Non-parametric methods

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Parametric methods

- Assume some model (Gaussian, Bernoulli, Multinomial, logistic, network of logistic units, Linear, Quadratic) with fixed number of parameters
  - Gaussian Bayes, Naïve Bayes, Logistic Regression, Neural Networks

- Estimate parameters (μ,σ^2,θ,w,β) using MLE/MAP and plug in

- **Pro** – need few data points to learn parameters
- **Con** – Strong distributional assumptions, not satisfied in practice

Non-Parametric methods

- Typically don’t make any distributional assumptions
- As we have more data, we should be able to learn more complex models
- Let number of parameters scale with number of training data

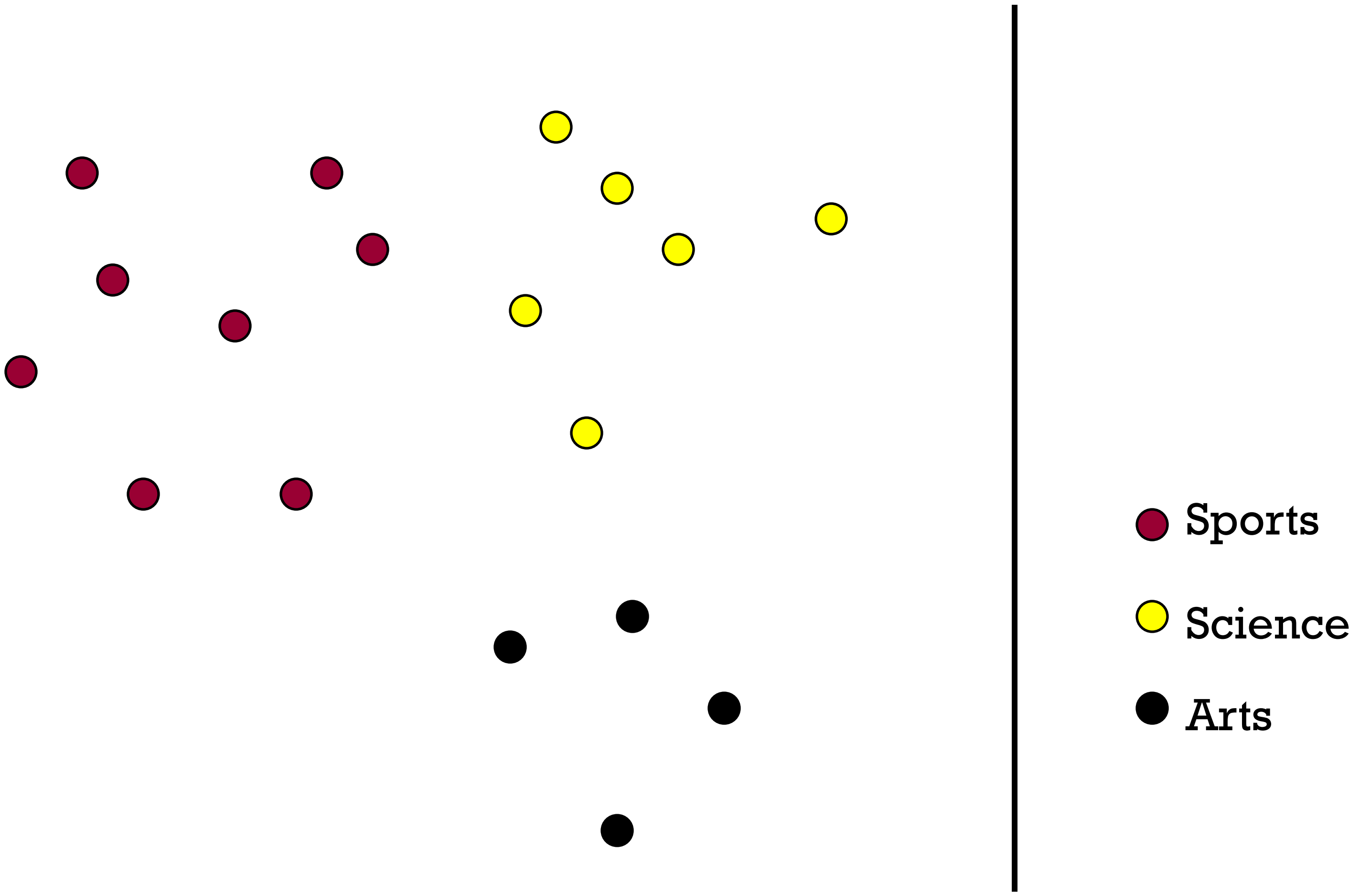
- Some nonparametric methods today (more later)

  Classification: k-NN (k-Nearest Neighbor) classifier

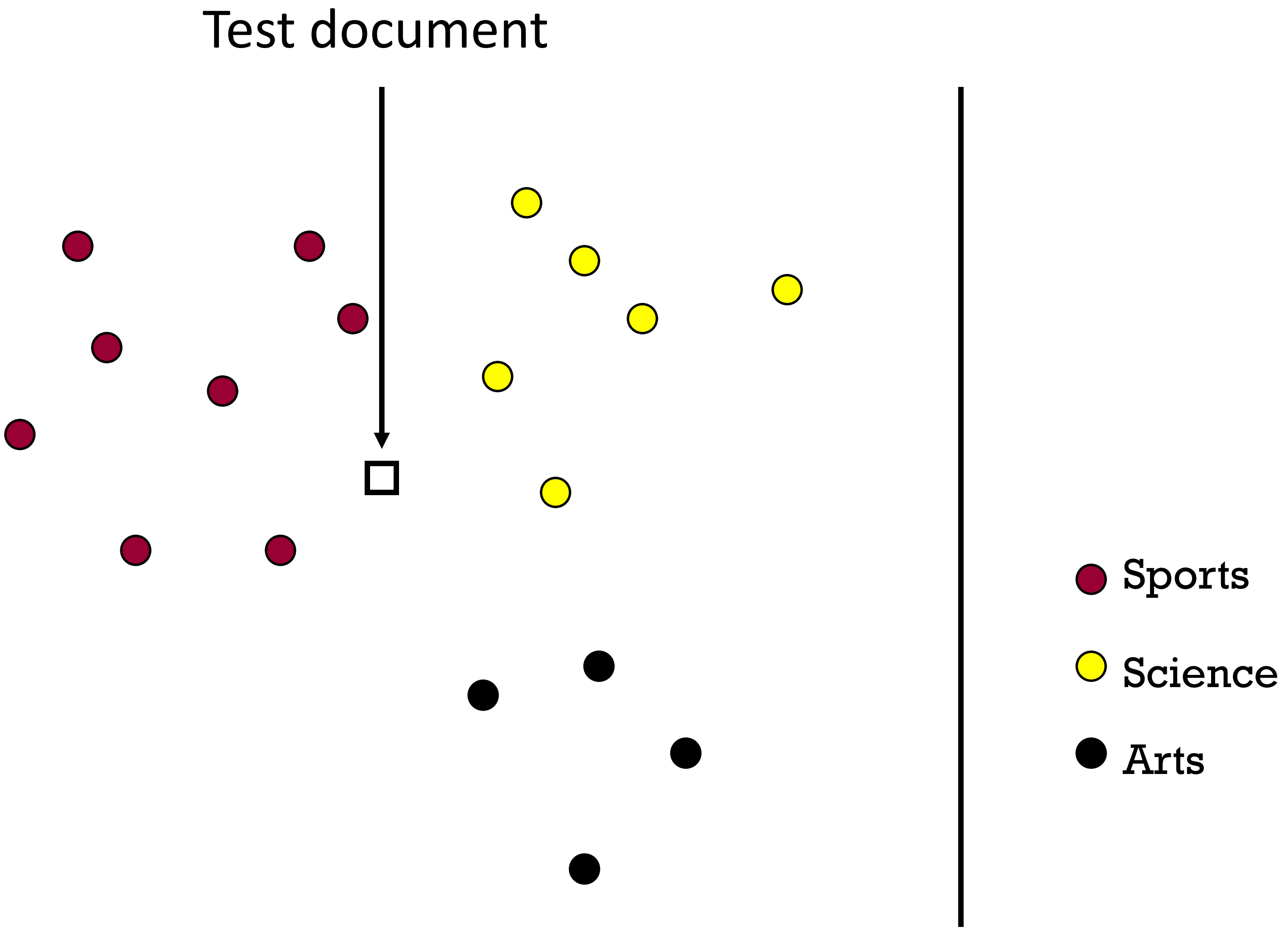
  Density estimation: k-NN, Histogram, Kernel density estimate

