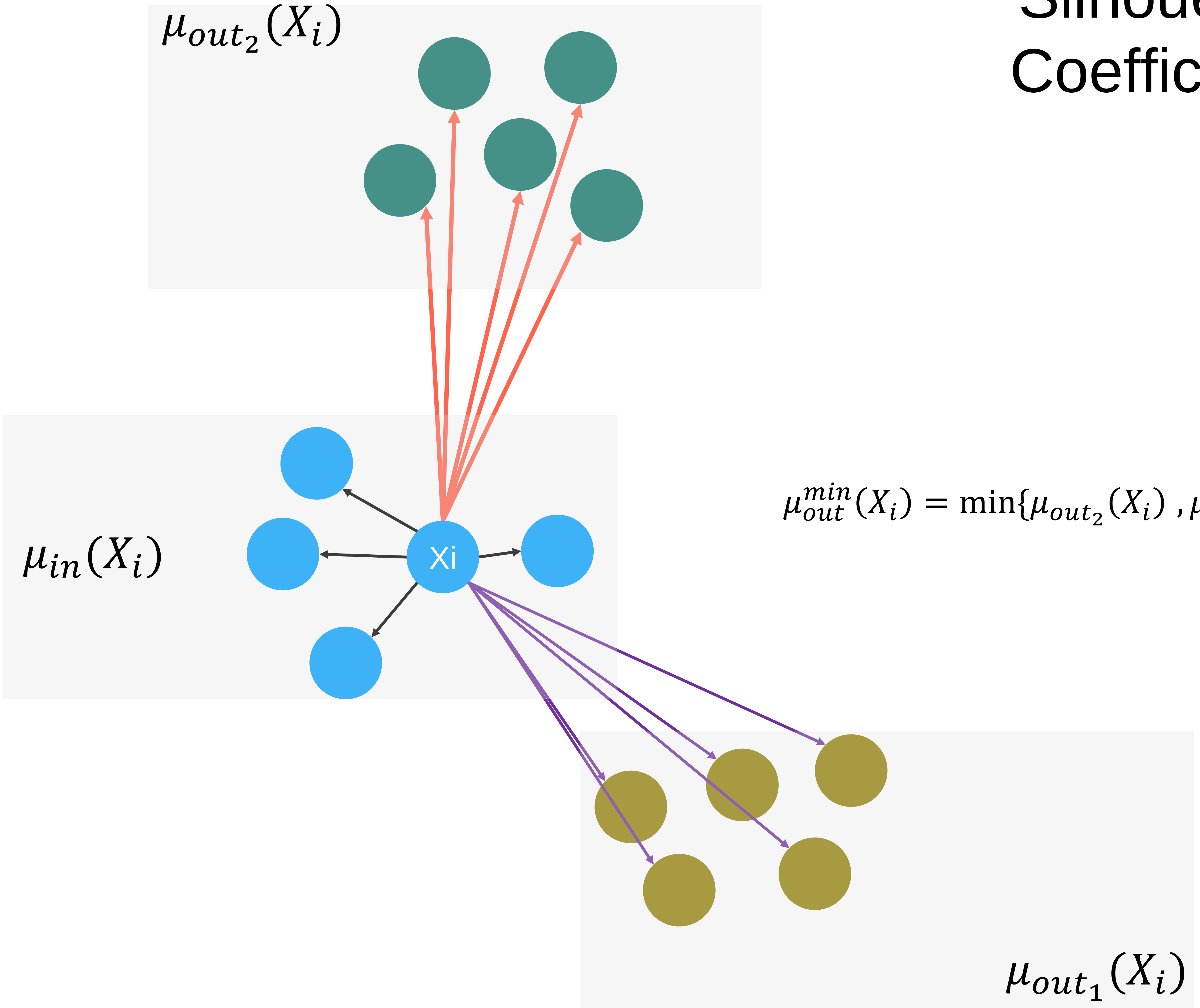
Silhouette Coefficient



$$\mu_{out}^{min}(X_i) = \min\{\mu_{out_2}(X_i)\ ,\mu_{out_1}(X_i)\}$$

Silhouette Coefficient

Define the silhoutte coefficient of a point $\mathbf{x}_i$ as

$$s_i = \frac{\mu_{out}^{\min}(\mathbf{x}_i) - \mu_{in}(\mathbf{x}_i)}{\max\left\{\mu_{out}^{\min}(\mathbf{x}_i), \mu_{in}(\mathbf{x}_i)\right\}}$$

where $\mu_{in}(\mathbf{x}_i)$ is the mean distance from $\mathbf{x}_i$ to points in its own cluster $\hat{y}_i$:

$$\mu_{in}(\mathbf{x}_i) = \frac{\sum_{\mathbf{x}_j \in C_{\hat{y}_i}, j \neq i} \delta(\mathbf{x}_i, \mathbf{x}_j)}{n_{\hat{y}_i} - 1}$$

and $\mu_{out}^{\min}(\mathbf{x}_i)$ is the mean of the distances from $\mathbf{x}_i$ to points in the closest cluster:

$$\mu_{out}^{\min}(\mathbf{x}_i) = \min_{j \neq \hat{y}_i} \left\{ \frac{\sum_{\mathbf{y} \in C_j} \delta(\mathbf{x}_i, \mathbf{y})}{n_j} \right\}$$

The Silhouette Coefficient for clustering C: $SC = \frac{1}{n} \sum_{i=1}^{n} s_i$.

SC close to 1 implies a good clustering (Points are close to their own clusters but far from other clusters)

Density Estimation

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Adopted from slides from Le Song, Mahdi Roozbahani.

Outline

- Overview ⬅
- Parametric Density Estimation
- Nonparametric Density Estimation

Continuous variable

Continuous probability distribution

Probability density function

Density value

Temperature (real number)

Gaussian Distribution

$$\int f_X(x)dx = 1$$

Discrete variable

Discrete probability distribution

Probability mass function

Probability value

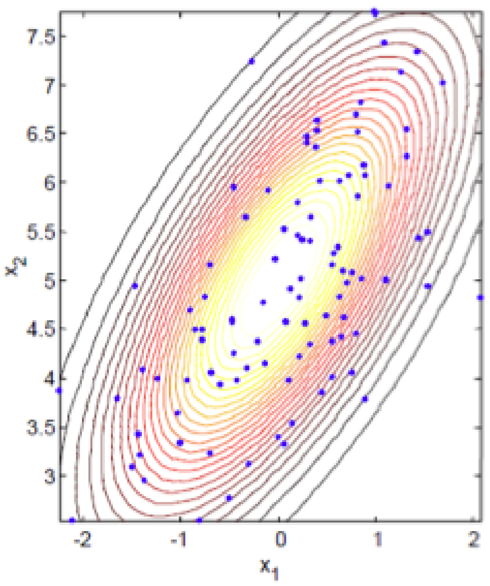
Coin flip (integer)

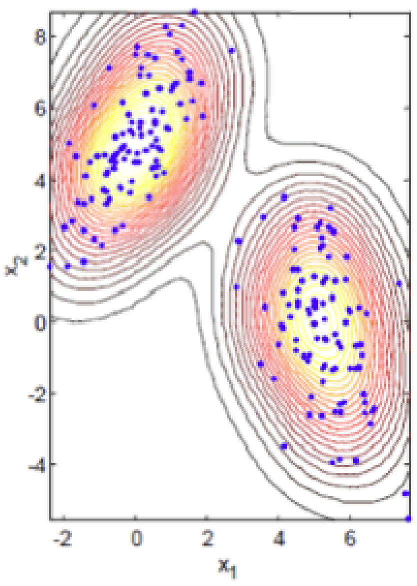
Bernoulli distribution

$$\sum_{x \epsilon A} f_X(x) = 1$$

Why Density Estimation?

- Learn more about the "shape" of the data cloud

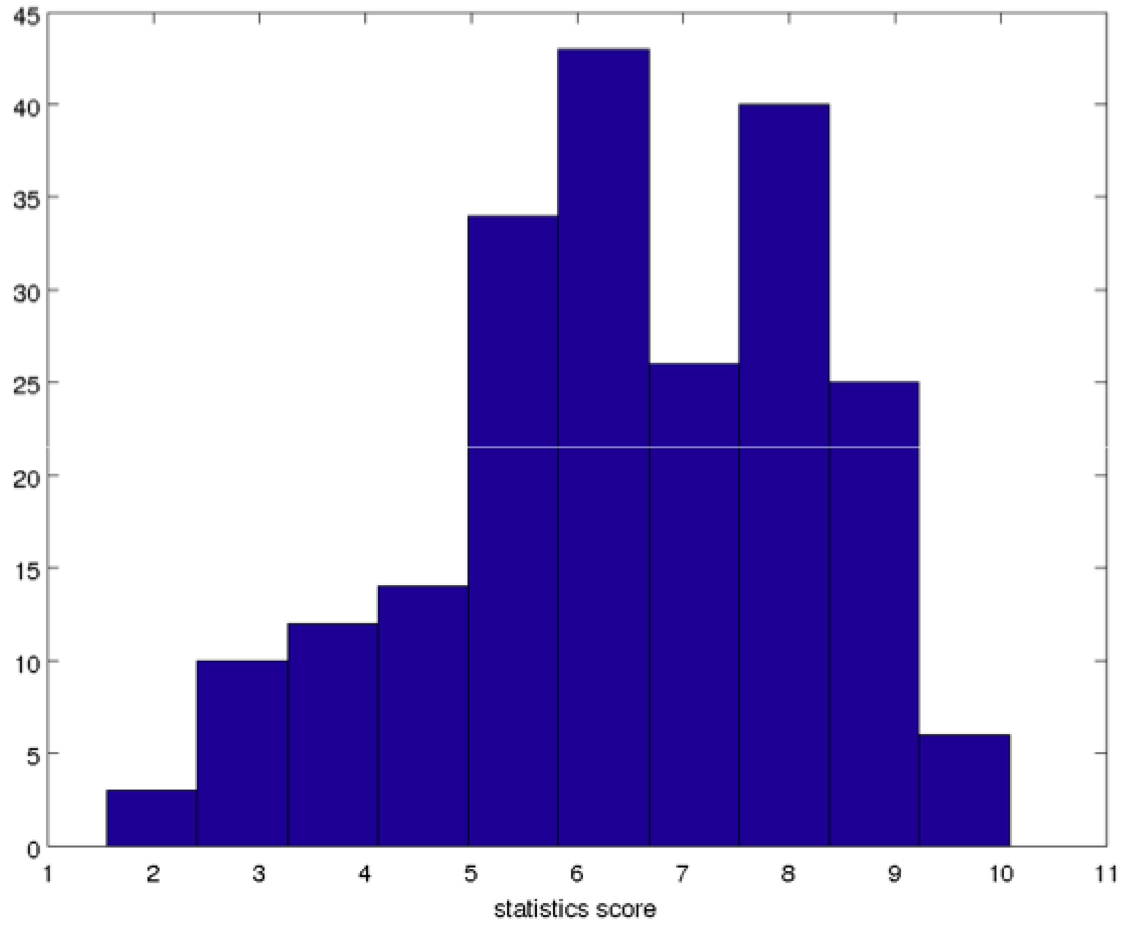


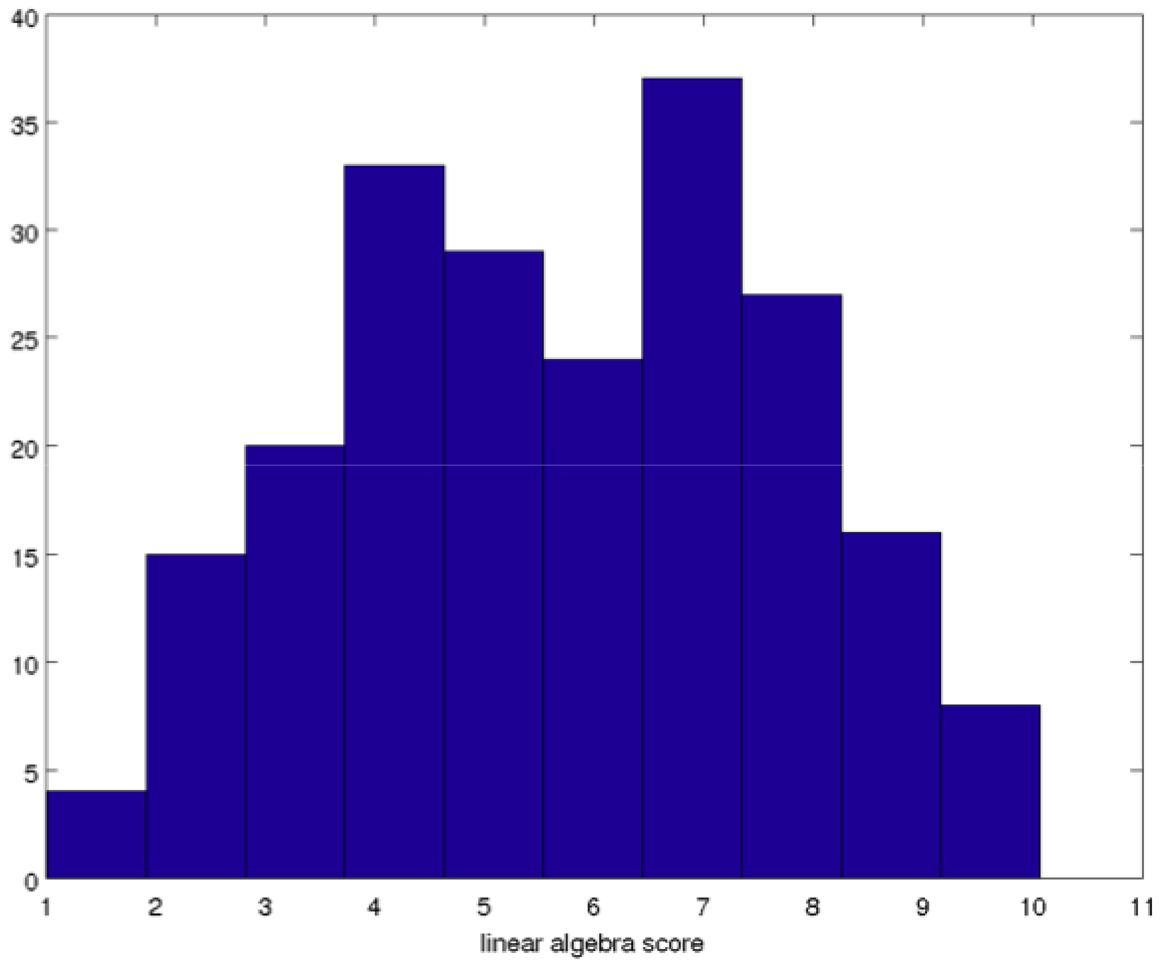


- Access the density of seeing a particular data point
  - Is this a typical data point? (high density value)
  - Is this an abnormal data point / outlier? (low density value)

- Building block for more sophisticated learning algorithms
  - Classification, regression, graphical models …
  - A simple recommendation system

