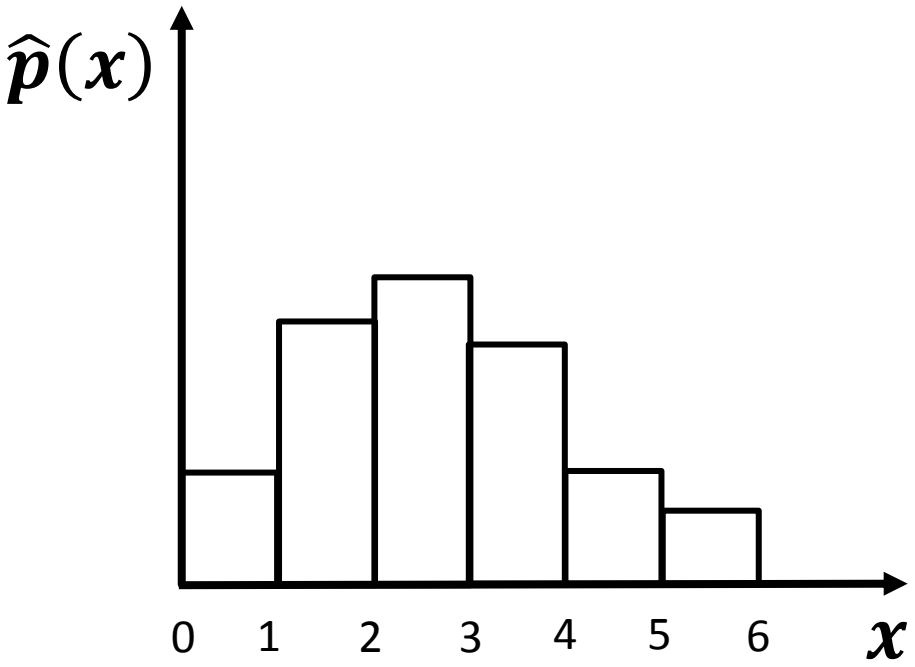
Recall:

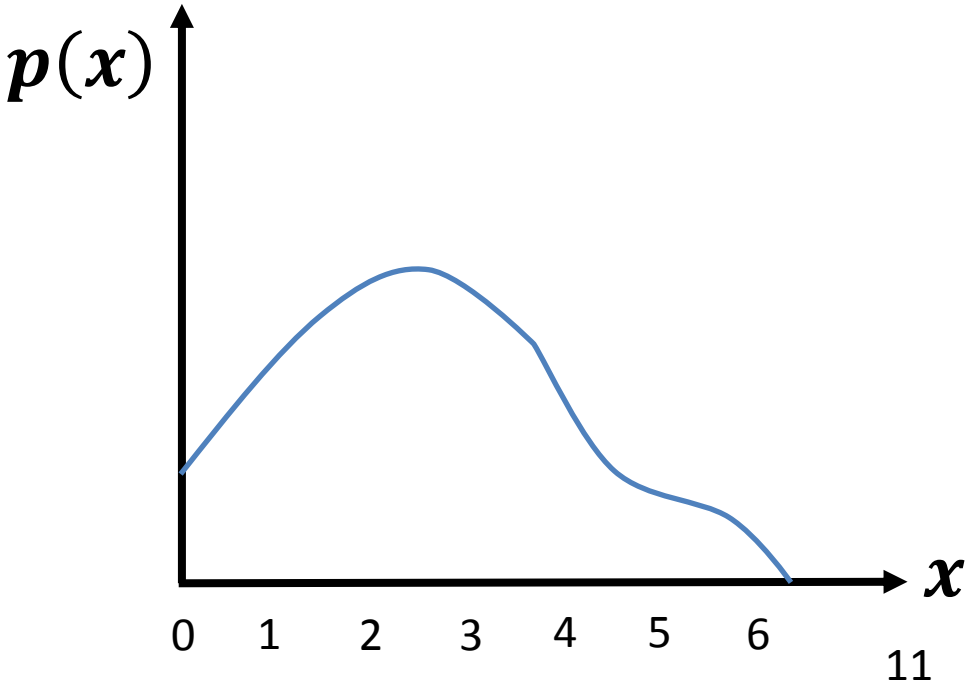
$$\hat{p}(x) = \frac{m}{M\ *(size\ of\ bin)}$$