  Regression: Kernel regression

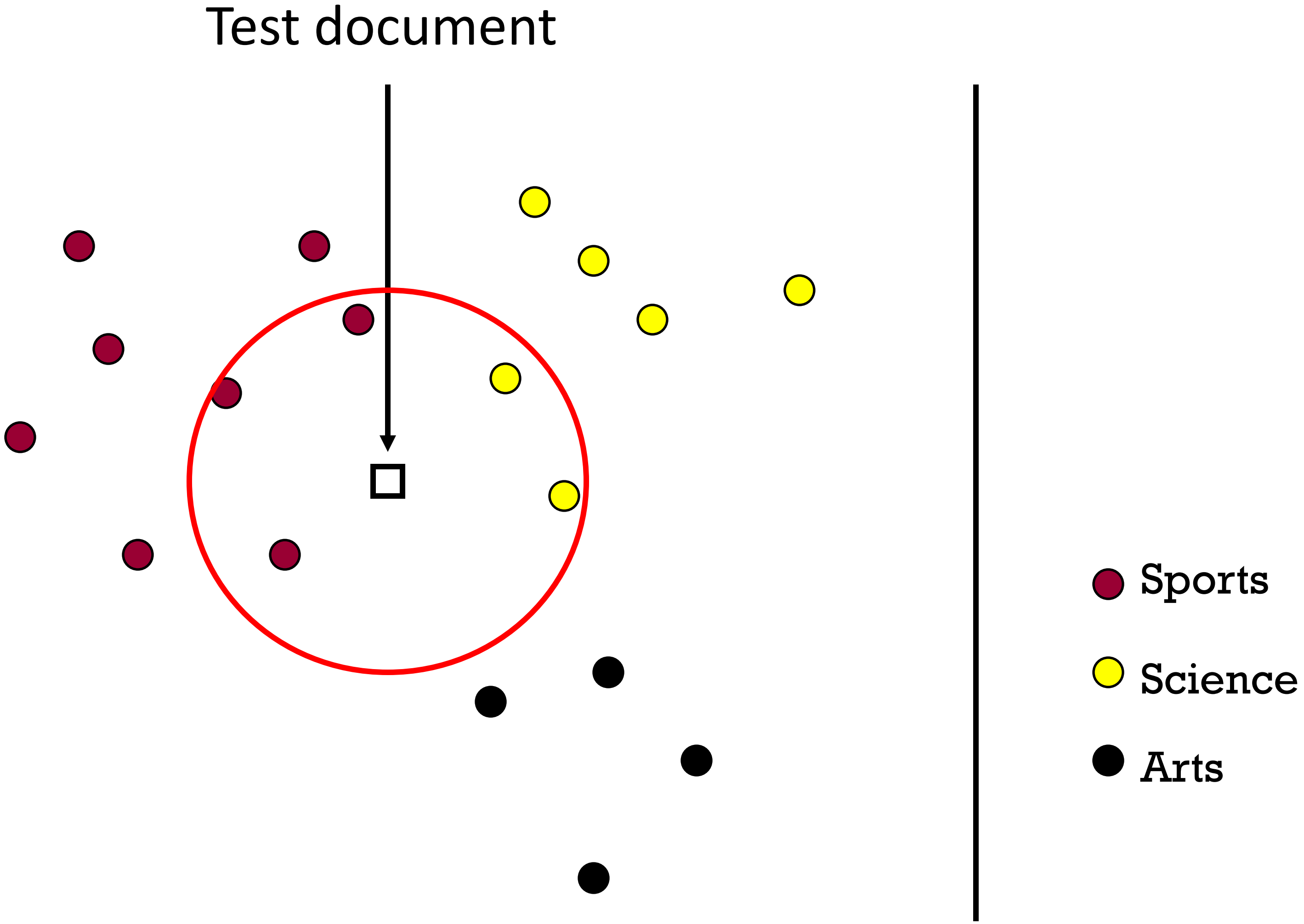
k-NN classifier



k-NN classifier



k-NN classifier (k=5)



What should we predict? … Average? Majority? Why?

k-NN classifier

- Optimal Classifier: $$\begin{aligned} f^*(x) &= \arg\max_y P(y|x) \\ &= \arg\max_y P(x|y)P(y) \end{aligned}$$

- k-NN Classifier: $$\begin{aligned} \widehat{f}_{kNN}(x) &= \arg\max_y \; \widehat{P}_{kNN}(x|y)\widehat{P}(y) \\ &= \arg\max_y \; k_y \end{aligned}$$