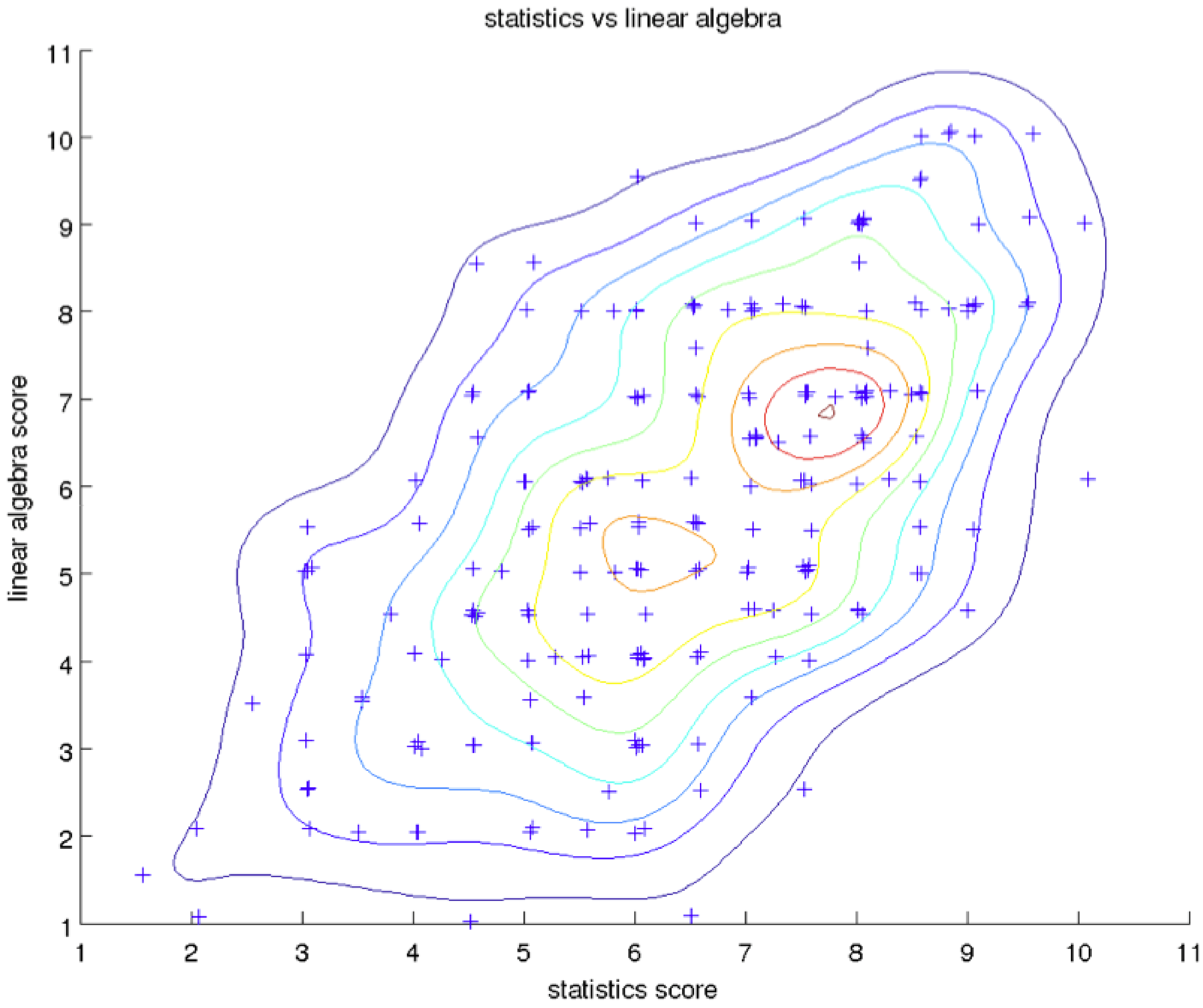
Example: Test Scores





Histogram is an estimate of the probability distribution of a continuous variable

Example: Test Scores



Parametric Density Estimation

- Models which can be described by a fixed number of parameters

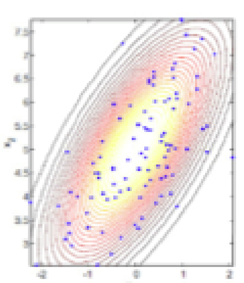
- Discrete case: eg. Bernoulli distribution

$$P(x|\theta) = \theta^x (1-\theta)^{1-x}$$

$1 \rightarrow Head$
$0 \rightarrow Tails$

one parameter, $x \in [0,1]$, which generate a family of models, $\mathcal{F} = \{P(x|\theta) \mid x \in [0,1]\}$, θ *probability of possible outcome*

- Continuous case: eg. Gaussian distribution in R^d

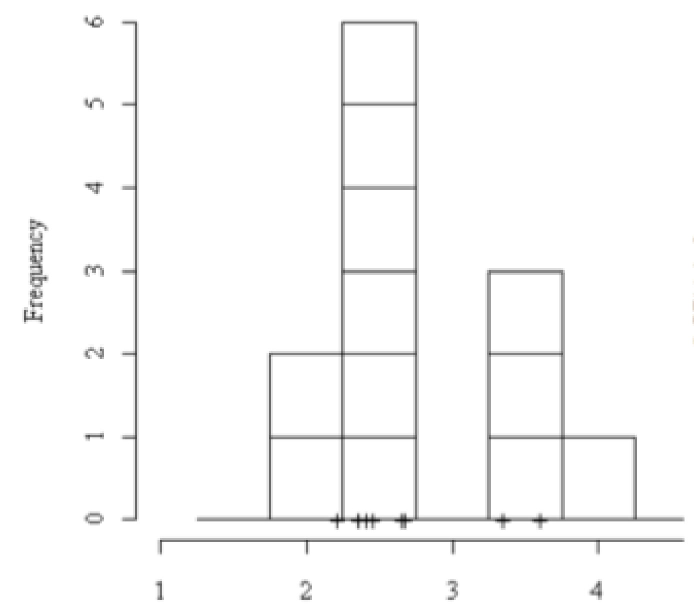


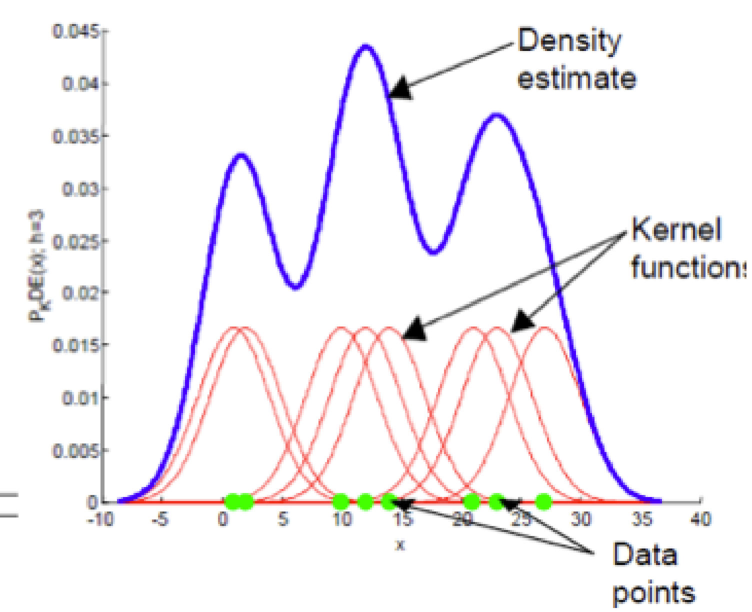
$$p(x|\mu,\Sigma) = \frac{1}{|\Sigma|^{\frac{1}{2}}(2\pi)^{\frac{d}{2}}} exp\left(-\frac{1}{2}(x-\mu)^{\top}\Sigma^{-1}(x-\mu)\right)$$

Two sets of parameters $\{\mu, \Sigma\}$, which again generate a family of models, $\mathcal{F} = \{p(x|\mu,\Sigma) \mid \mu \in R^d, \Sigma \in R^{d\times d} \text{ and } PSD\}$,

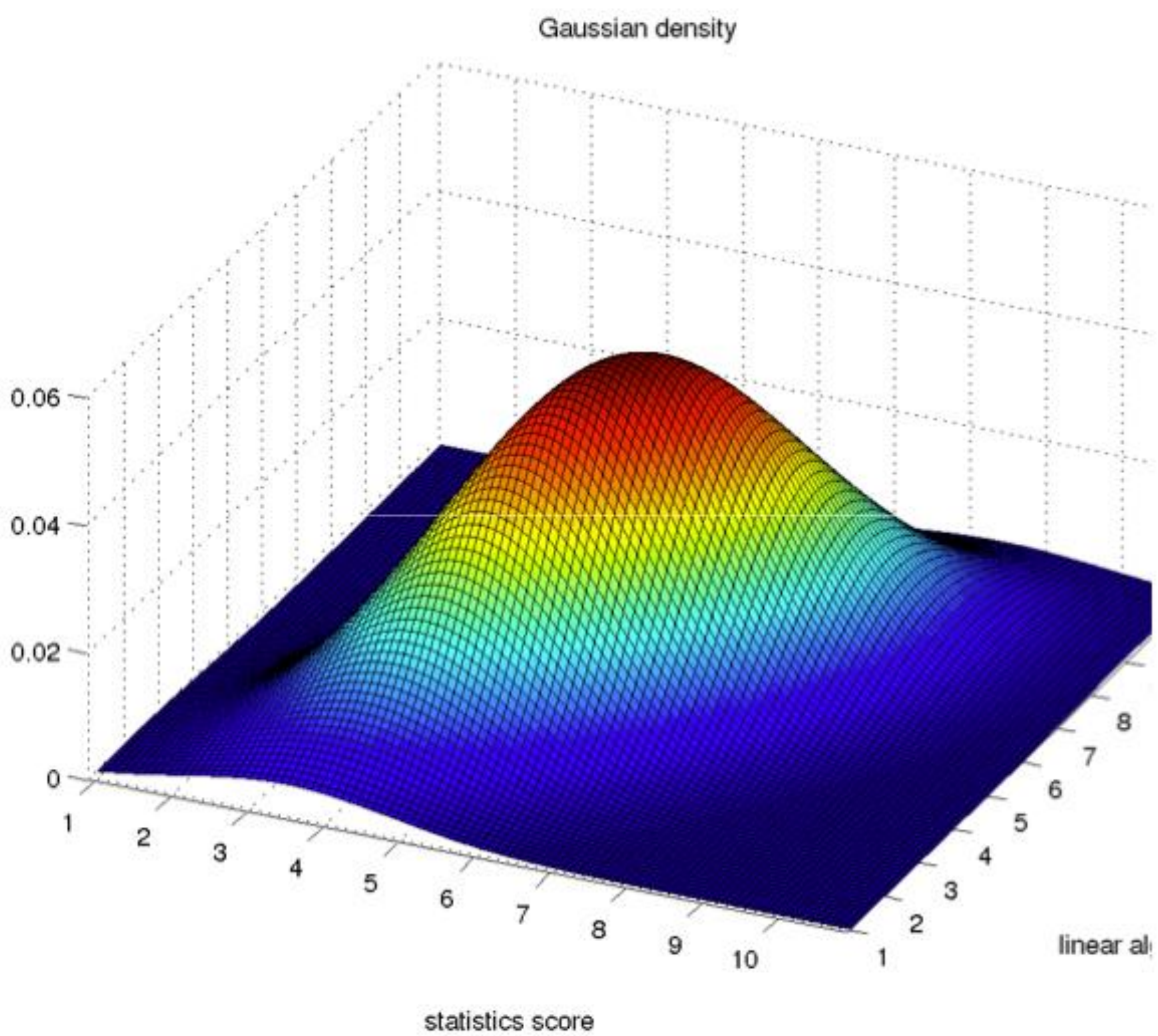
Nonparametric Density Estimation

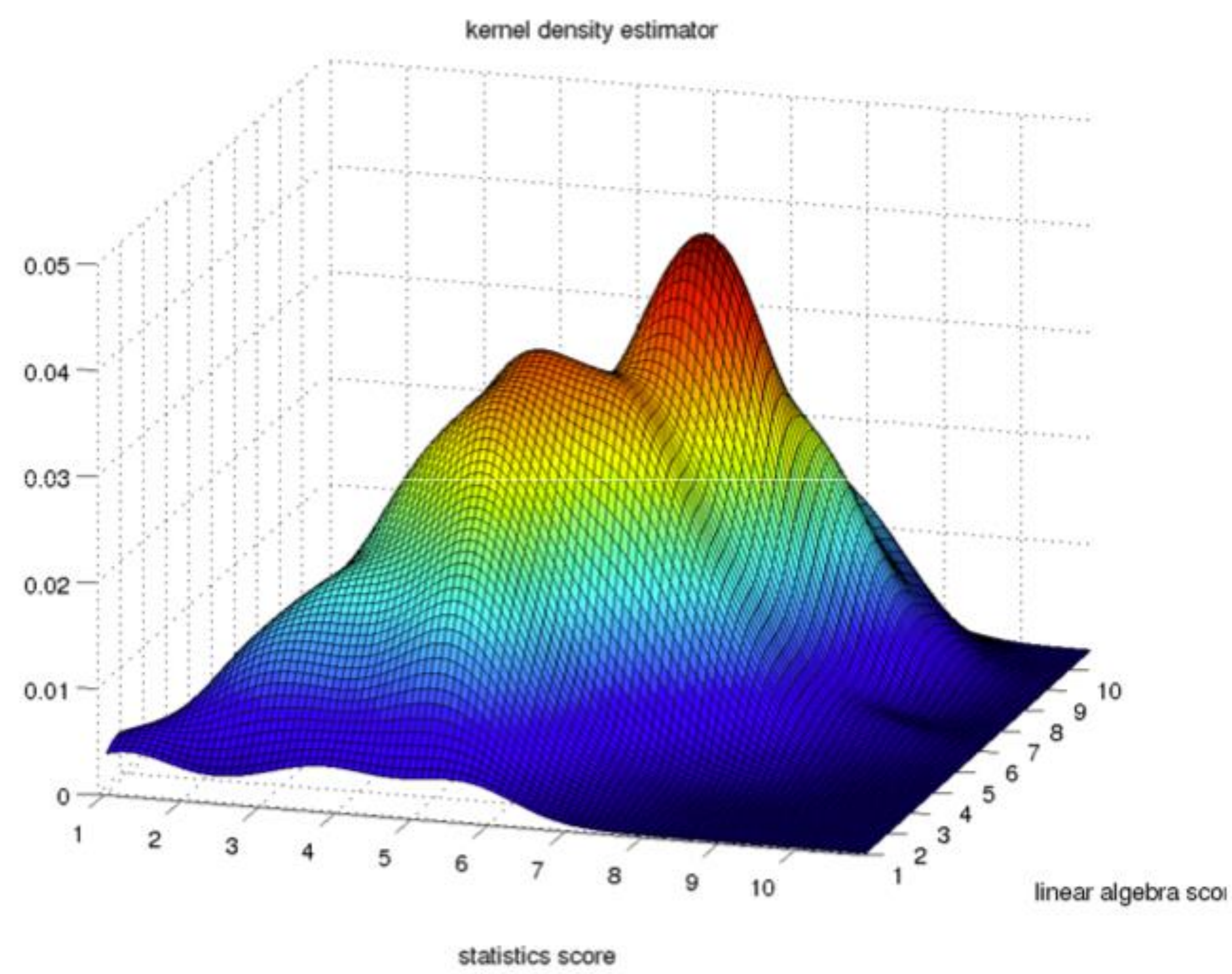
- What are nonparametric models?
  - "nonparametric" does not mean there are no parameters
  - can not be described by a fixed number of parameters
  - one can think of there are many parameters
- Eg. Histogram
- Eg. Kernel density estimator