Histogram Analysis

- Weak method of estimation

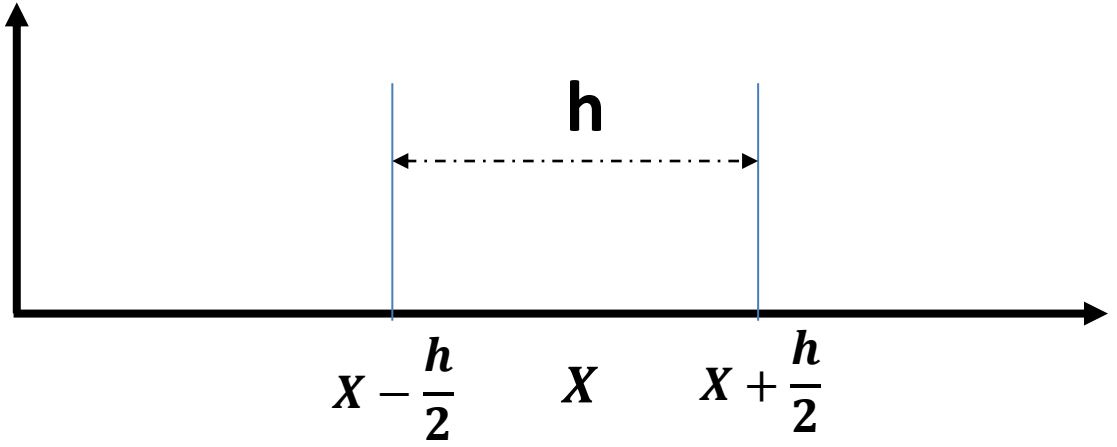
- Discontinuity of these density estimates, even though the true densities are assumed to be smooth





Naïve Estimator

- Instead of partitioning X, i.e., feature space, into a number of prespecified ranges, we perform a similar range analysis for every X



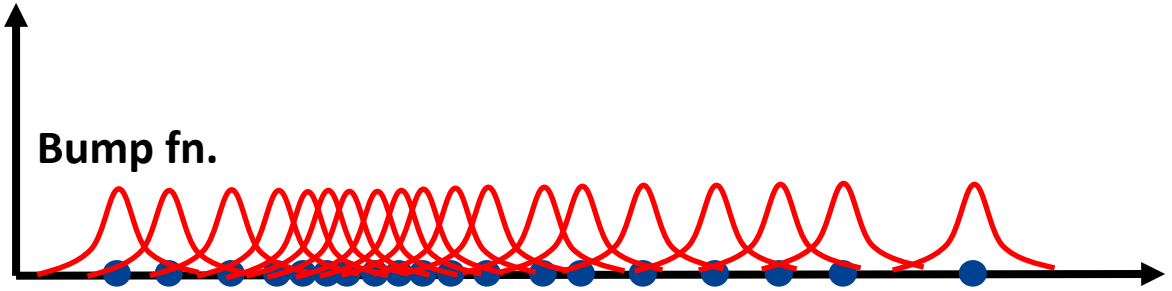
$$\hat{P}(X) = \frac{\#points\ falling\ in\ \left[X - \frac{h}{2}\ ,\ \ X + \frac{h}{2}\right)}{Mh}$$

Naïve Estimator

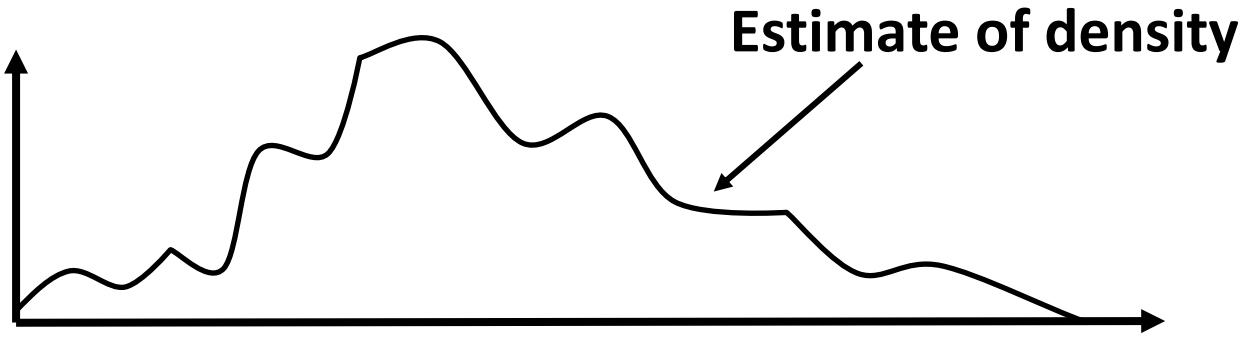
- Drawbacks:
  - Discontinuity of the density estimates
  - All data points are weighted equally regardless of their distance to the estimation point, i.e, X