$$\widehat{P}_{kNN}(x|y) = \frac{k_y}{n_y}$$

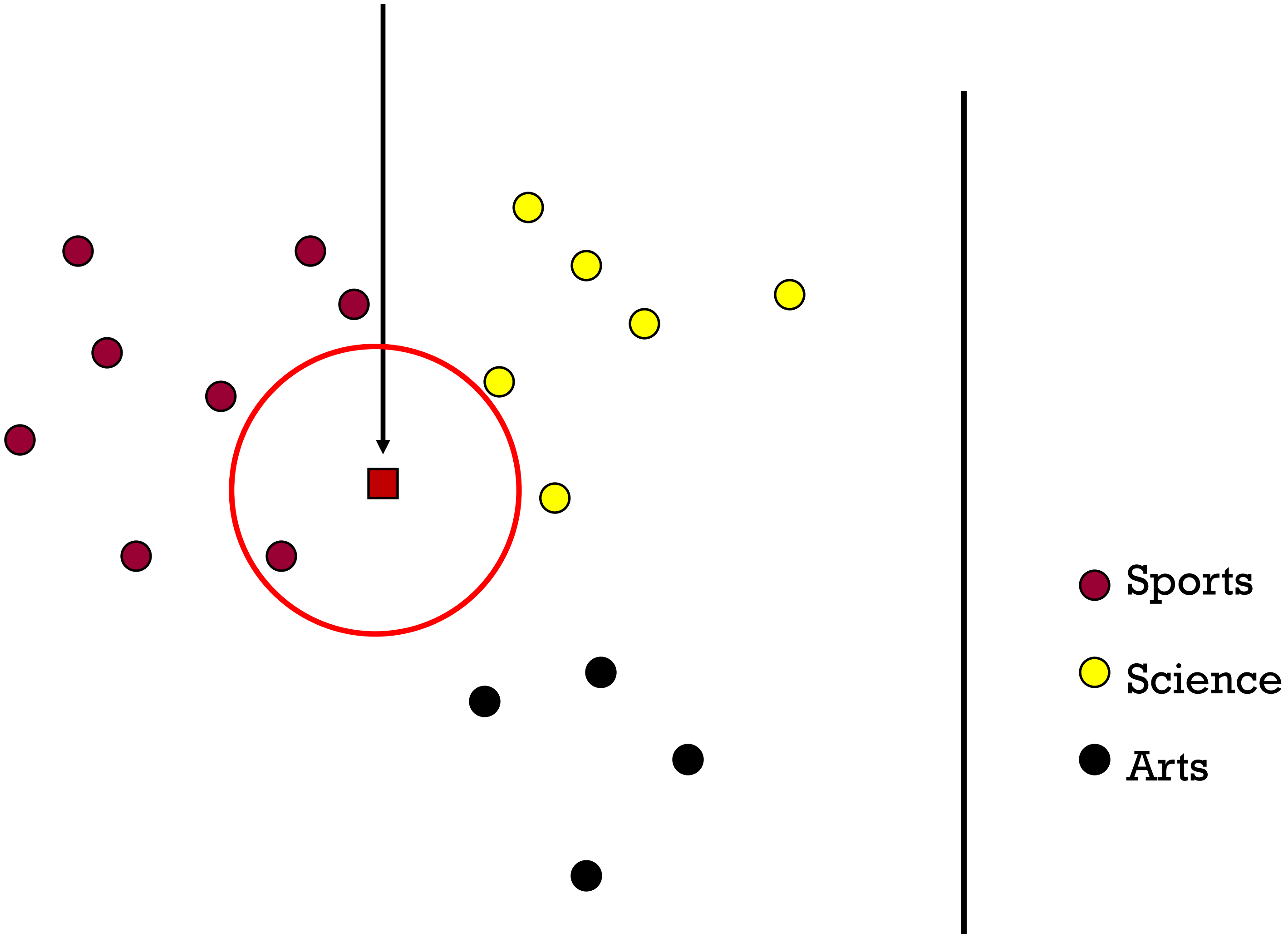
k_y → # training pts of class y amongst k NNs of x