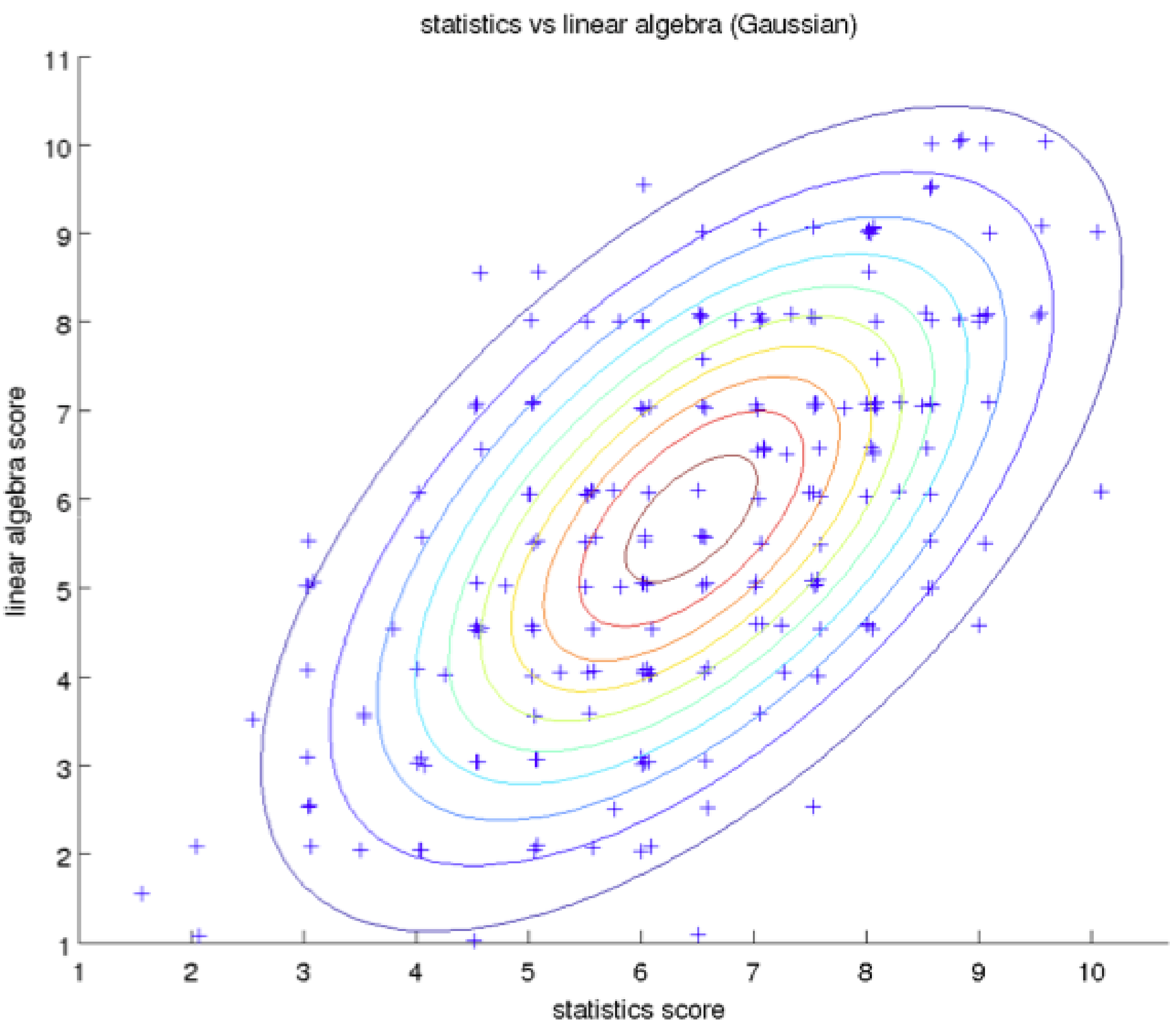


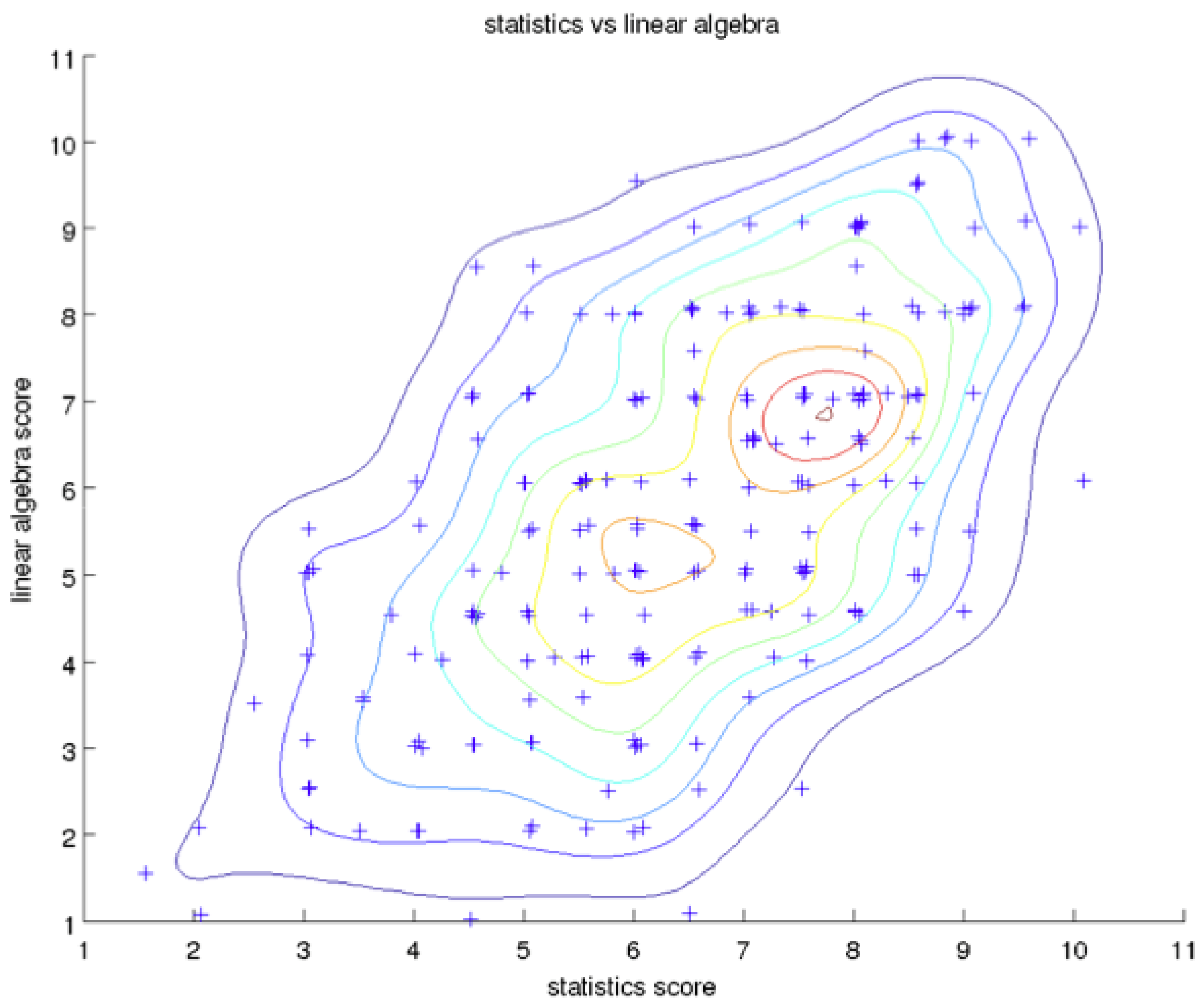
Parametric v.s. Nonparametric Density Estimation





Parametric v.s. Nonparametric Density Estimation





Outline

- Overview
- Parametric Density Estimation
- Nonparametric Density Estimation

Estimating Parametric Models

- A very popular estimator is the maximum likelihood estimator (MLE), which is simple and has good statistical properties

- Assume that n data points $X = \{x_1, x_2, \dots, x_n\}$ drawn independently and identically (iid) from some distribution $P^*(x)$

Using the parameters, we can estimate each data point

- Want to fit the data with a model $P(x|\theta)$ with parameter θ

$$\theta = argmax_\theta \log P(X|\theta) = argmax_\theta \log \prod_{i=1}^{N} P(x_i|\theta)$$

Example Problem

- Estimate the probability θ of landing in heads using a biased coin

- Given a sequence of n independently and identically distributed (iid) flips
  - Eg. $X = \{x_1, x_2, \ldots, x_n\} = \{1,0,1,\ldots,0\}, x_i \in \{0,1\}$

- Model: $P(x|\theta) = \theta^x(1-\theta)^{1-x}$
  - $P(x|\theta) = \begin{cases} 1-\theta, for\ x=0 \\ \theta, \quad for\ x=1 \end{cases}$

- Likelihood of a single observation x_i ?
  - $L(\theta|x_n) = p(x_n|\theta) = \theta^{x_n}(1-\theta)^{1-x_n}$

MLE for Biased Coin

- Objective function, log-likelihood

$$l(\theta|\mathbf{X}) = \log L(\theta|\mathbf{X}) = \log \prod_{n=1}^{N} \theta^{x_n}(1-\theta)^{1-x_n} = \log(\theta^{N_H}(1-\theta)^{N_T})$$

$$= N_H \times \log\theta + N_T \times \log(1-\theta)$$

N_H = number of heads, N_T = number of tails

- Maximize $l(\theta|\mathbf{X})$ w.r.t. $\theta \rightarrow$ take derivative w.r.t. θ and set it to zero

$$\frac{\partial l(\theta|\mathbf{X})}{\partial\theta} = \frac{N_H}{\theta} - \frac{N - N_H}{1-\theta} = 0 \rightarrow \theta_{MLE} = \frac{N_H}{N}$$

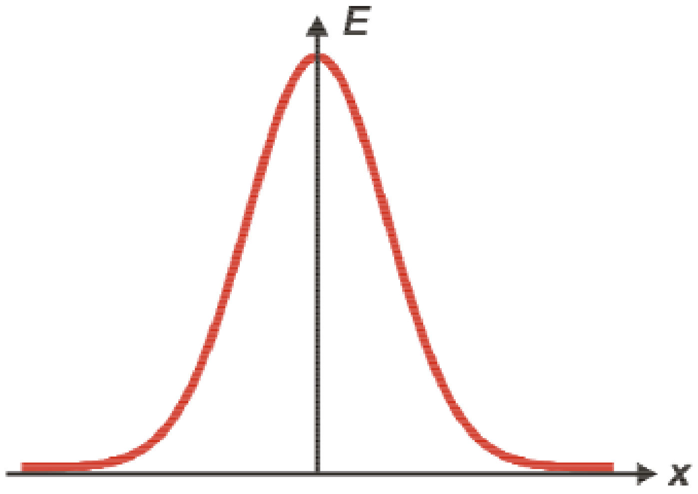
- Example: $N_H = 78, N_H = 22 \rightarrow \theta = 0.78$

Estimating Gaussian Distributions

- Gaussian distribution in R

$$p(x|\mu,\sigma) = \frac{1}{(2\pi)^{\frac{1}{2}}\sigma} exp\left(-\frac{1}{2\sigma^2}(x-\mu)^2\right)$$

- Need to estimate two sets of parameters μ, σ



- Given n iid samples

$$X = \{x_1, x_2, \dots, x_n\}, x_i \in R$$

- Density of a data point:

$$p(x_i|\mu,\sigma) \propto exp\left(-\frac{1}{2\sigma^2}(x_i-\mu)^2\right)$$

Estimating Gaussian Distributions

- Gaussian distribution in R

$$p(x|\mu,\sigma) = \frac{1}{(2\pi)^{\frac{1}{2}}\sigma} exp\left(-\frac{1}{2\sigma^2}(x-\mu)^2\right)$$

- Mean

$$\mu = \frac{1}{n}\sum_{i=1}^{n} x_i$$

- Variance

$$\sigma^2 = \frac{1}{n}\sum_{i=1}^{n}\left(x_i - \mu\right)^2$$

MLE for Gaussian Distribution

- Objective function, log likelihood

$$l(\mu, \sigma; X) = \log \prod_{i=1}^{N} \frac{1}{(2\pi)^{\frac{1}{2}}\sigma} exp\left(-\frac{1}{2\sigma^2}(x_i - \mu)^2\right)$$

$$= -\frac{n}{2}\log 2\pi - \frac{n}{2}\log \sigma^2 - \sum_{i=1}^{N}\frac{(x_i - \mu)^2}{2\sigma^2}$$

- Maximize $l(\mu, \sigma; X)$ with respect to μ, σ

- Take derivatives w.r.t. μ, σ^2

$$\frac{\partial l}{\partial \mu} = 0$$

$$\frac{\partial l}{\partial \sigma^2} = 0$$

MLE for Gaussian Distribution

$$l(\mu, \sigma; X) = -\frac{n}{2}\log 2\pi - \frac{n}{2}\log\sigma^2 - \sum_{i=1}^{N}\frac{(x_i - \mu)^2}{2\sigma^2}$$

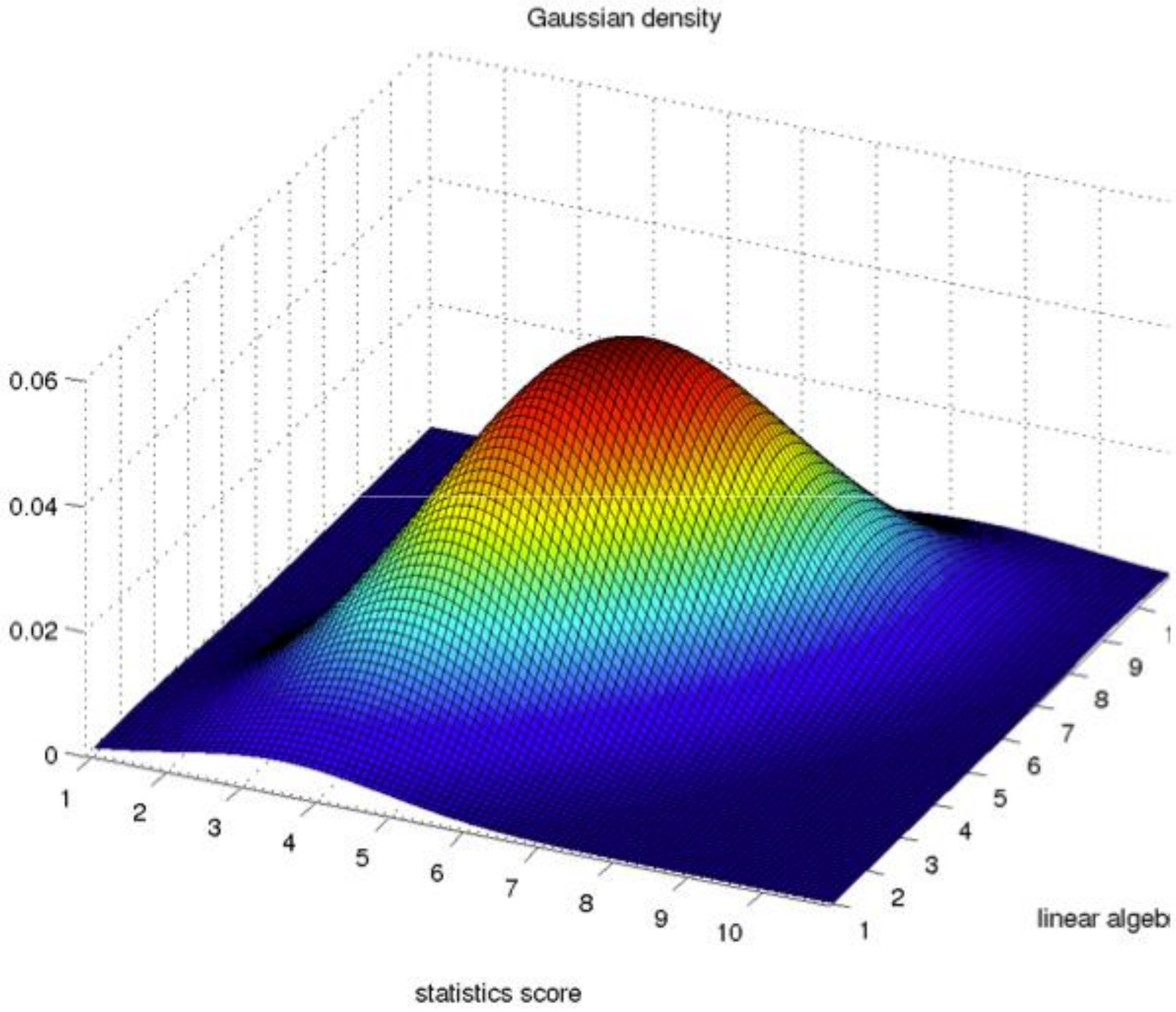
$$\frac{\partial l}{\partial \mu} = \frac{1}{\sigma^2}\sum_{i=1}^{N}(x_i - \mu) = 0$$