Kernel Density Estimator

- a.k.a. Parzen Window Density Estimator
- Choose a bump function



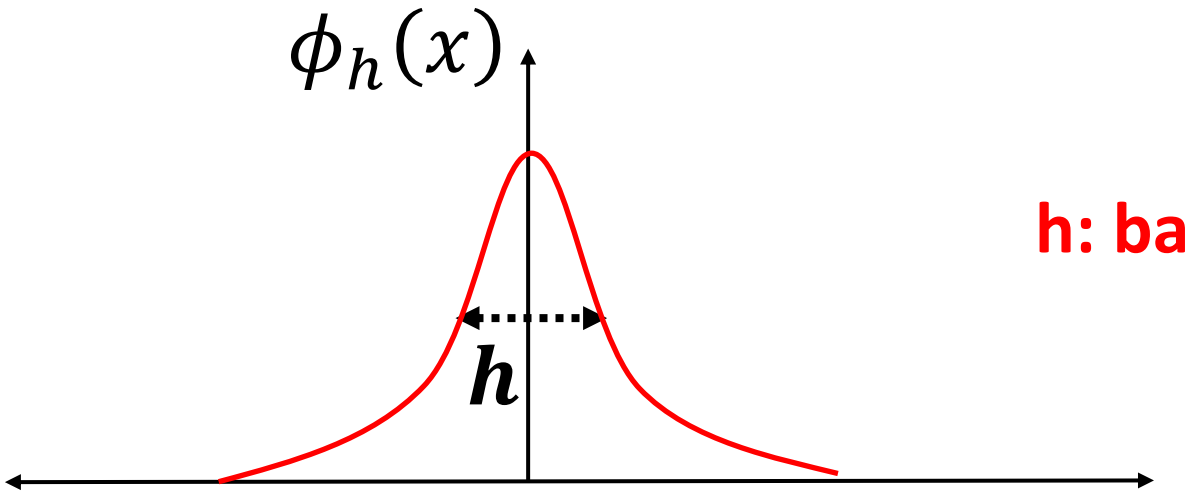
- Summation of bump functions:



Kernel Density Estimator

- Choose bump function as Gaussian with standard deviation (bandwidth) h:

$$\phi_h(x) = \frac{e^{\frac{-x^2}{2h^2}}}{\sqrt{2\pi}h}$$



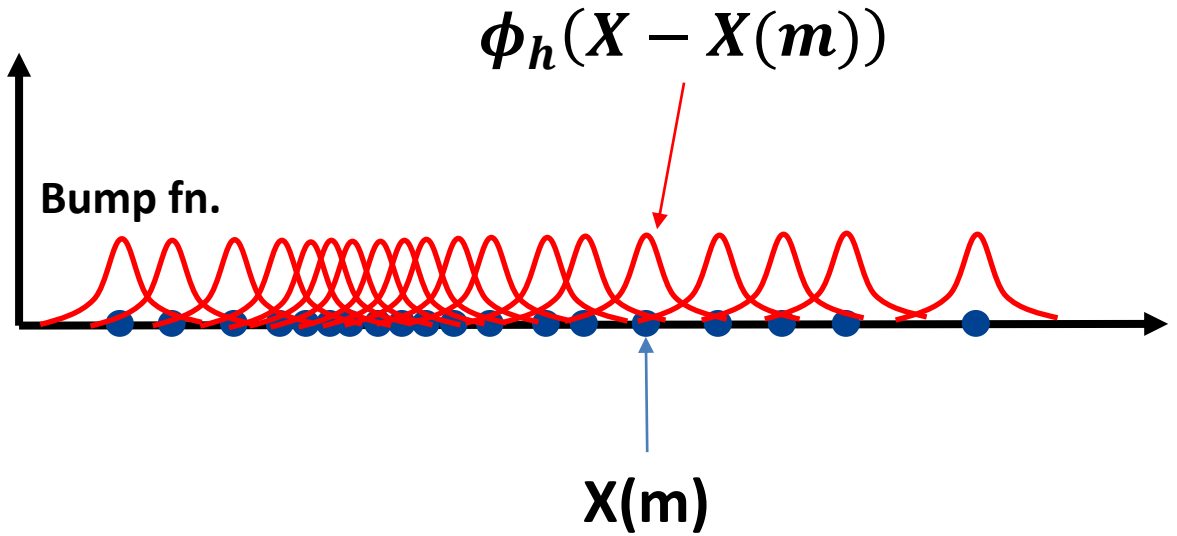
h: bandwidth

Kernel Density Estimator

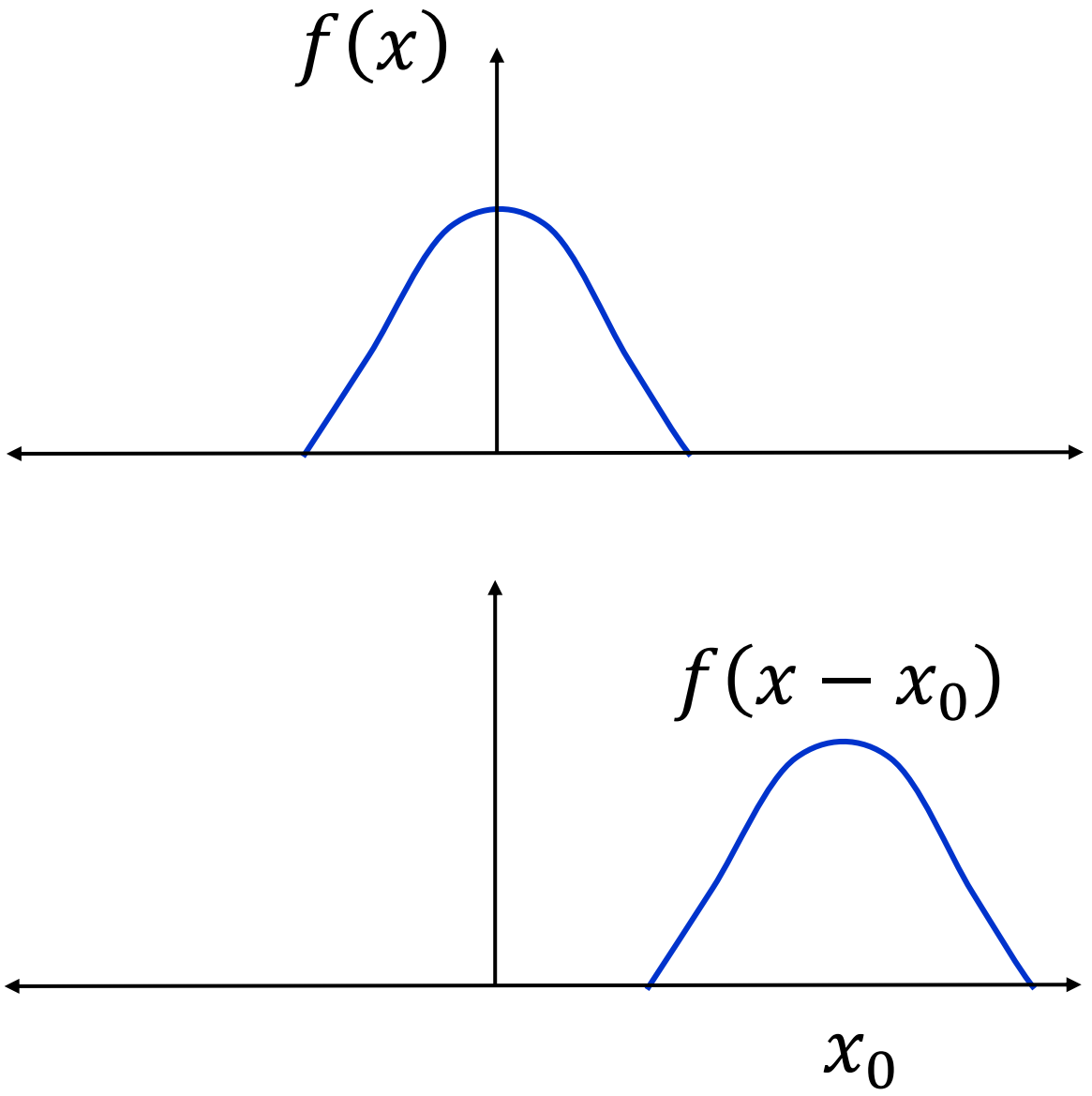
- Choose bump function as Gaussian with standard deviation (bandwidth) h:

$$\phi_h(x) = \frac{e^{\frac{-x^2}{2h^2}}}{\sqrt{2\pi}h}$$

- X(m) are the points generated from the density P(X) that we want to estimate



Kernel Density Estimator

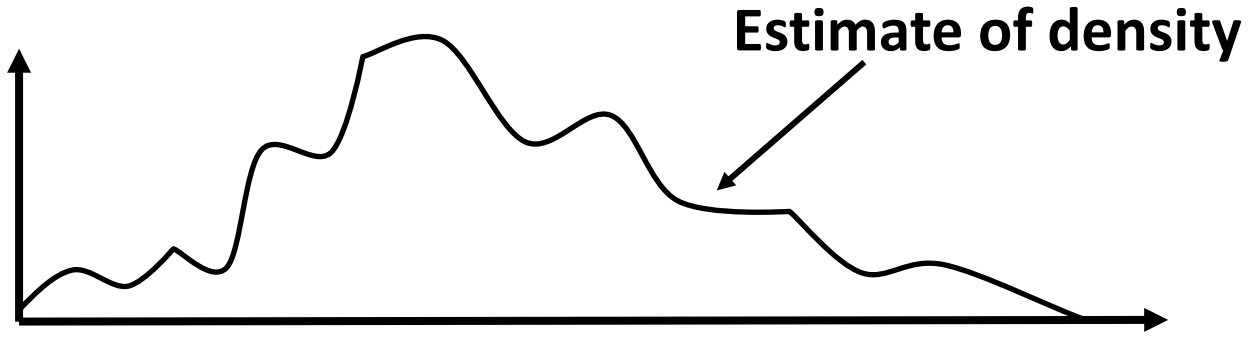


Kernel Density Estimator

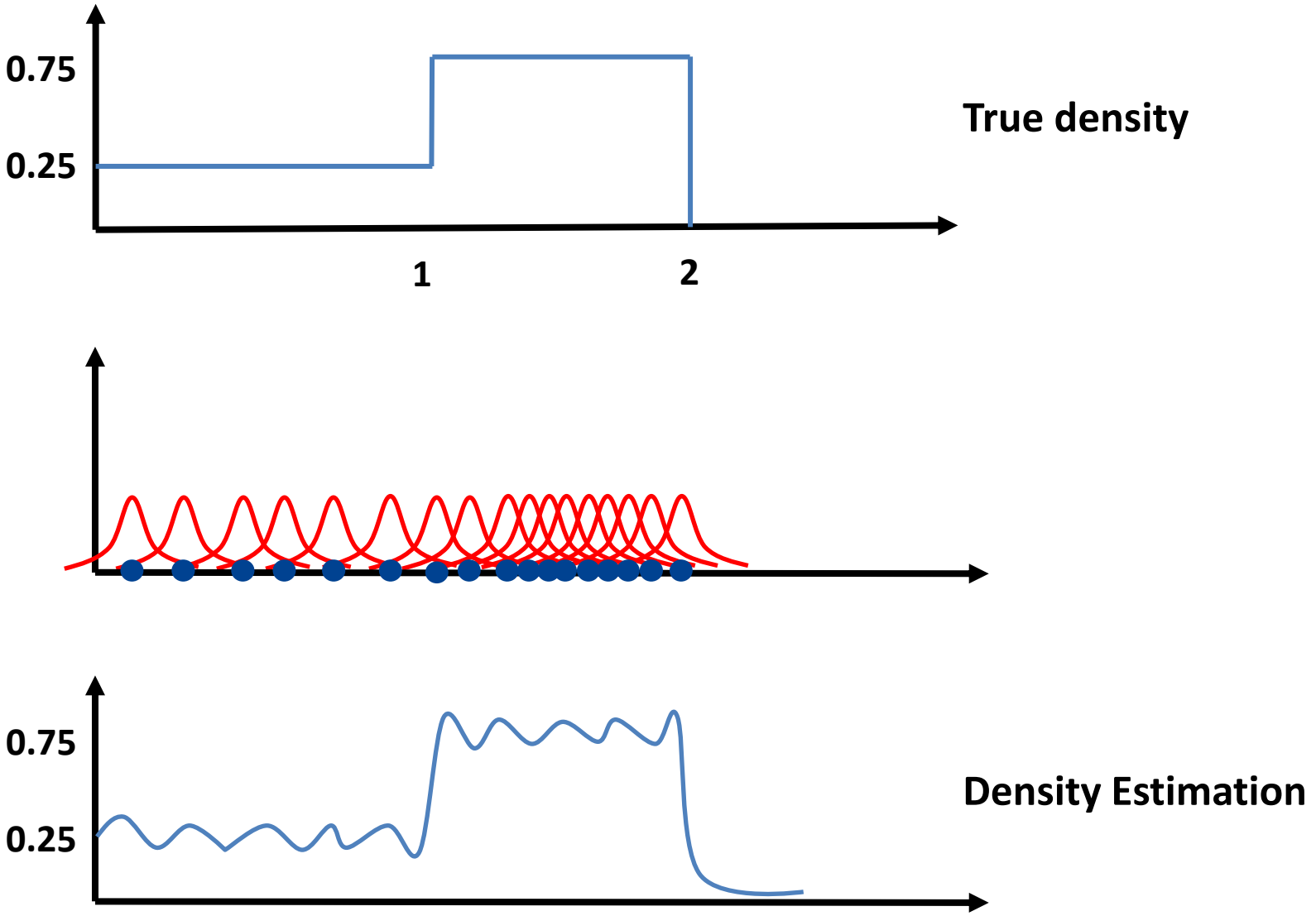
- Summation of bump functions:

$$\widehat{P}(X) = \frac{1}{M} \sum_{m=1}^{M} \phi_h(X - X(m))$$

Summation over # of generated points



Kernel Density Estimator



Kernel Density Estimator

- $\boldsymbol{\phi_h}$ does not have to be Gaussian

$$\boldsymbol{\phi_h = \frac{1}{h} g(\frac{X}{h})}$$

where $\boldsymbol{g(\cdot)}$ is any suitable bump function that integrates to 1:

$$\boldsymbol{\int_{-\infty}^{\infty} g(x)dx = 1}$$

e.g.

$$\mathrm{g(x)} = \frac{e^{\frac{-x^2}{2}}}{\sqrt{2\pi}} \quad \rightarrow \quad \phi_h(x) = \frac{e^{\frac{-x^2}{2h^2}}}{\sqrt{2\pi}h}$$

Kernel Density Estimator

- ϕ_h does not have to be Gaussian

$$\phi_h = \frac{1}{h} g\left(\frac{X}{h}\right)$$

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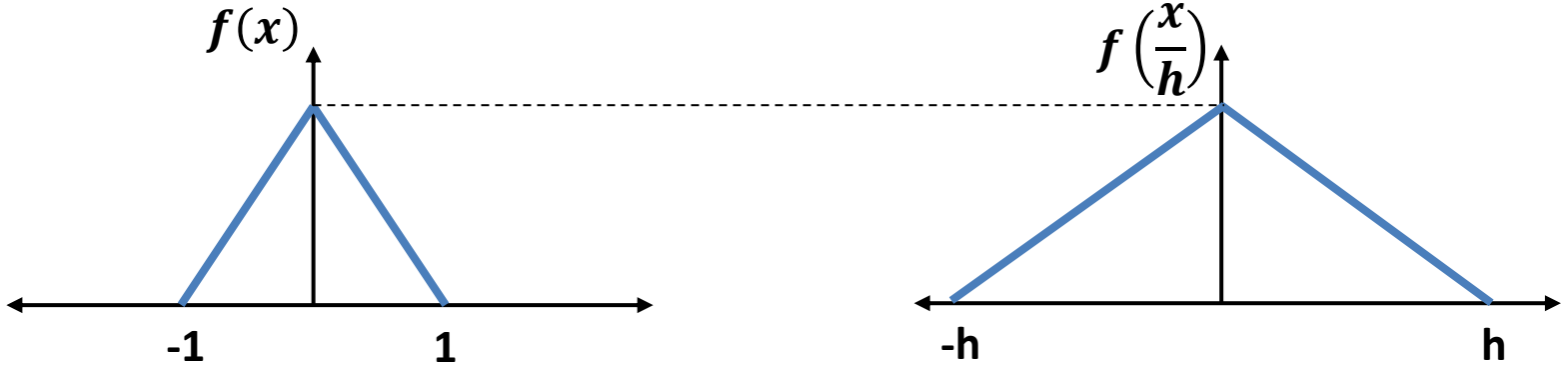