n_y → # total training pts of class y

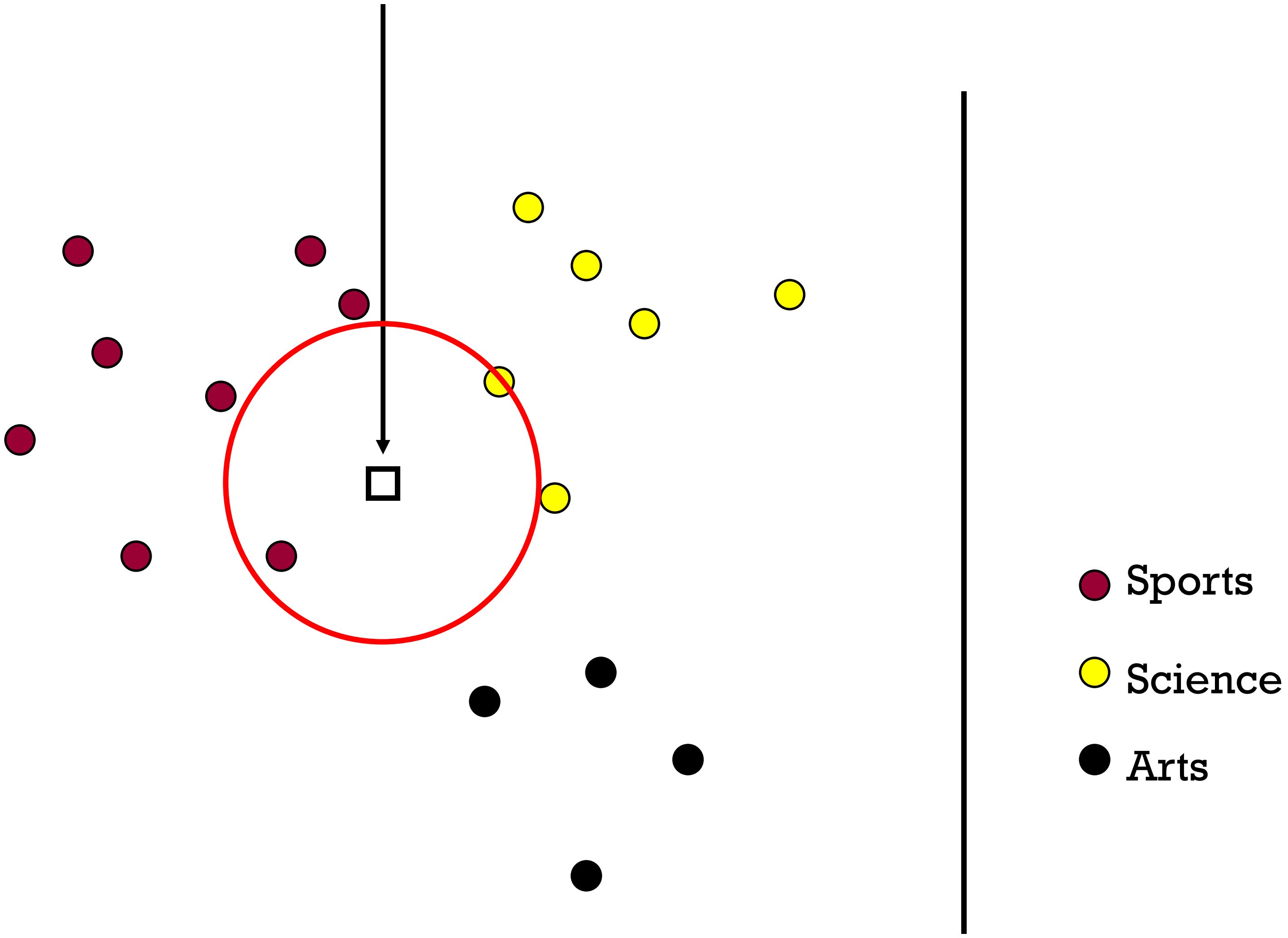
$$\sum_y k_y = k$$

$$\widehat{P}(y) = \frac{n_y}{n}$$

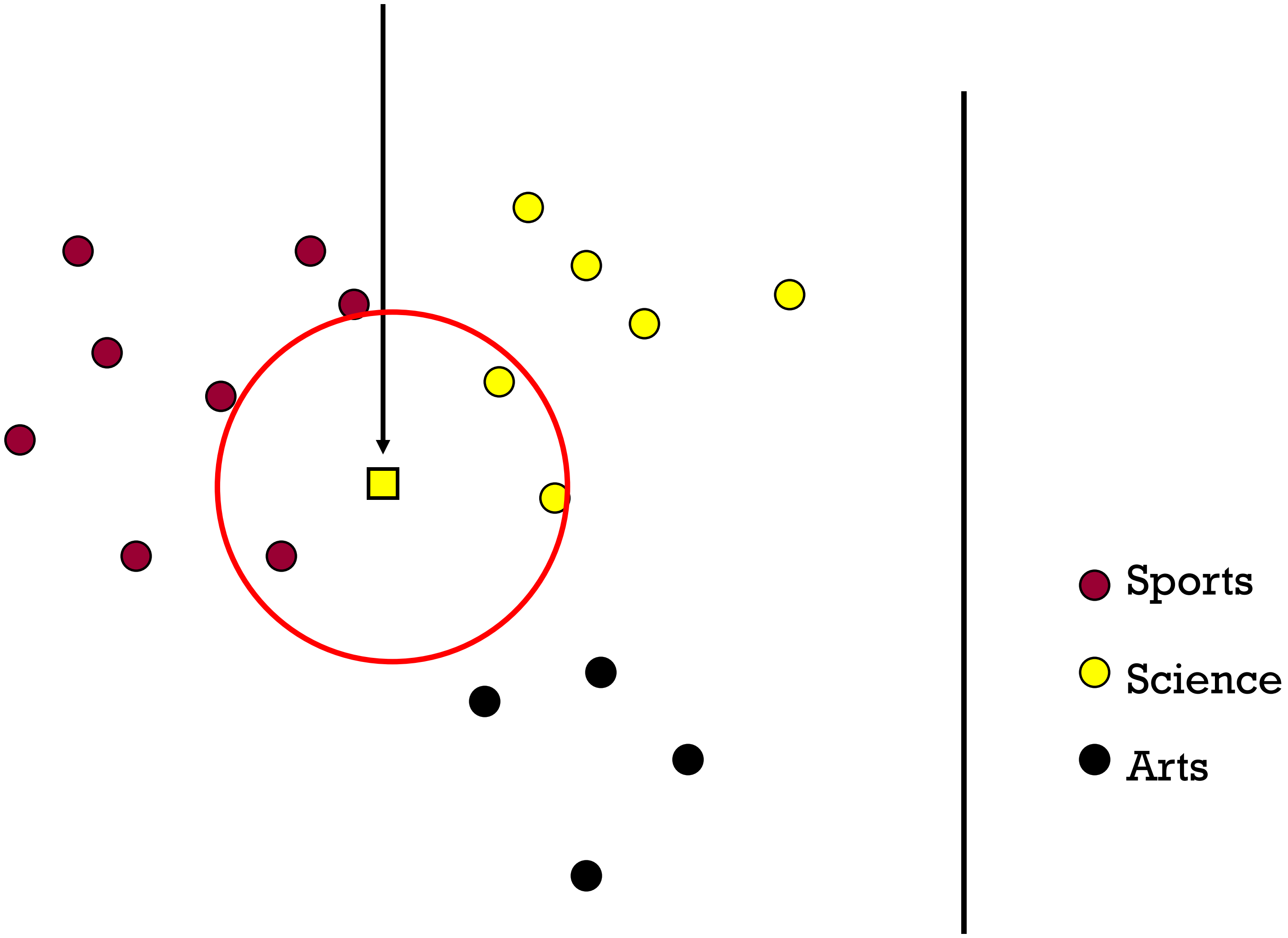
1-Nearest Neighbor (kNN) classifier



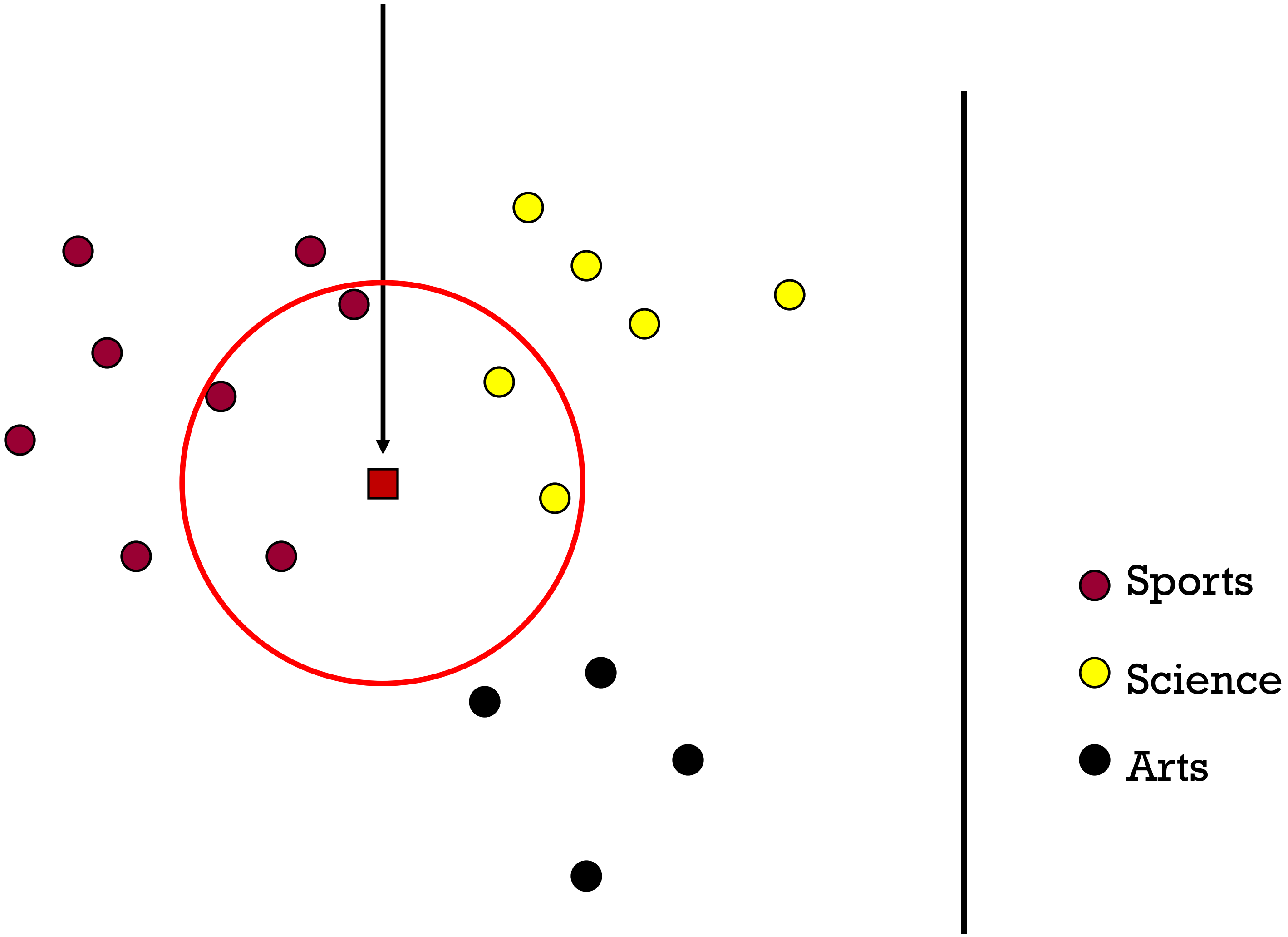
2-Nearest Neighbor (kNN) classifier



3-Nearest Neighbor (kNN) classifier

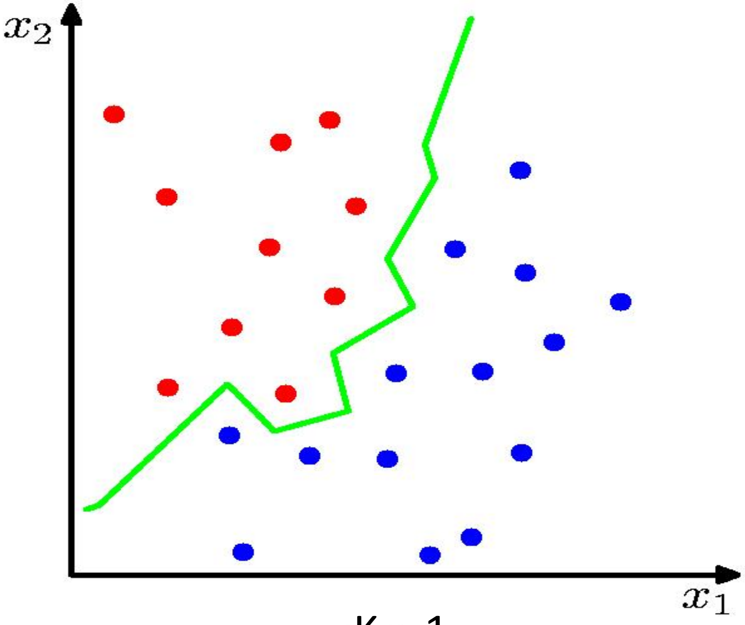


5-Nearest Neighbor (kNN) classifier



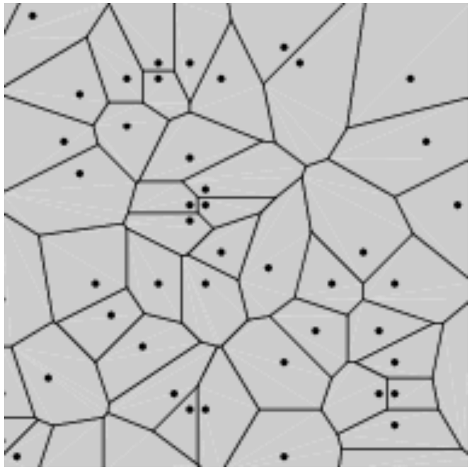
What is the best k?

1-NN classifier decision boundary



K = 1

Voronoi Diagram



As k increases, boundary becomes smoother (less jagged).

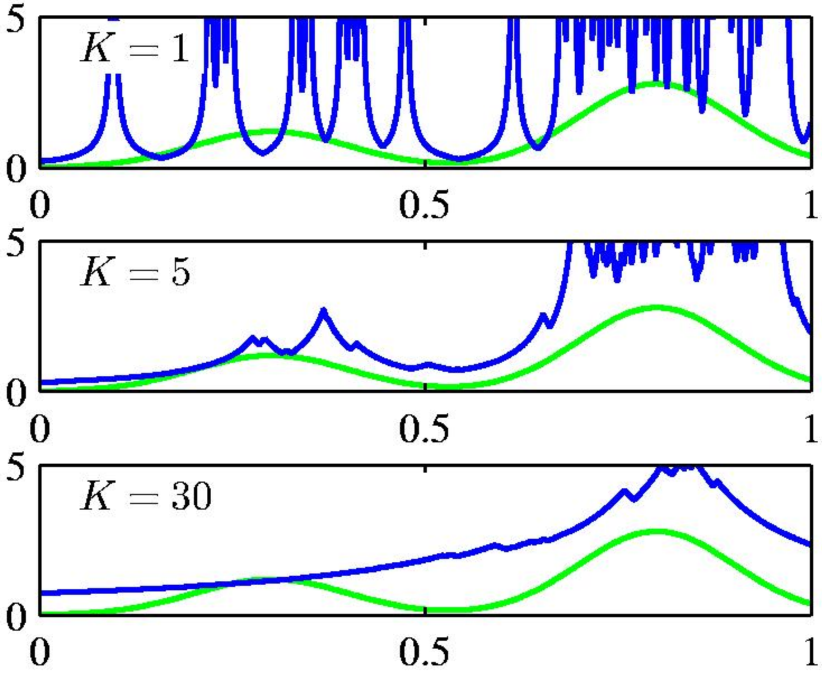
What is the best k?

Approximation vs. Stability (aka Bias vs Variance) Tradeoff