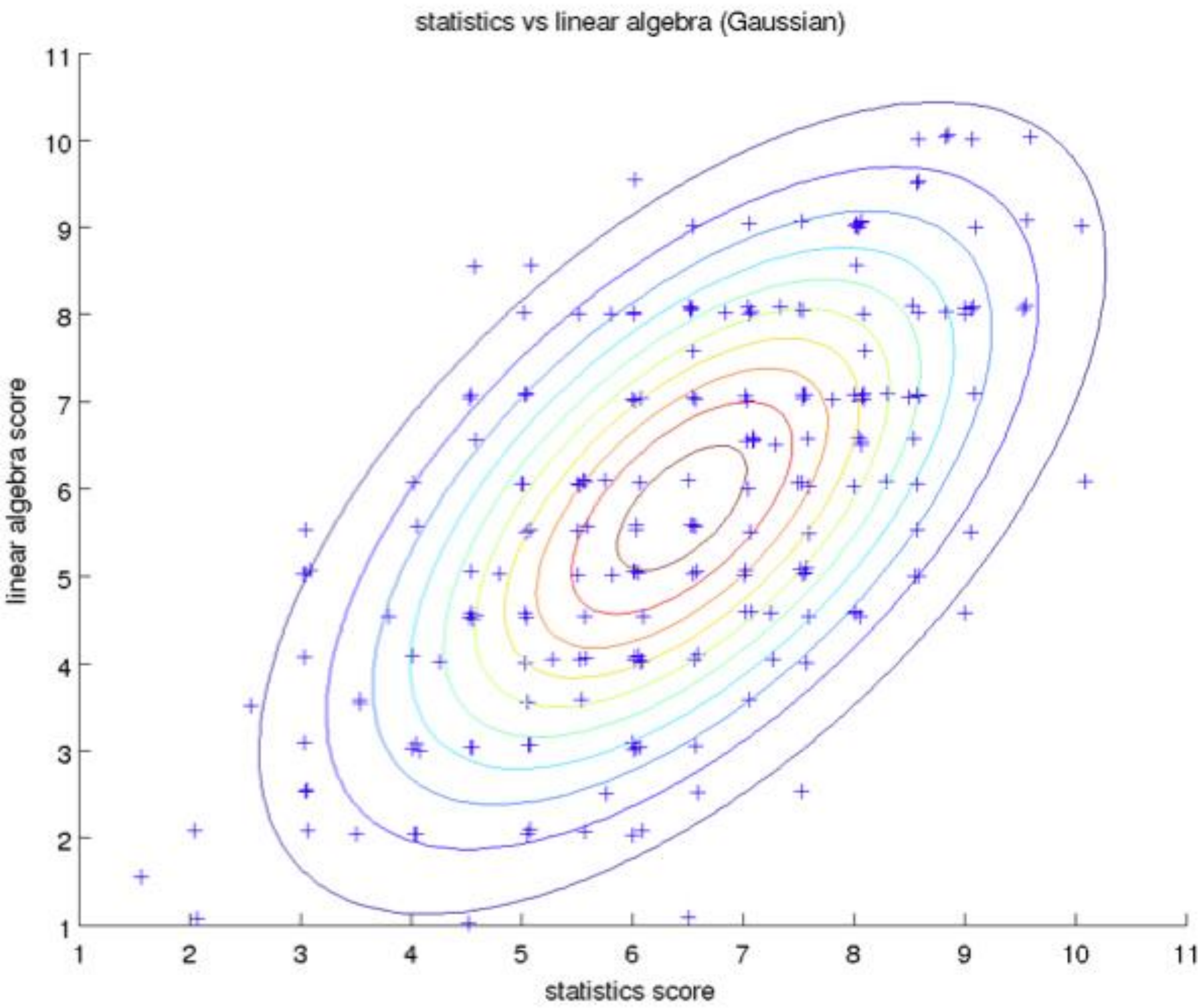
$$\Rightarrow \sum_{i}^{N} x_i = n\,\mu \Rightarrow \mu = \frac{1}{n}\sum_{i=1}^{N} x_i$$

$$\frac{\partial l}{\partial \sigma^2} = -\frac{n}{2\sigma^2} + \frac{1}{2\sigma^4}\sum_{i}^{N}(x_i - \mu)^2 = 0$$

$$\Rightarrow \sum_{i}^{N}(x_i - \mu)^2 = n\,\sigma^2 \Rightarrow \frac{1}{n}\sum_{i=1}^{N}(x_i - \mu)^2$$

Example


Gaussian density
0.06
0.04
0.02
0
1
2
3
4
5
6
7
8
9
10
statistics score
linear algeb


statistics vs linear algebra (Gaussian)
linear algebra score
statistics score
1
2
3
4
5
6
7
8
9
10
11

Outline

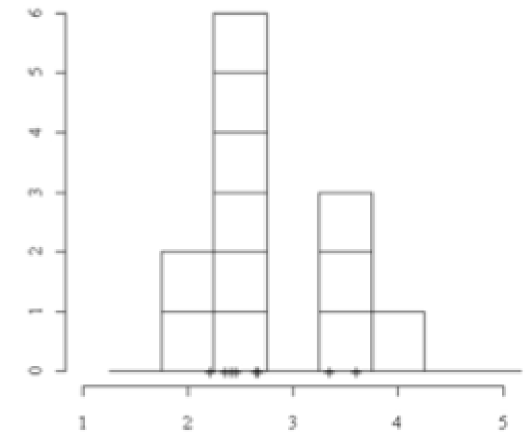
- Overview
- Parametric Density Estimation
- Nonparametric Density Estimation ⬅

Can be used for:

- Visualization
- Classification
- Regression

1-D Histogram

- One the simplest nonparametric density estimator



- Given n iid samples $X = \{x_1, x_2, \dots, x_n\} = x_i \in [0,1)$
- Split [0,1) into m bins

$$B_1 = \left[0, \frac{1}{m}\right), B_2 = \left[\frac{1}{m}, \frac{2}{m}\right), \dots B_m = \left[\frac{m-1}{m}, 1\right)$$

- Count the number of points, c_1 within B_1, c_2 within B_2...
- For a new test point x

Identity matrix

$$p(x) = \sum_{j=1}^{m} \frac{m c_j}{n} I(x \in B_j) = \frac{\textit{number of points in bin c}}{\textit{total number of data points} \times \textit{bin width}}$$

$$\frac{1}{m}$$

$$P = \int p(x)dx$$

The probability that point x is drawn from a distribution p(x)

Why is Histogram Valid?

- Requirement for density $p(x)$
- $p(x) \geq 0, \int_{\Omega} p(x)dx = 1$

- For histogram, One dimensional case:

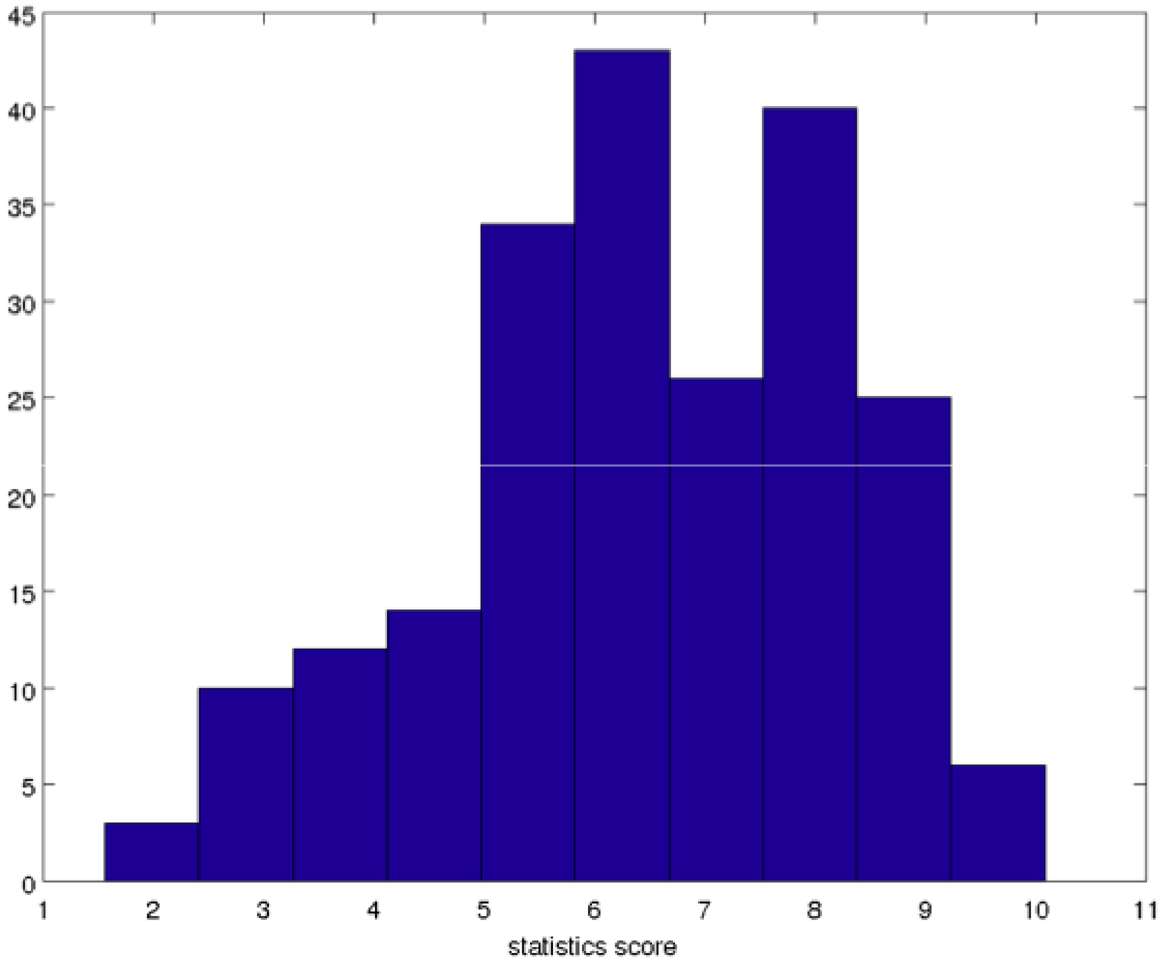
$$\int_{[0,1)} p(x)dx = \int_{[0,1)} \sum_{j=1}^{m} \frac{mc_j}{n} dx$$

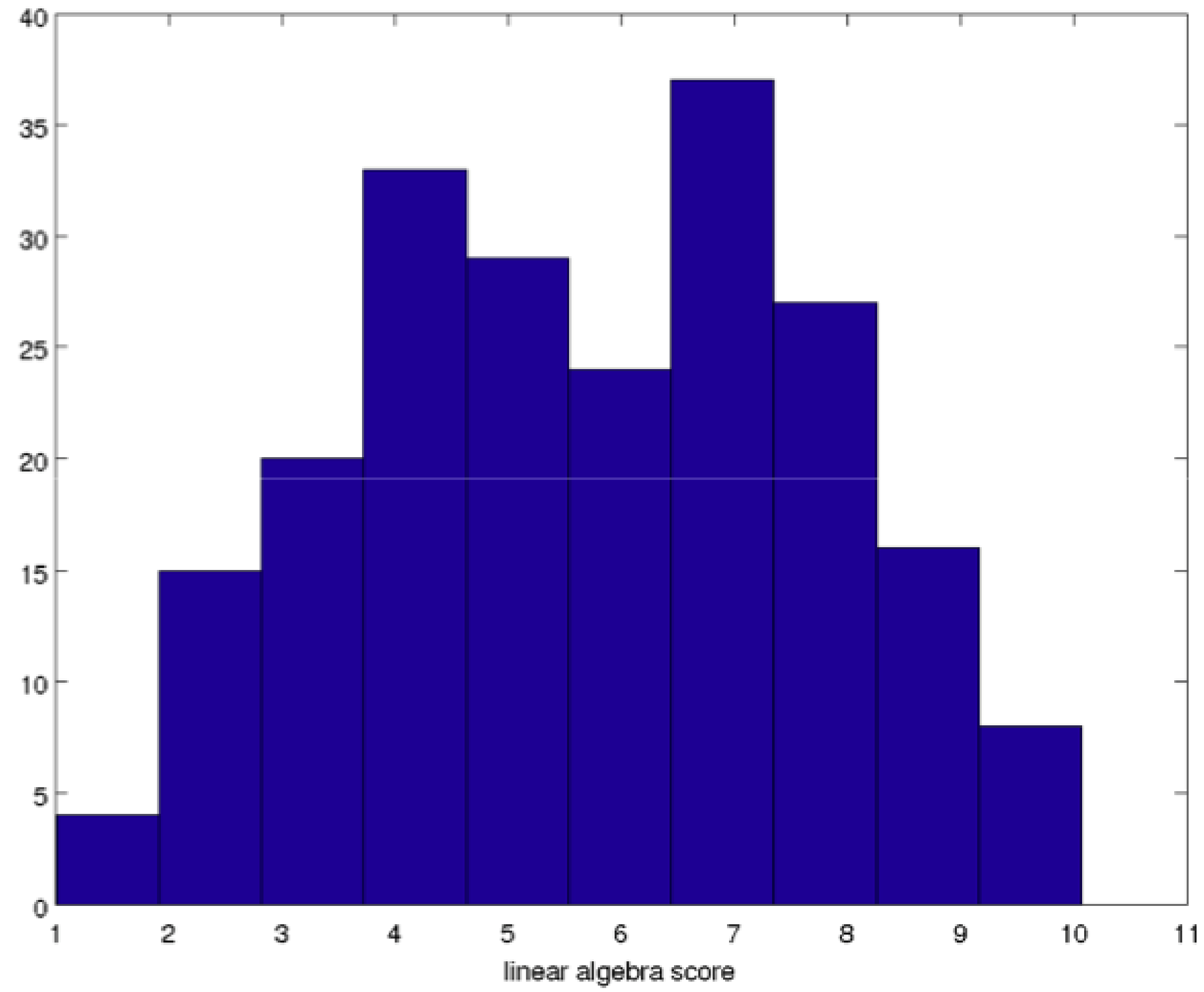
$$= \int_{0}^{\frac{1}{m}} \sum_{j=1}^{m} \frac{mc_j}{n} dx + \int_{\frac{1}{m}}^{\frac{2}{m}} \sum_{j=1}^{m} \frac{mc_j}{n} dx + \ldots + \int_{\frac{j-1}{m}}^{\frac{j}{m}} \sum_{j=1}^{m} \frac{mc_j}{n} dx = \sum_{j=1}^{m} \int_{[\frac{j-1}{m}, \frac{j}{m})} \frac{mc_j}{n} dx$$

$$= \sum_{j=1}^{m} \frac{mc_j}{n} [\frac{j}{m} - \frac{j-1}{m}] = \sum_{j=1}^{m} \frac{c_j}{n} = 1$$

Example: Test Scores

- What is missing if we want density?