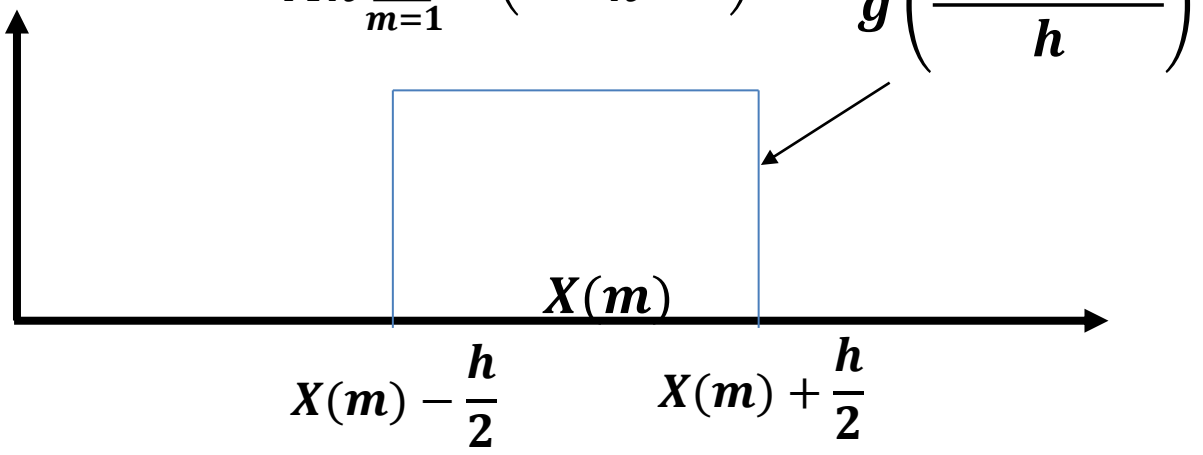
Kernel Density Estimator

- Naïve estimator is equivalent to a Parzen window estimator with:

$$g(x) = \begin{cases} 1, & -\frac{1}{2} \le x < \frac{1}{2} \\ 0, & otherwise \end{cases}$$

- In this case:

$$\widehat{P}(X) = \frac{1}{Mh} \sum_{m=1}^{M} g\left(\frac{X - X(m)}{h}\right)$$



Kernel Density Estimator

1-D form:

$$\widehat{P}(X) = \frac{1}{M}\sum_{m=1}^{M} \phi_h(X - X(m))$$

$$= \frac{1}{Mh}\sum_{m=1}^{M} g\left(\frac{X - X(m)}{h}\right)$$

$$\int_{-\infty}^{\infty} g(x)dx = 1$$

$$\int_{-\infty}^{\infty} \widehat{P}(x)dx = 1$$

Kernel Density Estimator

Multi-dimension Form:

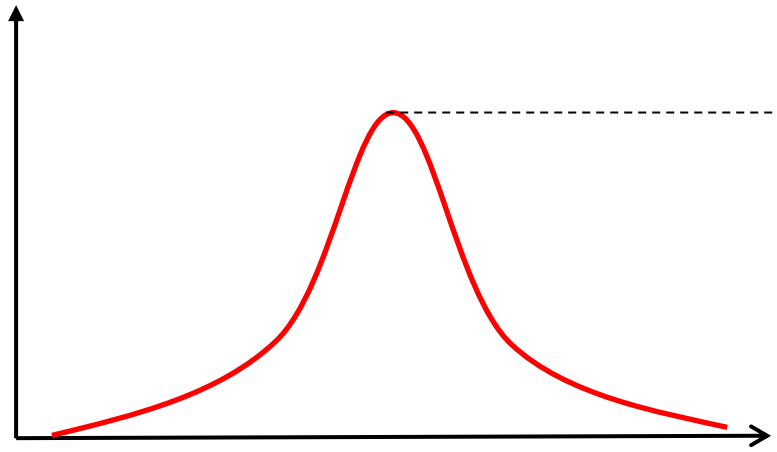
$$\widehat{\boldsymbol{P}}(\underline{\boldsymbol{X}}) = \frac{\mathbf{1}}{\boldsymbol{M}\boldsymbol{h}^{\boldsymbol{N}}} \sum_{\boldsymbol{m}=\mathbf{1}}^{\boldsymbol{M}} \boldsymbol{g}\left(\frac{\underline{\boldsymbol{X}} - \underline{\boldsymbol{X}}(\boldsymbol{m})}{\boldsymbol{h}}\right)$$

$$\int_{-\infty}^{\infty} \boldsymbol{g}(\underline{\boldsymbol{X}}) d\underline{\boldsymbol{X}} = \mathbf{1}$$