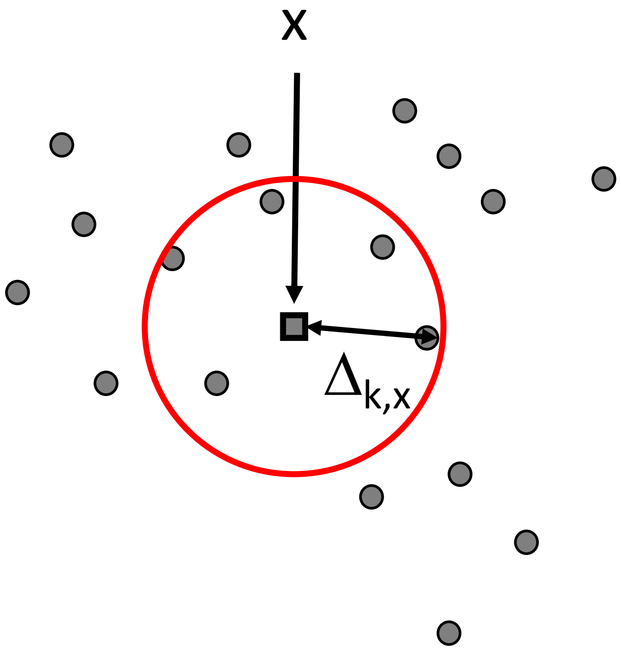
- Larger K => predicted label is more stable
- Smaller K => predicted label can approximate best classifier well given enough data

k-NN density estimation

$$\widehat{p}(x) = \frac{k}{n\Delta_{k,x}}$$



k acts as a smoother.



Not very popular for density estimation – spiked estimates

Histogram density estimate

Partition the feature space into distinct bins with widths Δ_i and count the number of observations, n_i, in each bin.

$$\widehat{p}(x) = \frac{n_i}{n\Delta_i}\mathbf{1}_{x\in \mathrm{Bin}_i}$$

"Local relative frequency"

- Often, the same width is used for all bins, $\Delta_i = \Delta$.
- Δ acts as a smoothing parameter.