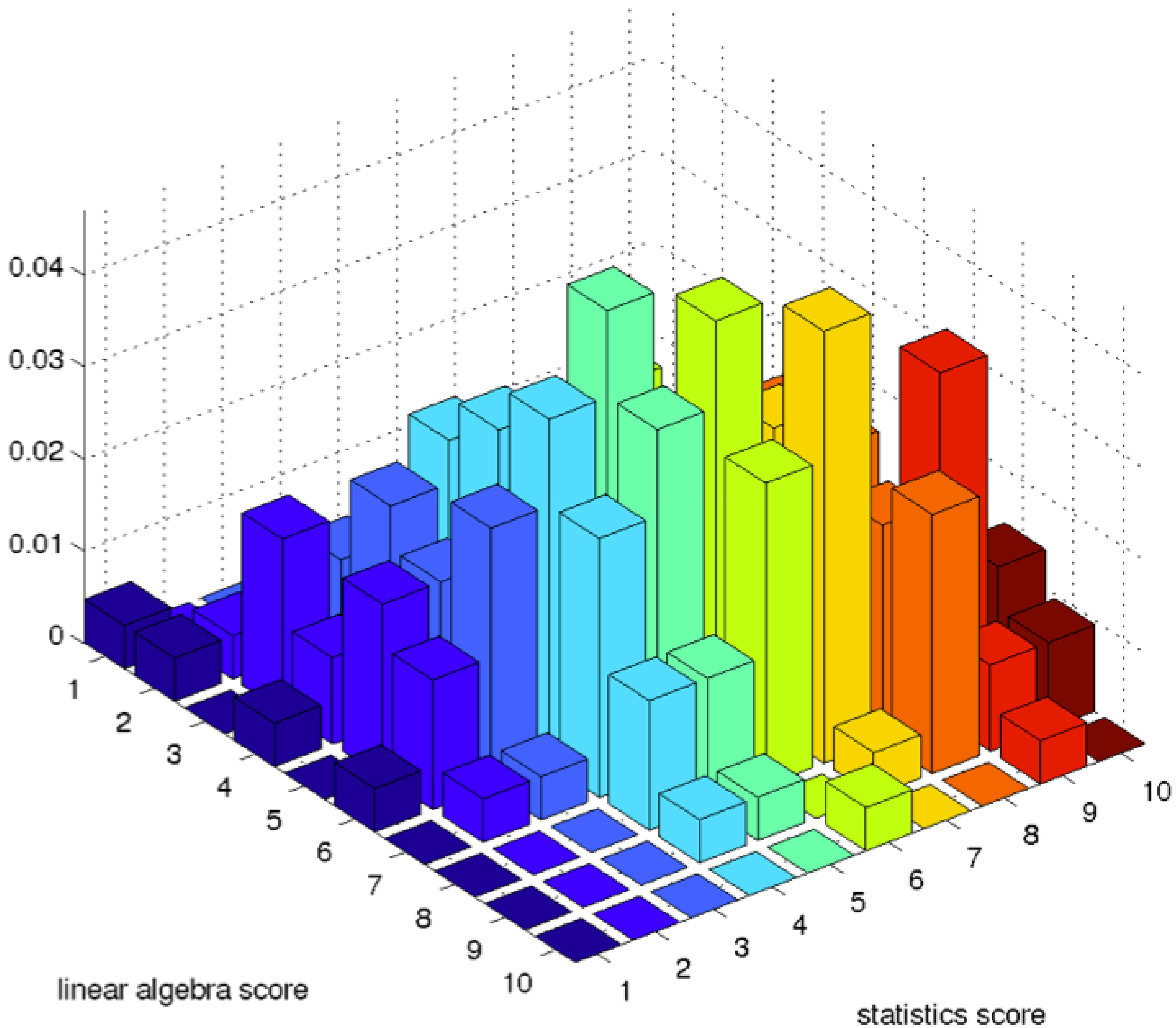
Higher-Dimensional Histogram

- Given n iid samples $X = \{x_1, x_2, \dots, x_n\}, x_i \in [0,1)^d$
- Split $[0,1)^d$ evenly into m^d bins
- Bin size is $h = \frac{1}{m}$

$Two\ Dimensional\ data$:

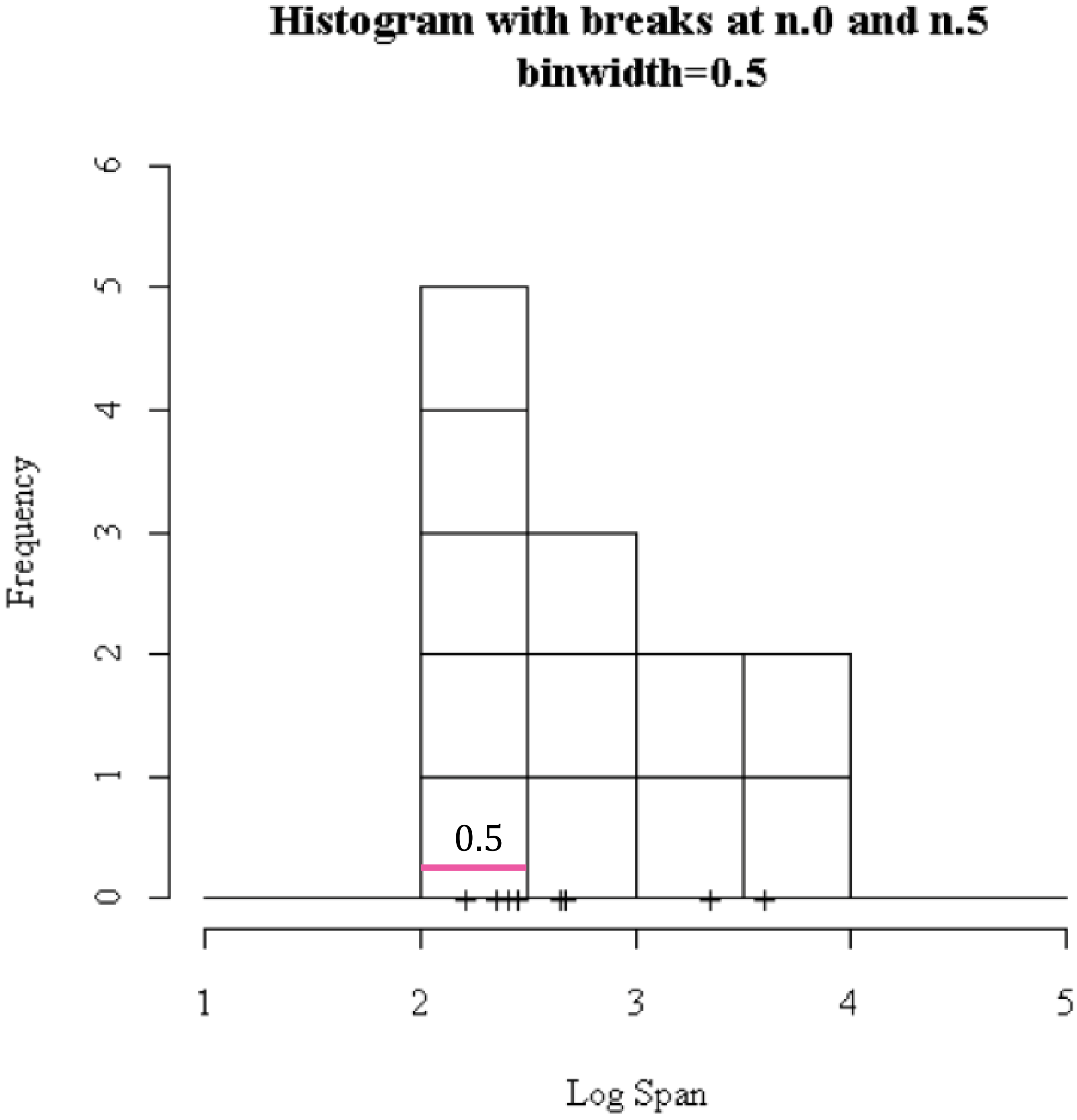
$m = 10$ (number of bins in each dimension)

$m^2 = 100$ (total number of bins for two dimensional data)

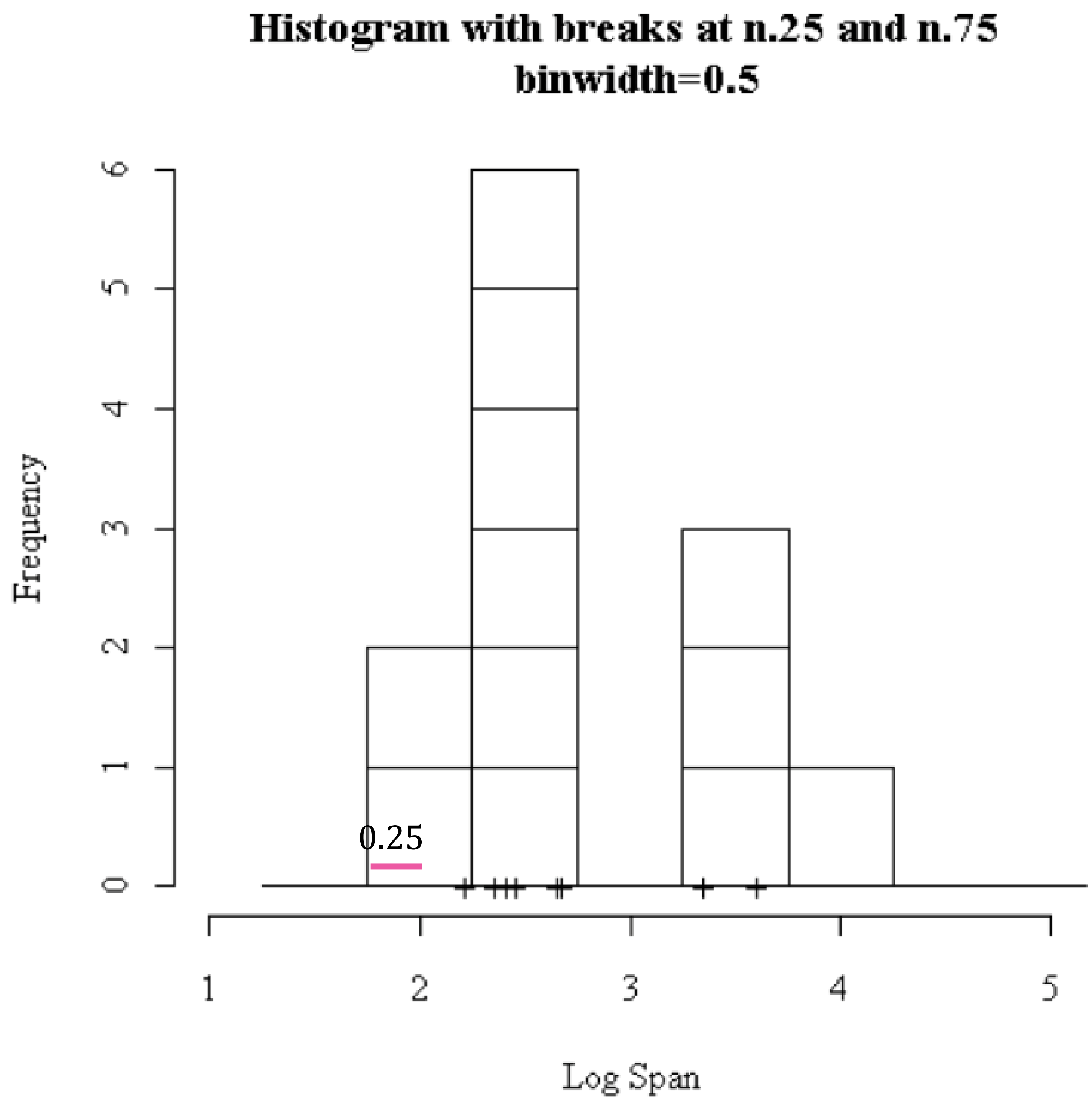


0.04
0.03
0.02
0.01
0
1
2
3
4
5
6
7
8
9
10
linear algebra score
1
2
3
4
5
6
7
8
9
10
statistics score

Output Depends on Where You Put the Bins



Output Depends on Where You Put the Bins



Kernel Density Estimation

- Kernel density estimator

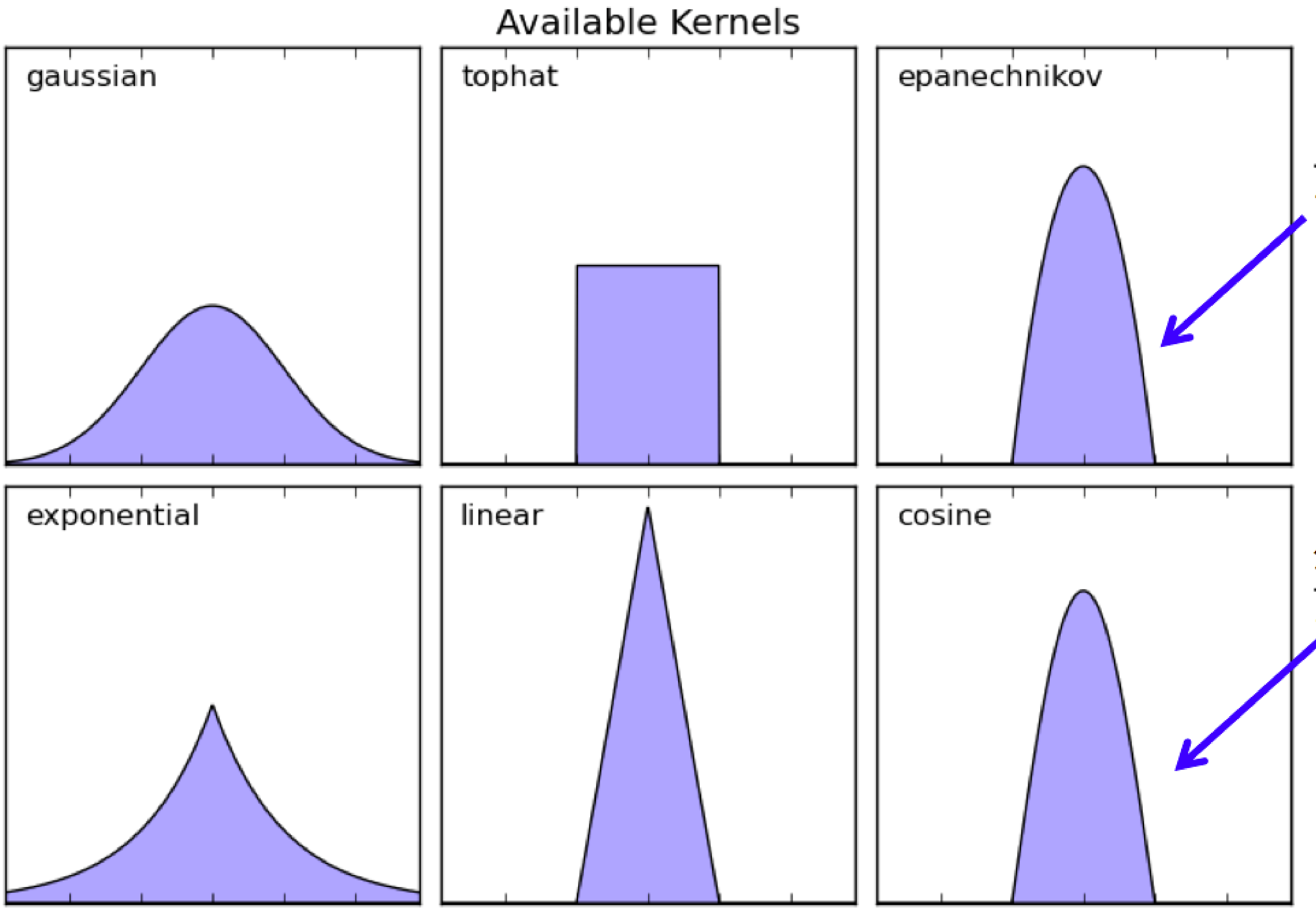
$$p(x) = \frac{1}{N}\sum_{i}^{N}\frac{1}{h}K\left(\frac{x_i - x}{h}\right)$$

- Smoothing kernel function
  - $K(u) \geq 0,$
  - $\int K(u)du = 1,$
  - $\int uK(u) = 0,$
  - $\int u^2K(u)du \leq \infty$