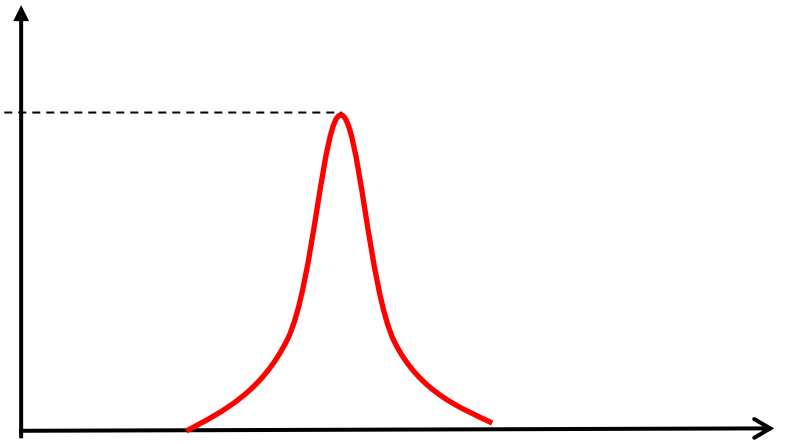
For example: multi-dimension independent Gaussian density:

$$g(\underline{X}) = \frac{e^{-\sum_{i=1}^{N} \frac{x_i^2}{2}}}{(2\pi)^{N/2}}$$

How to choose h?



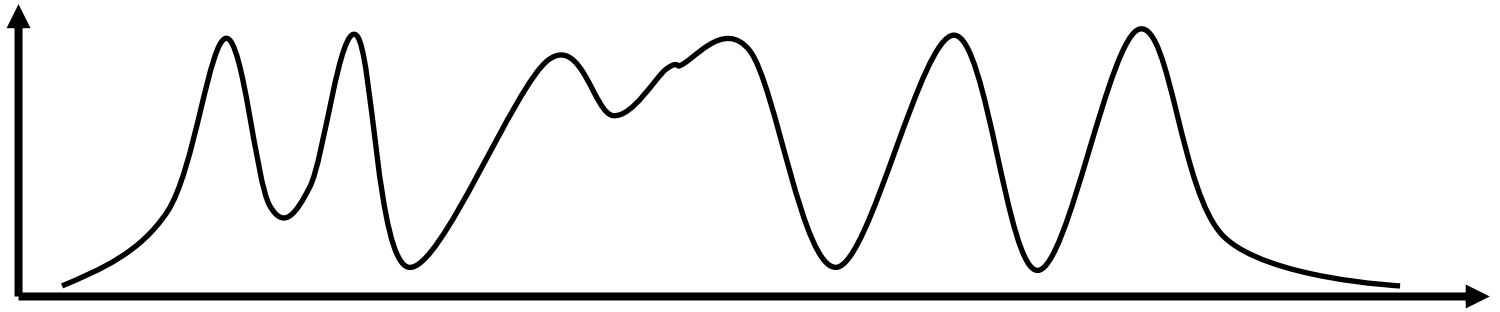
Large h



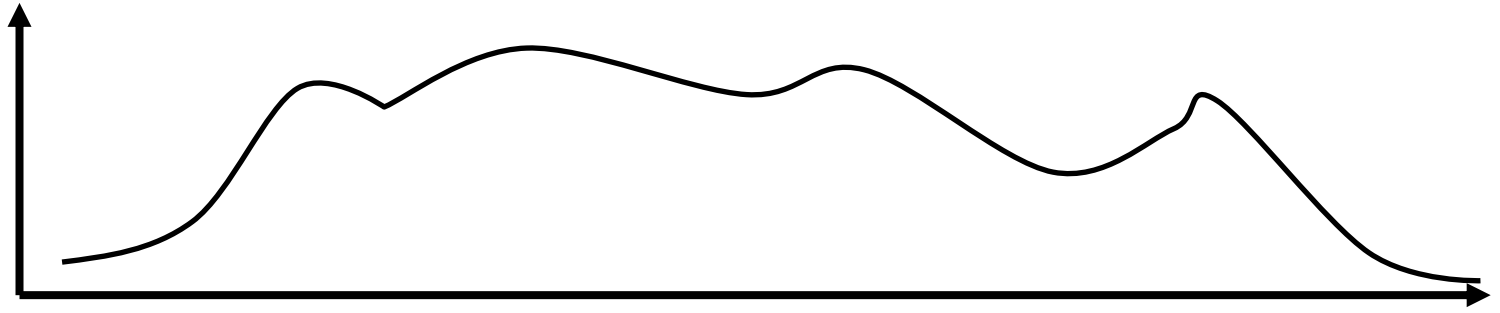
Small h

How to choose h?