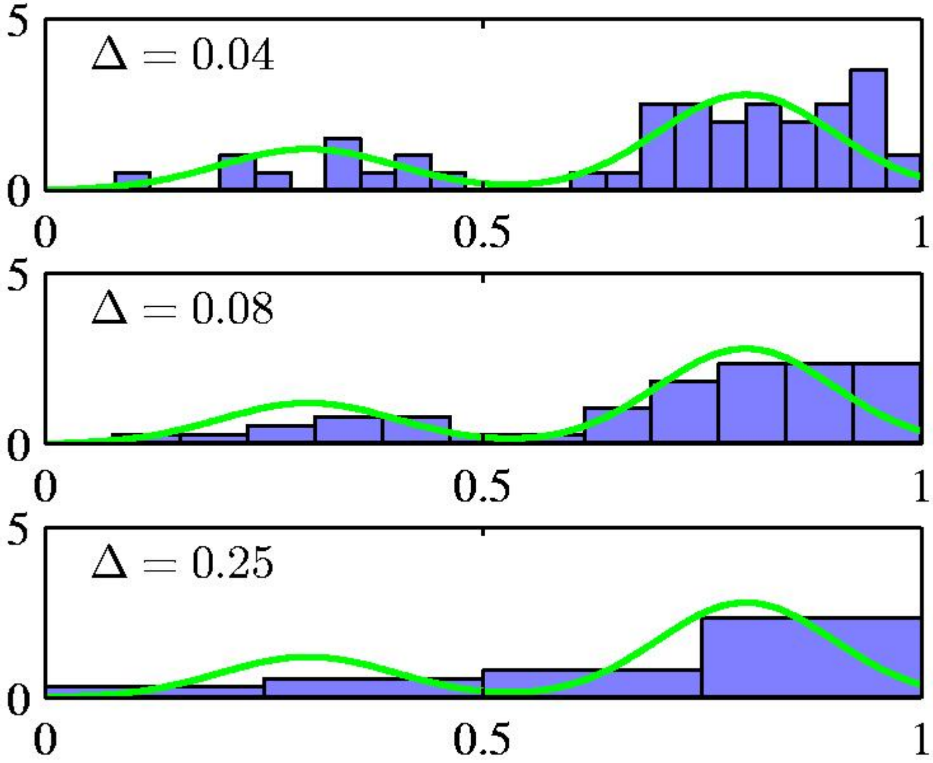


Image src: Bishop book

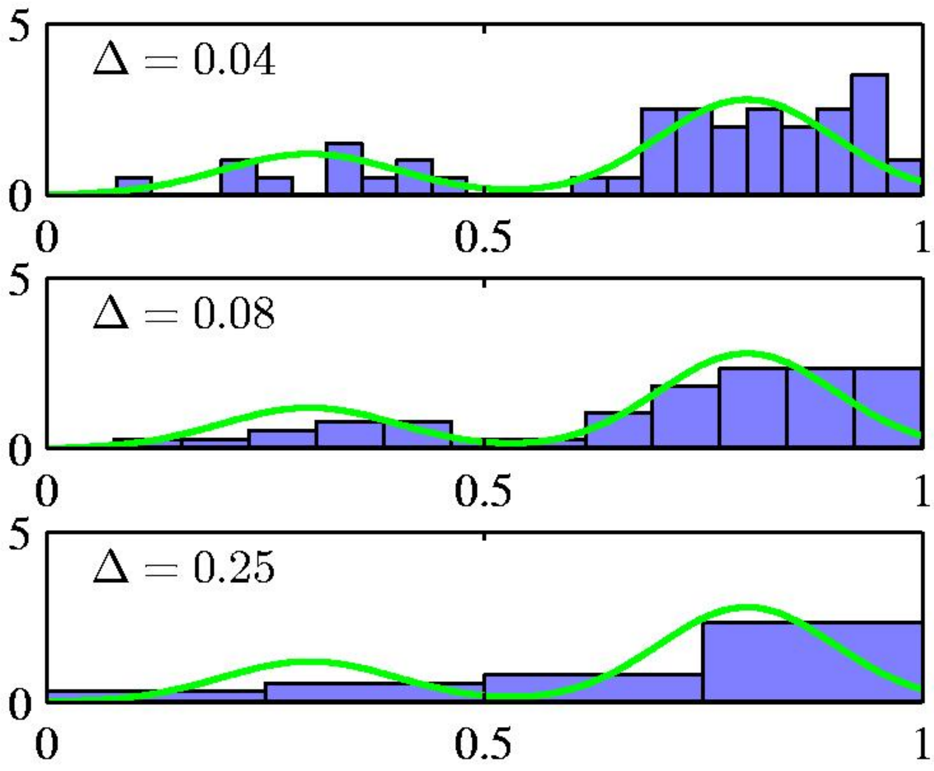
Effect of histogram bin width

$$\widehat{p}(x) = \frac{n_i}{n\Delta}\mathbf{1}_{x\in \text{Bin}_i}$$

# bins = 1/Δ

Small Δ, large #bins
Good fit but unstable
(few points per bin)
"**Small bias**, **Large variance**"

Large Δ, small #bins
Poor fit but stable
(many points per bin)
"**Large bias**, **Small variance**"



Histogram as MLE

- Underlying model – density is constant on each bin

  Parameters p_j : density in bin j

  Note $\sum_j p_j = 1/\Delta$ since $\int p(x)dx = 1$

- Maximize likelihood of data under probability model with parameters p_j

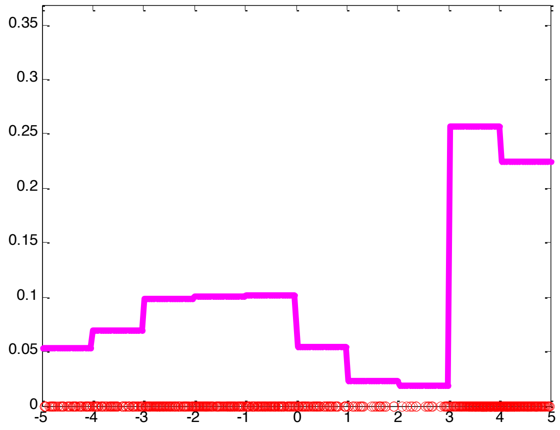
$$\hat{p}(x) = \arg\max_{\{p_j\}} P(X_1, \ldots, X_n; \{p_j\}_{j=1}^{1/\Delta}) \quad \text{s.t.} \quad \sum_j p_j = 1/\Delta$$

- Show that histogram density estimate is MLE under this model

Kernel density estimate

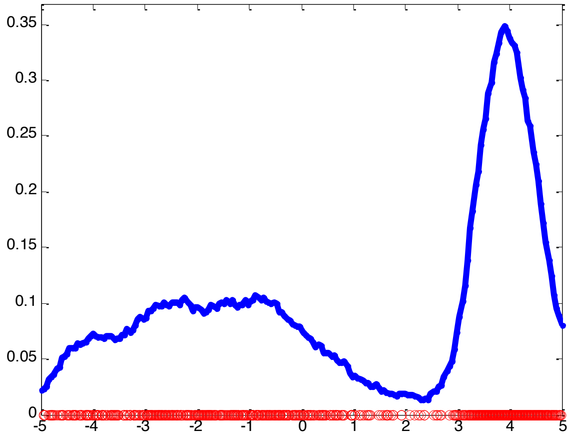
- Histogram – blocky estimate

$$\widehat{p}(x) = \frac{1}{\Delta}\frac{\sum_{j=1}^{n} \mathbf{1}_{X_j \in \text{Bin}_x}}{n}$$