- An example: Gaussian kernel $K(u) = \frac{1}{\sqrt{2\pi}}e^{-u^2/2}$

Smoothing Kernel Functions

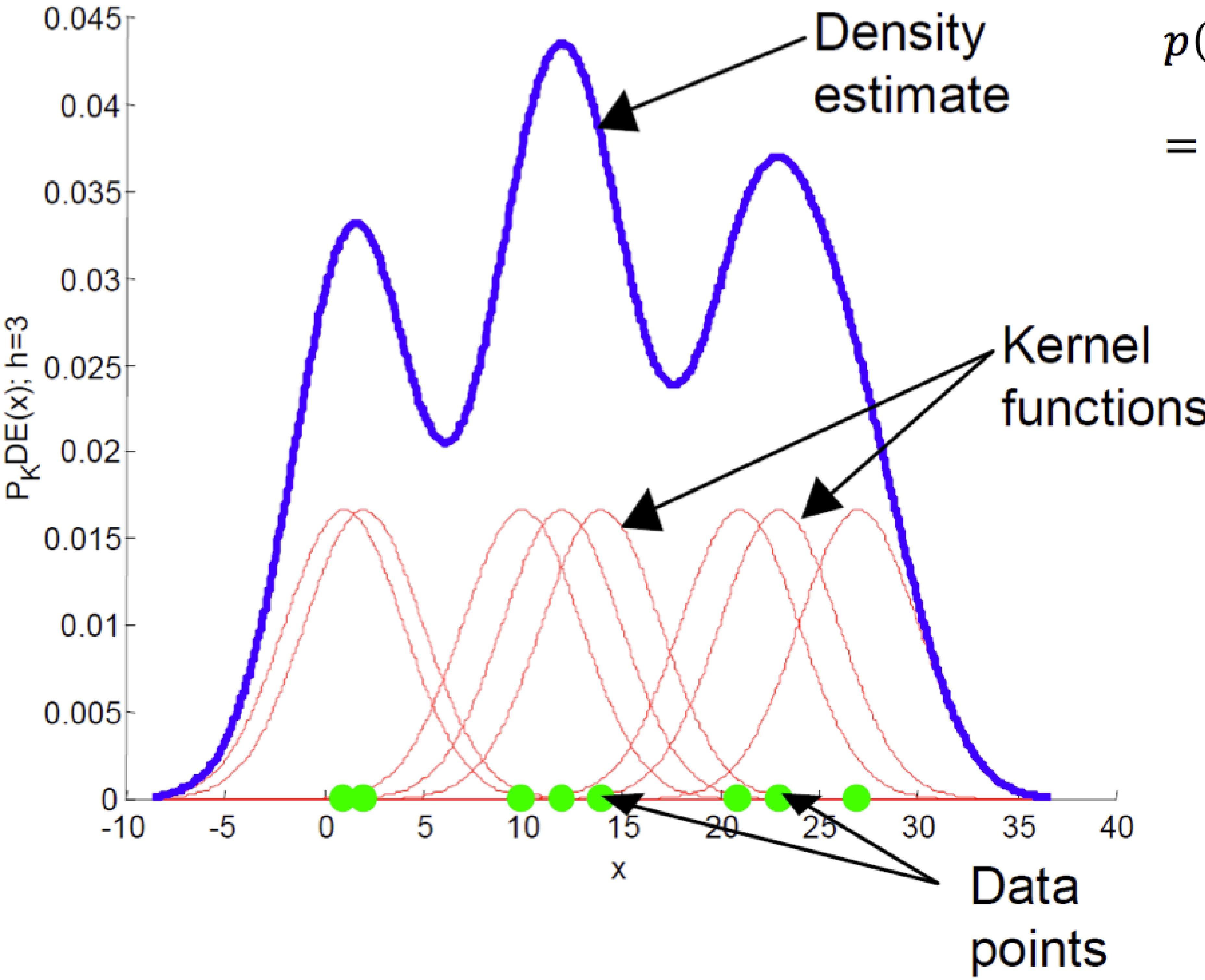
- An example: Gaussian kernel $K(u) = \frac{1}{\sqrt{2\pi}} e^{-u^2/2}$



$K(u) = \frac{3}{4}(1 - u^2) I(|u| \leq 1)$

$K(u) = \frac{\pi}{4} \cos\left(\frac{\pi}{2} u\right) I(|u| \leq 1)$

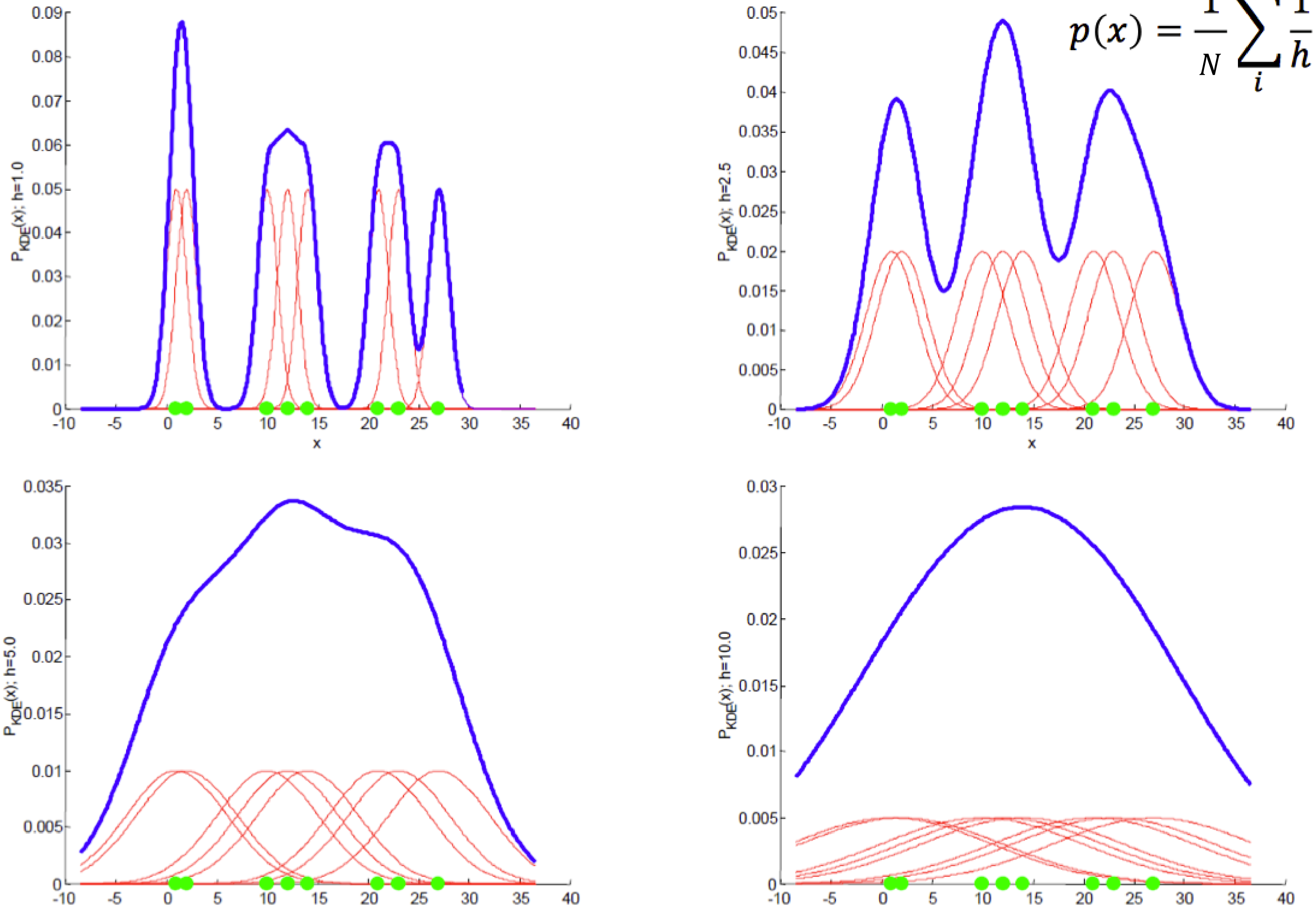
Example



$$p(x) = \frac{1}{N}\sum_{i}^{N}\frac{1}{h}K\left(\frac{x_i - x}{h}\right)$$

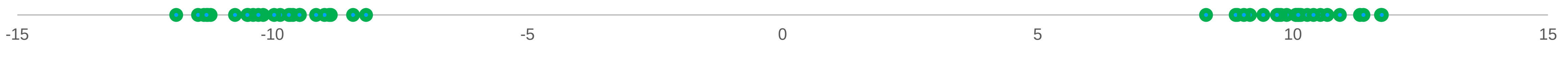
Effect of the Kernel Bandwidth

$$p(x) = \frac{1}{N}\sum_{i}^{N}\frac{1}{h}K\left(\frac{x_i - x}{h}\right)$$



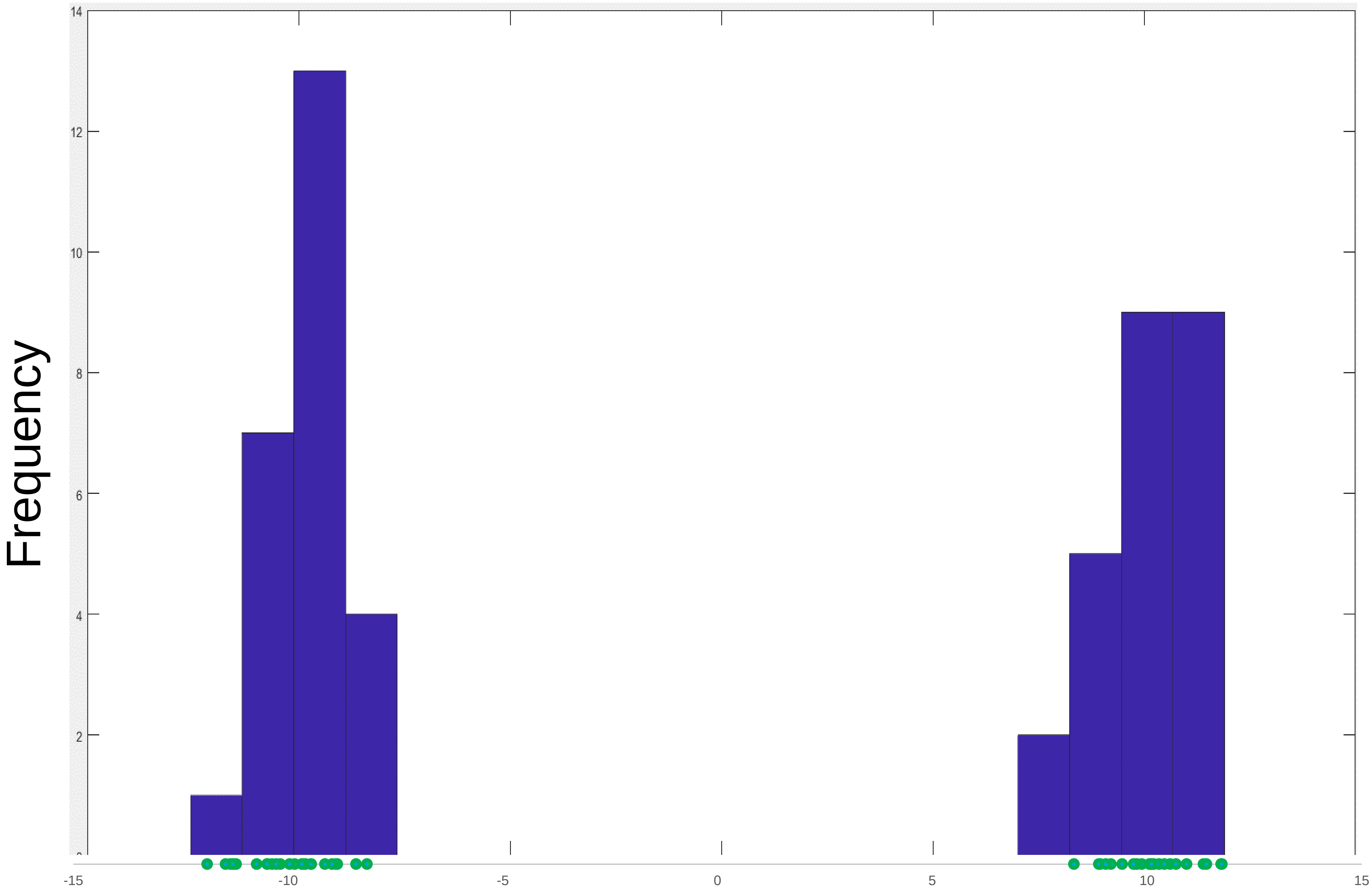
Visual Example

50 datapoints are given to us



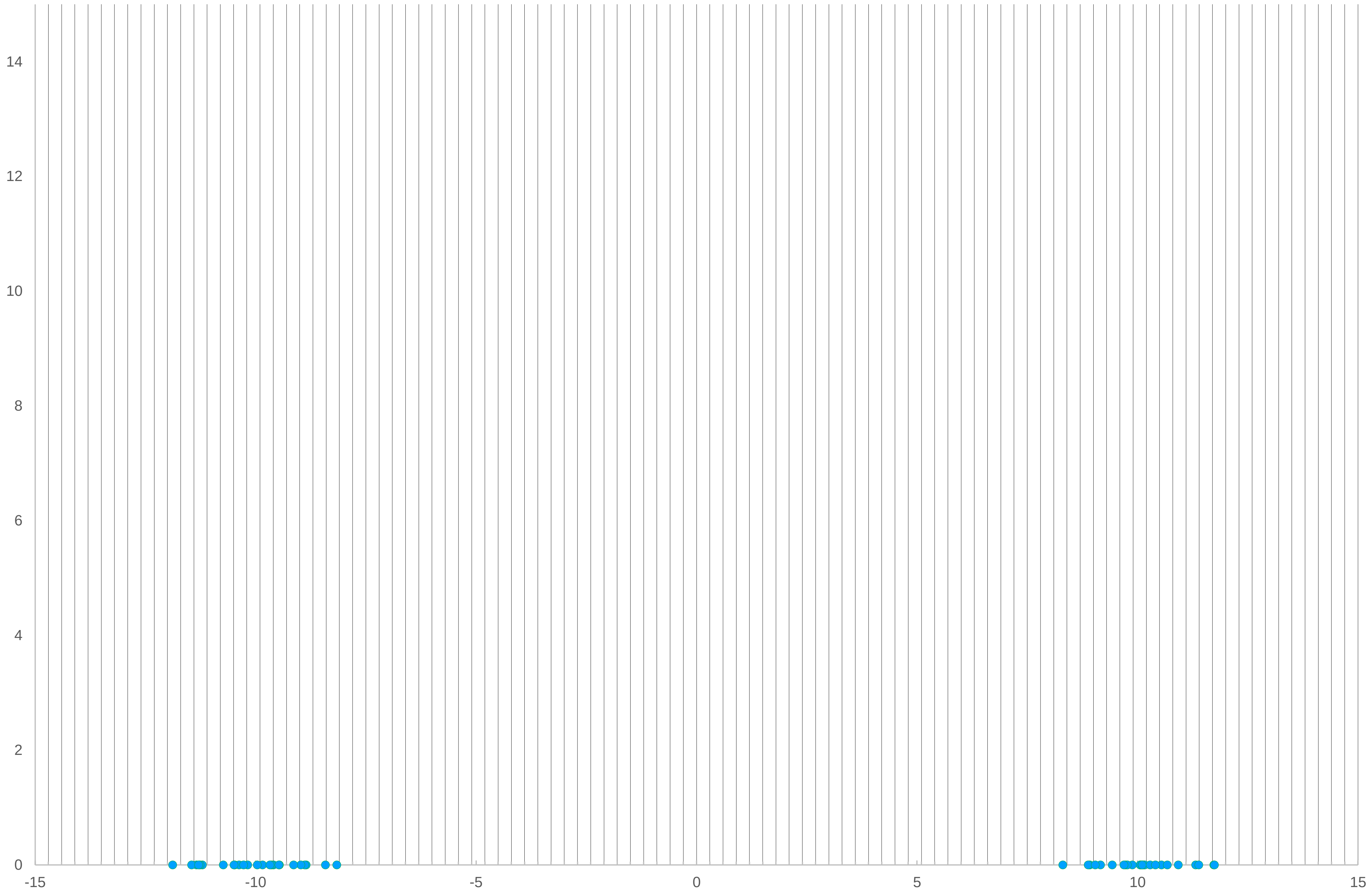
Visual Example

Let’s implement 20 bins histogram



Visual Example

Let’s create 200 uniform points to have a smoother density function
OR simply you can just implement this on each datapoint