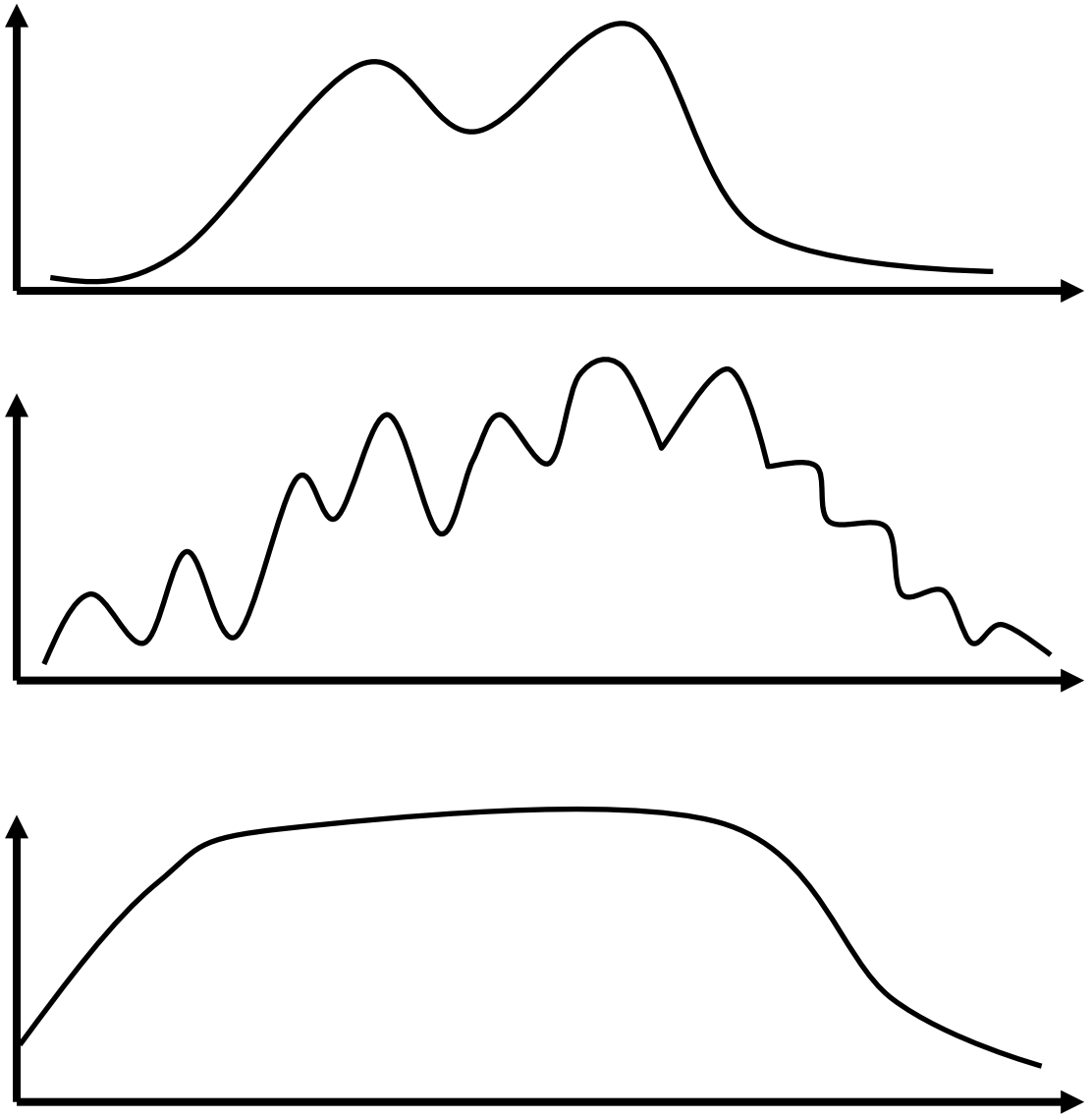
- Too small h → bumpy estimate or non-smooth



- Too large h → the estimate could be too smooth that essential details of the density will be lost or smoothed out



How to choose h?



True Density

Too small h

Too large h

Optimal h

- The optimal H (diagonal bandwidth matrix) can be approximated as :

$$\boldsymbol{H_i = \sigma_i \left[\frac{4}{(N+2)M}\right]^{\frac{1}{N+4}}}$$

normal reference rule

where

$$\sigma_i = \sqrt{[\Sigma_X]_{i,i}}$$

- Σ_X is the estimated covariance matrix, i.e.,

$$\Sigma_X = \frac{1}{M}\sum_{m=1}^{M}(\underline{X}(m) - \hat{\mu})(\underline{X}(m) - \hat{\mu})^T$$

$[\Sigma_X]_{i,i} \equiv i^{th}$ diagonal element of Σ_X

$N \equiv$ dimensions

$$\boldsymbol{h_{opt} = \frac{1}{N}\sum_{i=1}^{N} H_i}$$

For multi-variate normal kernel & diagonal bandwidth matrix

Bowman, A.W., and Azzalini, A. (1997), Applied Smoothing Techniques for Data Analysis, London: Oxford University Press [page 32].

Acknowledgment

- These slides have been created relying on lecture notes of Prof. Dr. Amir Atiya