- Kernel density estimate aka "Parzen/moving window method"

$$\widehat{p}(x) = \frac{1}{\Delta}\frac{\sum_{j=1}^{n} \mathbf{1}_{||X_j - x|| \leq \Delta}}{n}$$



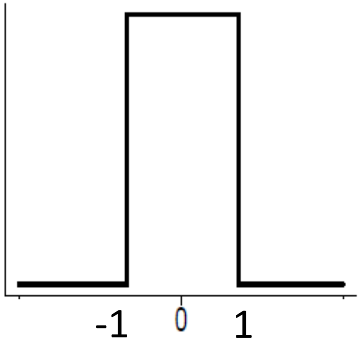
Kernel density estimate

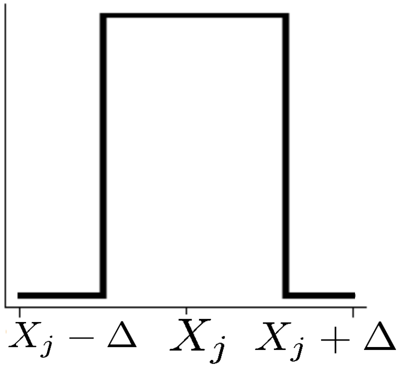
- $\widehat{p}(x) = \frac{1}{\Delta} \frac{\sum_{j=1}^{n} K\left(\frac{X_j - x}{\Delta}\right)}{n}$ more generally

$$K\left(\frac{X_j - x}{\Delta}\right)$$

boxcar kernel :

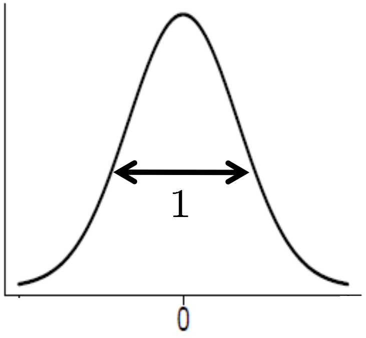
$$K(x) = \frac{1}{2} I(x),$$

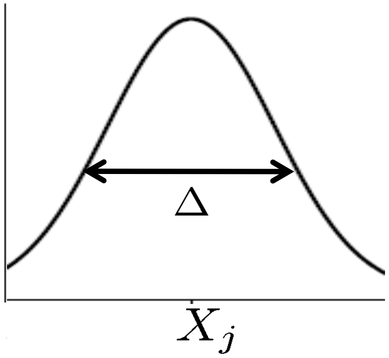




Gaussian kernel :

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

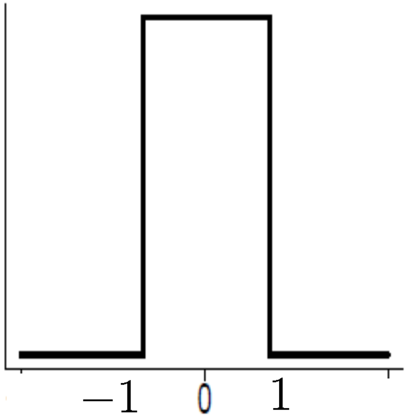




Kernels

boxcar kernel :

$$K(x) = \frac{1}{2} I(x),$$



Gaussian kernel :

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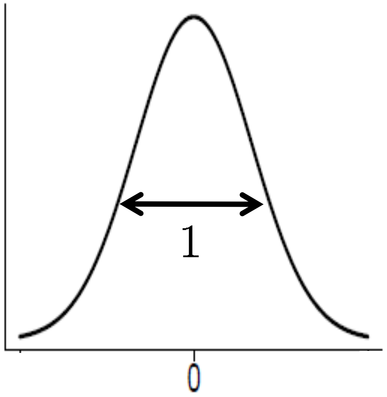


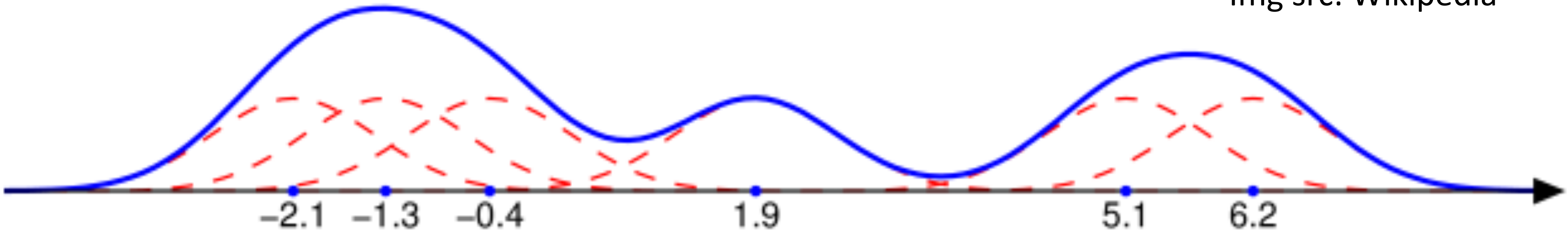
Any kernel function that satisfies

$$\begin{aligned} K(x) &\geq 0, \\ \int K(x)dx &= 1 \end{aligned}$$

Kernel density estimation

- Place small "bumps" at each data point, determined by the kernel function.
- The estimator consists of a (normalized) "sum of bumps”.

Img src: Wikipedia



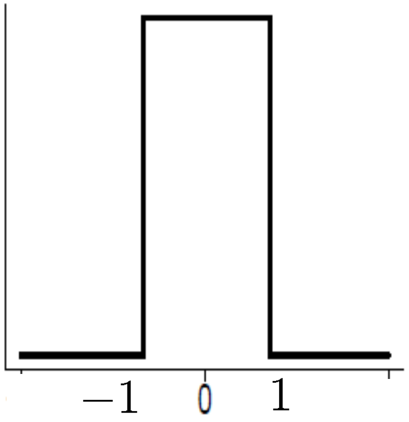
Gaussian bumps (red) around six data points and their sum (blue)

- Note that where the points are denser the density estimate will have higher values.