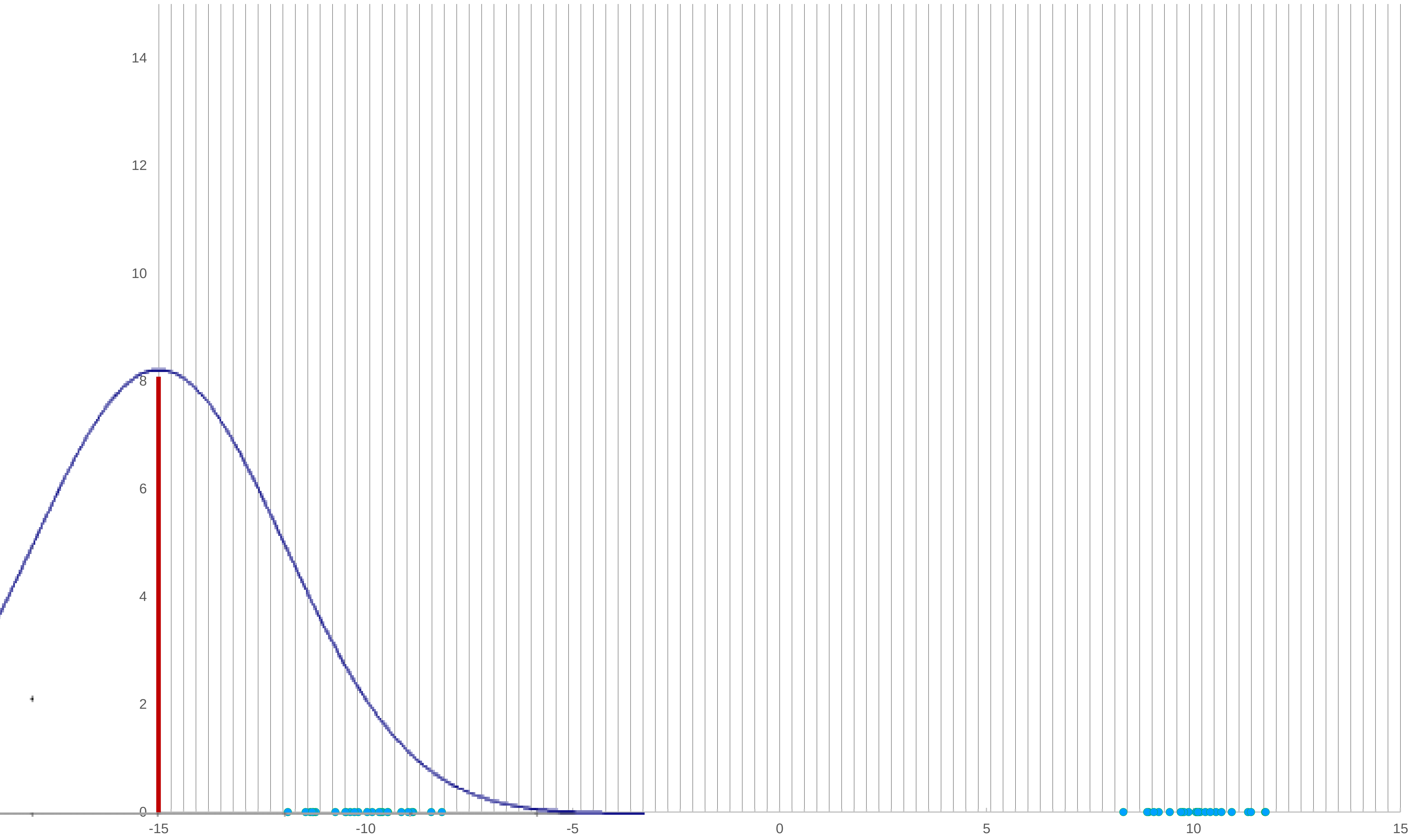


For **each** linearly spaced line, let's calculate the Gaussian kernel value over the given 50 points

$$p(x) = \frac{1}{N}\sum_{i}^{N}\frac{1}{h}K(u)$$

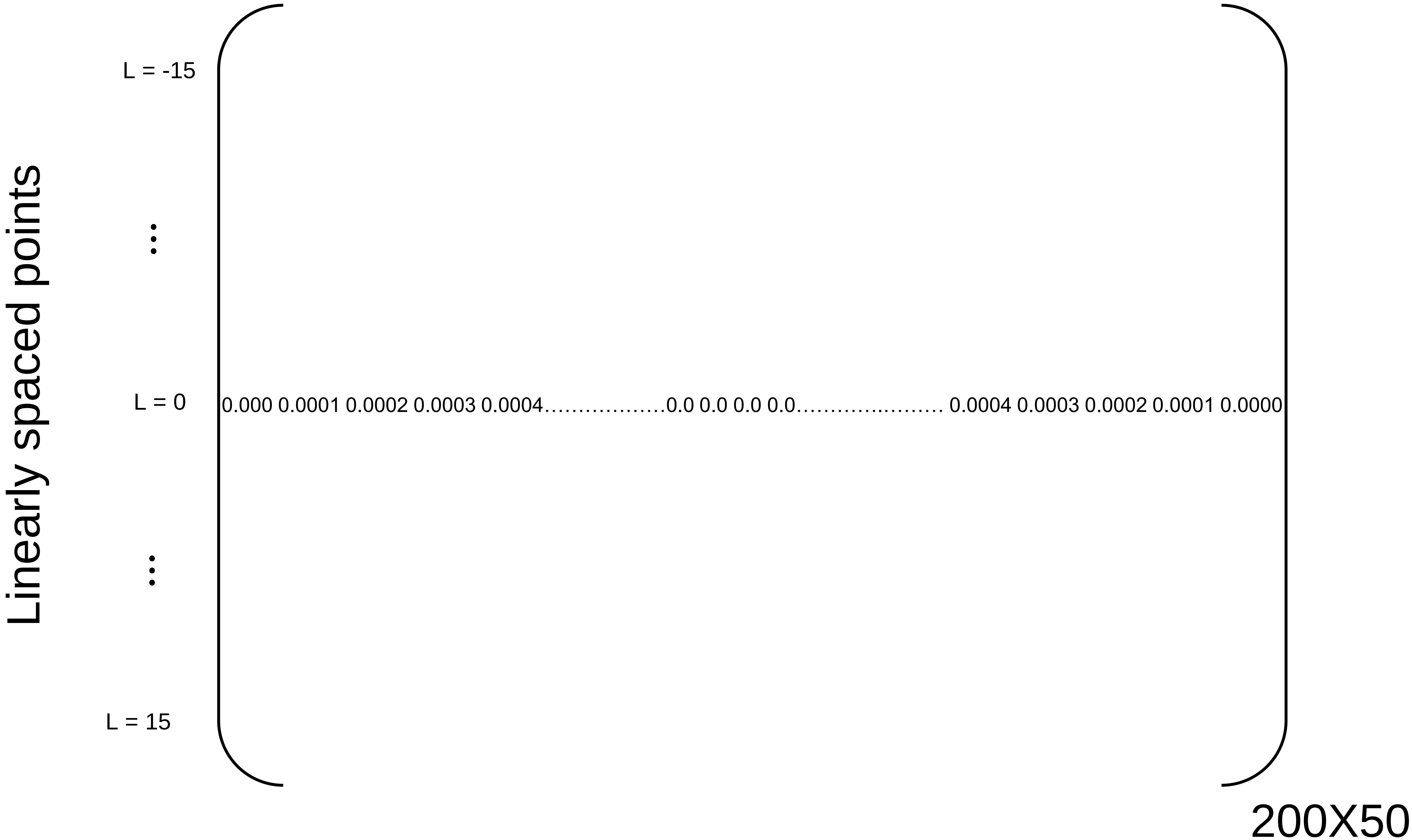
$$u = \frac{x_i - x}{h}$$

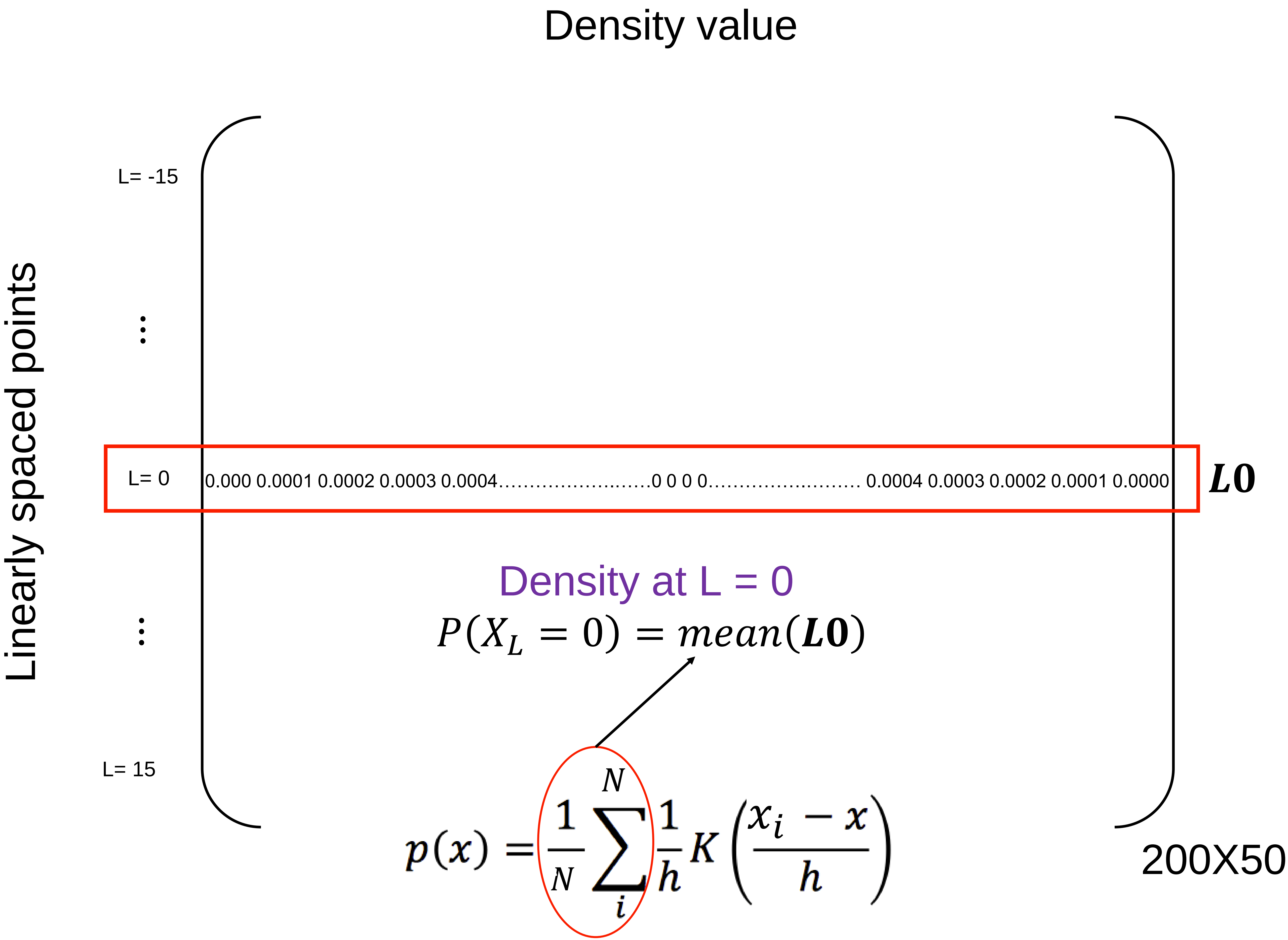
$$K(u) = \frac{1}{\sqrt{2\pi}}e^{-u^2/2}$$



Density value

As an example of kernel heights for line at 0

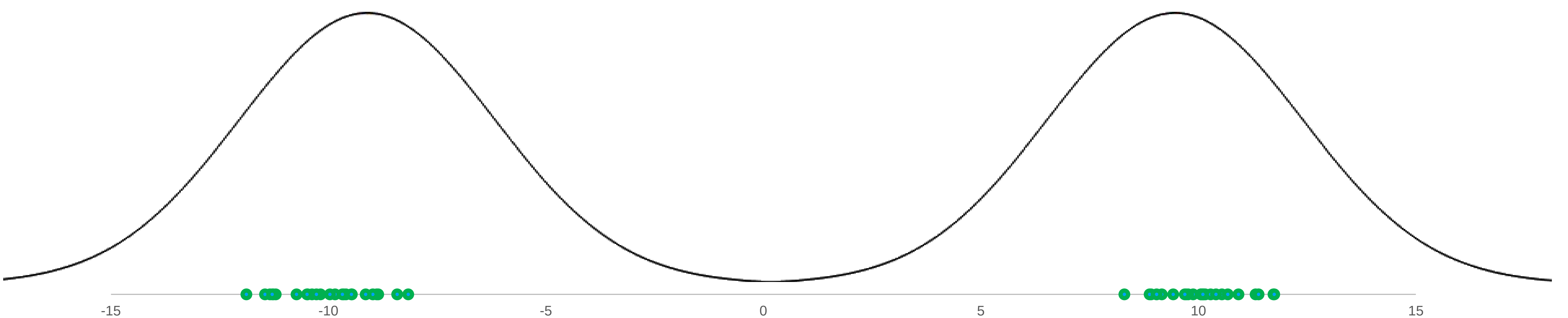



Density value
Linearly spaced points
L= -15
L= 0
0.000 0.0001 0.0002 0.0003 0.0004……………………0 0 0 0…………………… 0.0004 0.0003 0.0002 0.0001 0.0000
L0
L= 15
Density at L = 0
$P(X_L = 0) = mean(\boldsymbol{L0})$
$p(x) = \frac{1}{N}\sum_{i}^{N}\frac{1}{h}K\left(\frac{x_i - x}{h}\right)$
200X50

Visual Example

Based on Gaussian kernel estimator

Interactive Example



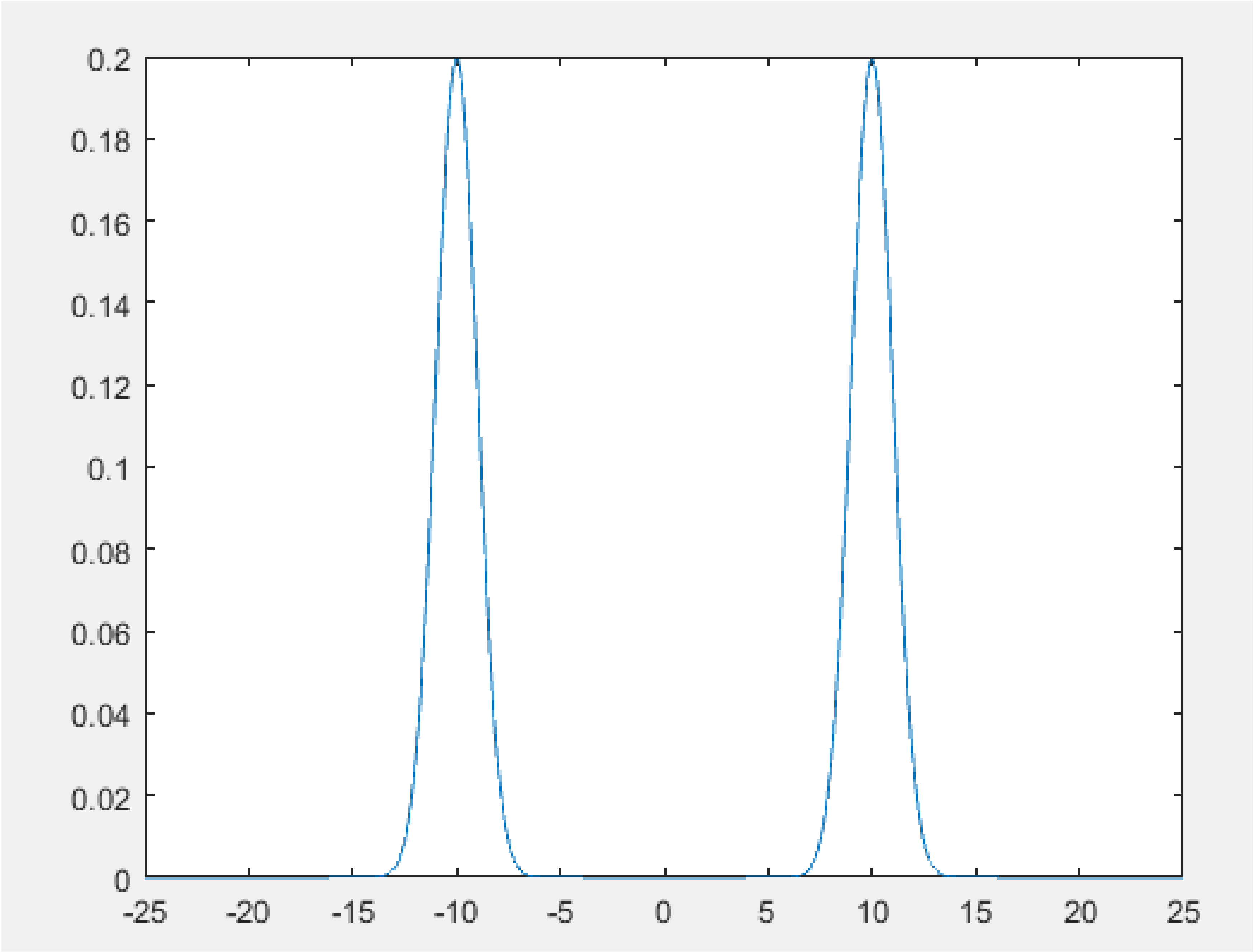
Numerical Example

$For\ \sigma = 1;$

```
% Data ; There are 200 data points (-13~<data<~13)
randn('seed',1)                                    % Used for reproducibility
data = [randn(100,1)-10; randn(100,1)+10]; % Two Normals mixed (GROUND TRUTH)
```

```
% Let's create apply density estimation over 1000 linearly spaced points

x = linspace(-25,+25,1000);   % grid lines

% Let's generate a "TRUE" density over all the bins given the "Ground Truth" information.

truepdf_firstnormal = exp(-.5*(x-10).^2)/sqrt(2*pi);
truepdf_secondnormal = exp(-.5*(x+10).^2)/sqrt(2*pi);
truepdf = truepdf_firstnormal/2 + truepdf_secondnormal/2;
% divided down by 2, because we are adding density value two times
```

```
plot(x,truepdf)                             % Plot True Density
```



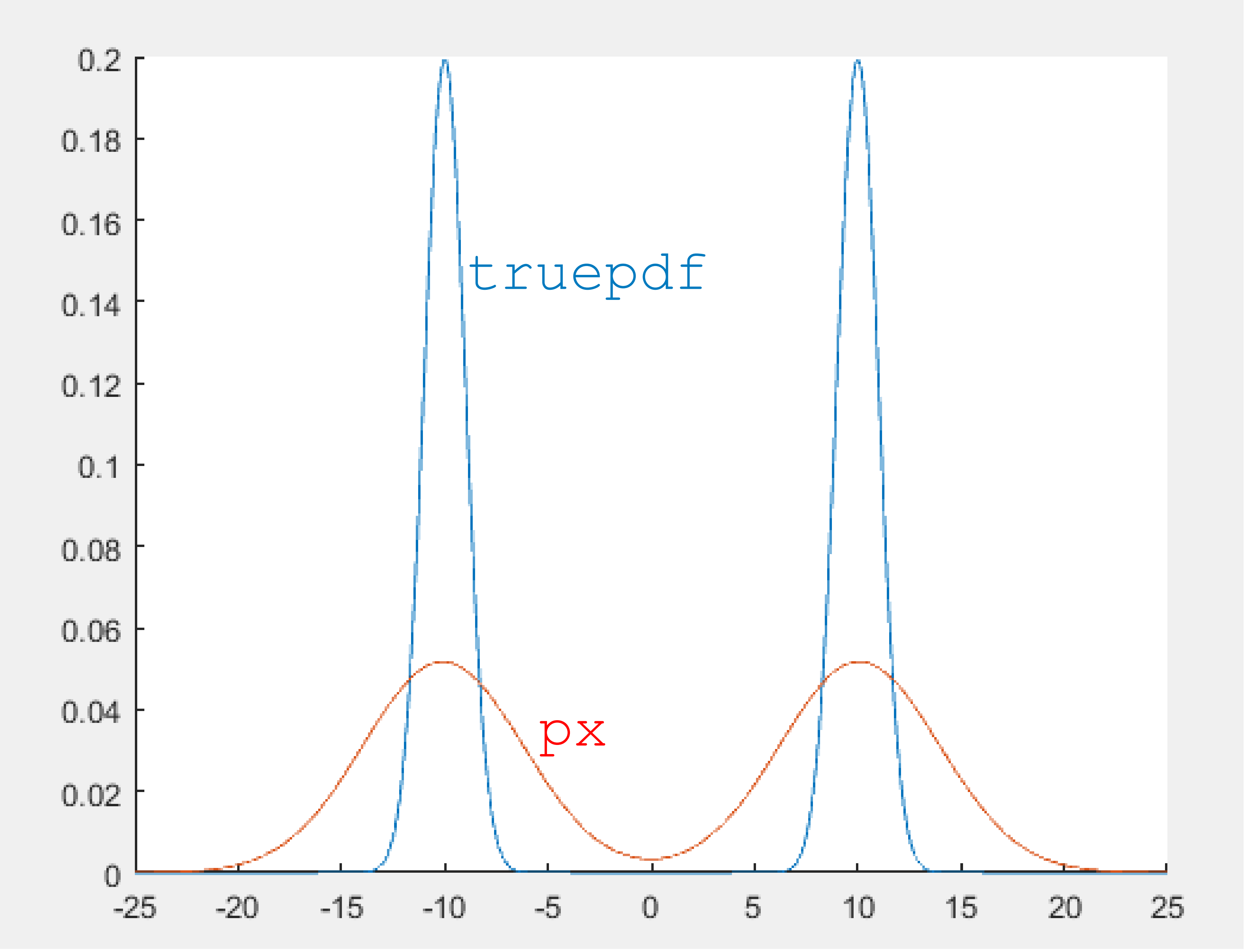
```
% Let's calculate Gaussian kernel density for each linearly spaced point over 200 Given data points
```

$$p(x) = \frac{1}{N}\sum_{i}^{N}\frac{1}{h}K\left(\frac{x_i - x}{h}\right) \qquad u = \frac{x_i - x}{h}$$

$$\text{Gaussian kernel } K(u) = \frac{1}{\sqrt{2\pi}}e^{-u^2/2}$$

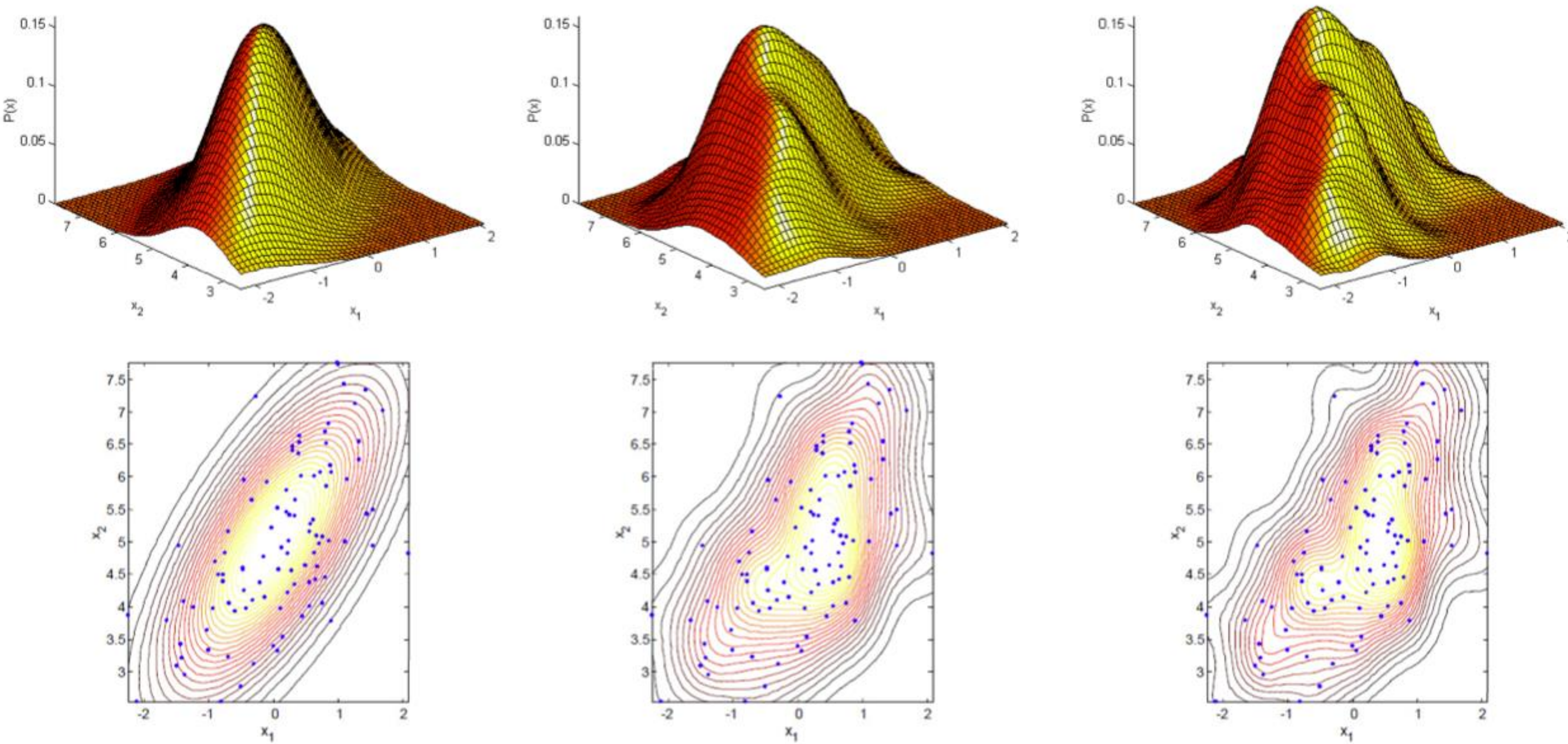
```
h = std(data)*(4/3/numel(data))^(1/5);% Bandwidth estimated by Silverman's Rule of Thumb

for i=1:size(x,1) % let's loop over grid lines
   u = (x(i)-data)./h; % length of u is 200
   Ku = exp(-.5*u.^2)/sqrt(2*pi);
   Ku = Ku./h;
   px(i) = mean(Ku);
end
```

```
plot(x,truepdf)
plot(x,px)
```

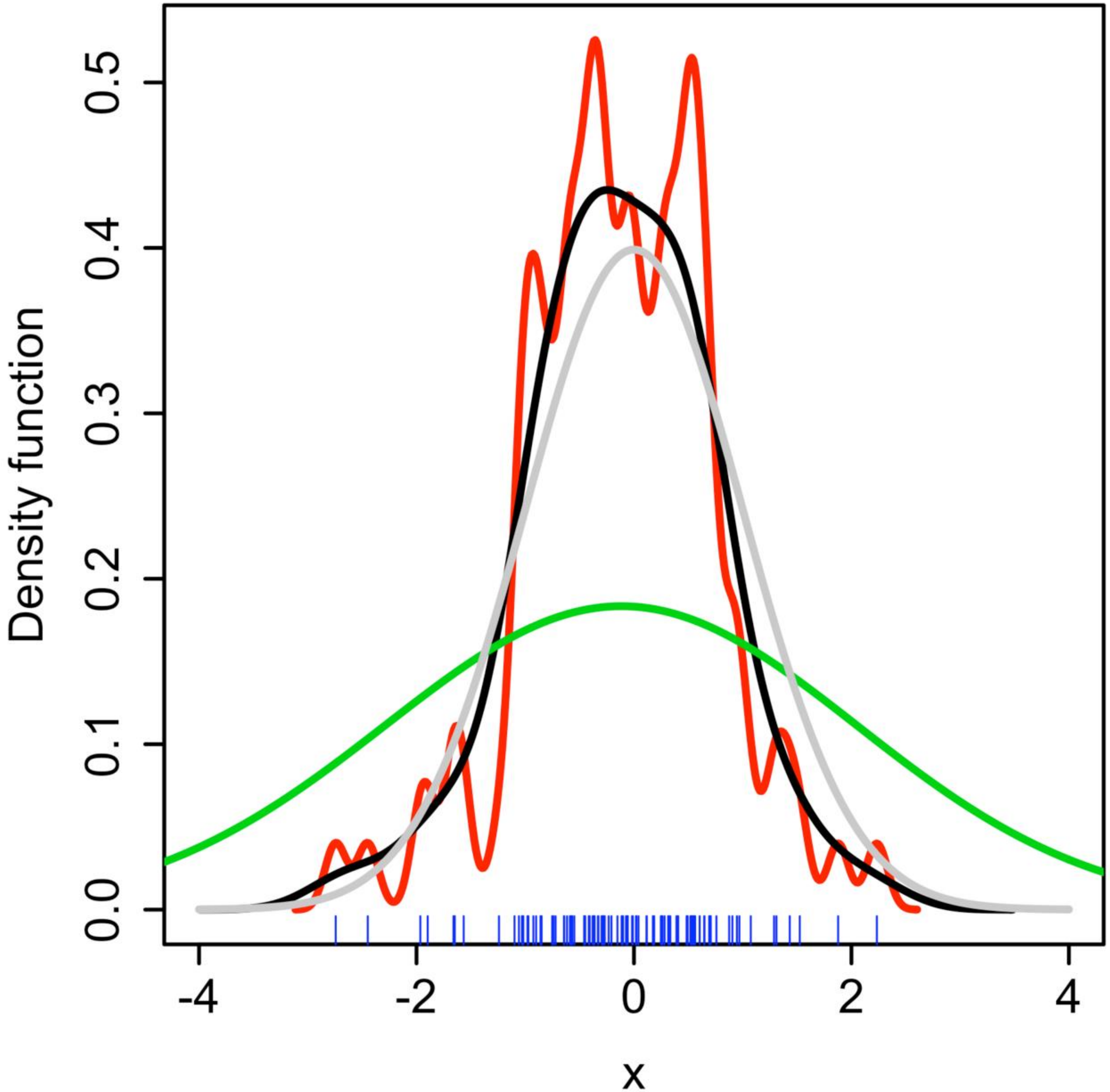


Two-Dimensional Examples

- This example shows the product KDE of a bivariate unimodal Gaussian
  - 100 data points were drawn from the distribution
  - The figures show the true density (left) and the estimates using $h = 1.06\sigma N^{-1/5}$ (middle) and $h = 0.9AN^{-1/5}$ (right)



Choosing Kernel Bandwidth



Choosing the Kernel Bandwidth

- Silverman's rule of thumb: If using the Gaussian kernel, a good choice for is

$$h = \left(\frac{4\hat{\sigma}^2}{3N}\right)^{\frac{1}{5}} \approx 1.06\hat{\sigma}N^{-\frac{1}{5}}$$

  $\hat{\sigma}$ is the standard deviation of the samples

- A better but more computational intensive approach:
  - Randomly split the data into two sets
  - Obtain a kernel density estimate for the first
  - Measure the likelihood of the second set
  - Repeat over many random splits and average

Non-parametric vs parametric

Summary

- Parametric density estimation
  - Maximum likelihood estimation
  - Different parametric forms
- Nonparametric density estimation
  - Histogram
  - Kernel density estimation