Choice of Kernels

boxcar kernel :

$$K(x) = \frac{1}{2} I(x),$$

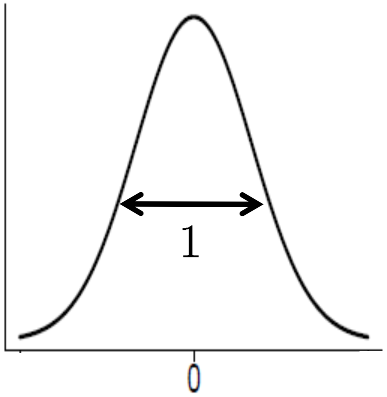


Finite support

– only need local points to compute estimate

Gaussian kernel :

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

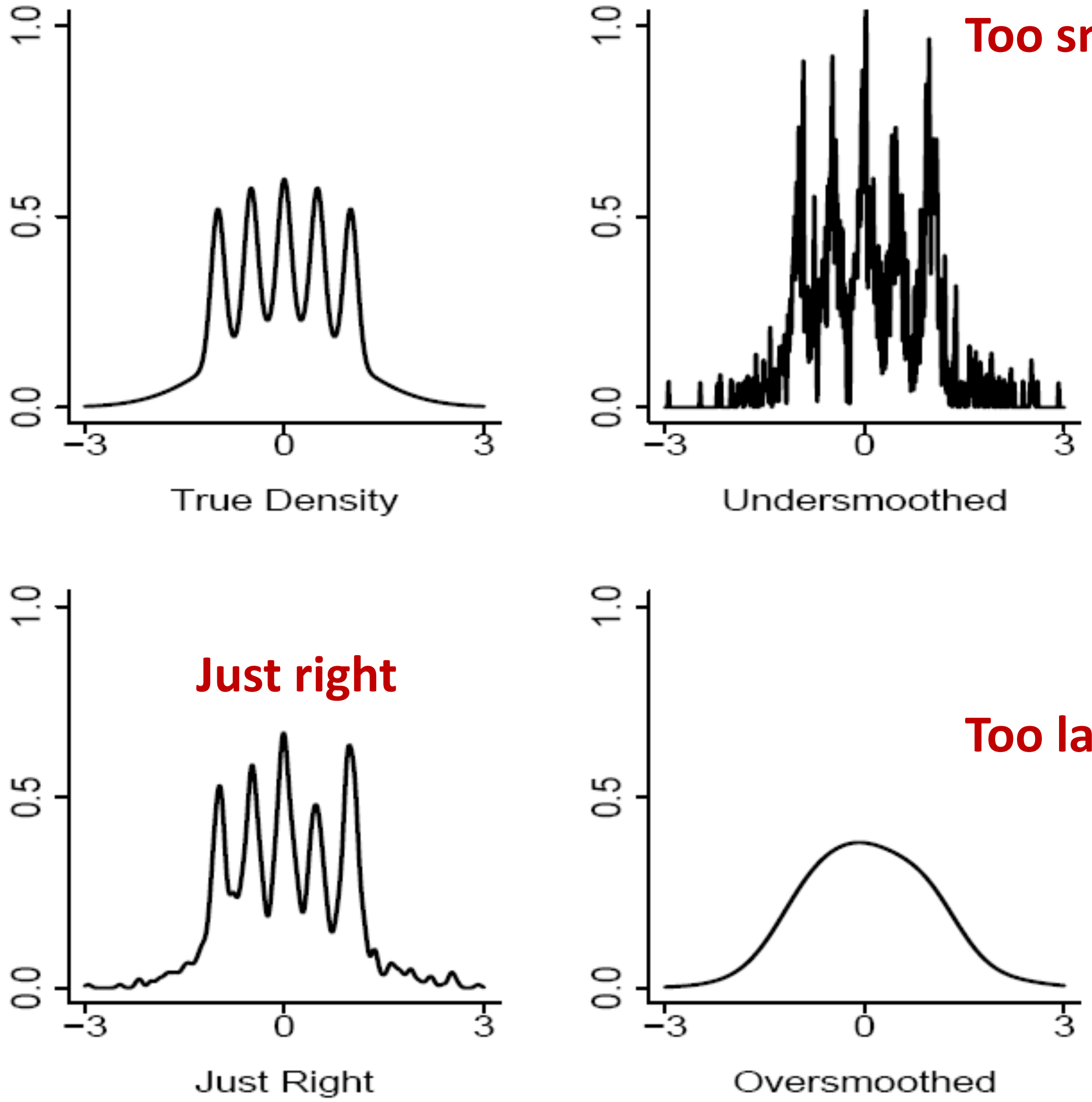


Infinite support

- need all points to compute estimate

-But quite popular since smoother

Choice of kernel bandwidth



True Density

Undersmoothed

Just Right

Oversmoothed

Too small

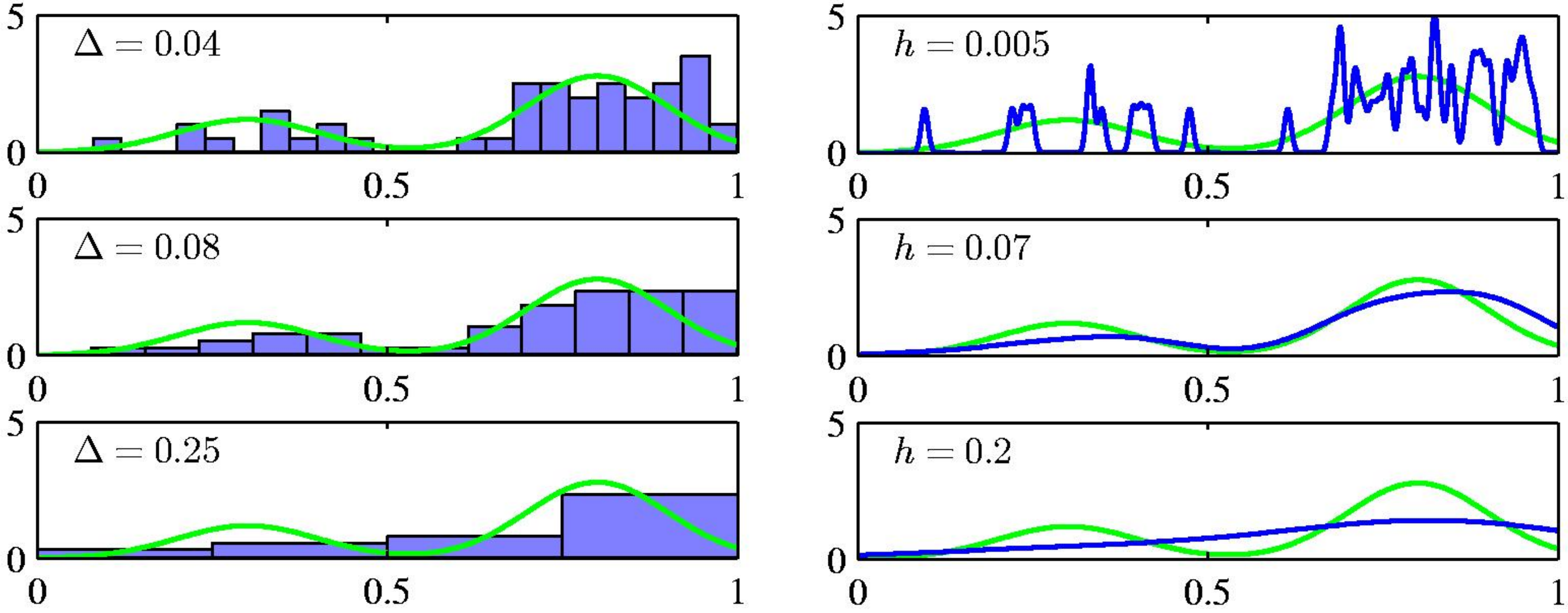
Just right

Too large

Image Source: Larry's book – All of Nonparametric Statistics

Bart-Simpson Density

Histograms vs. Kernel density estimation



$\Delta = \text{h}$ acts as a smoother.

Nonparametric density estimation

- Histogram $$\widehat{p}(x) = \frac{n_i}{n\Delta}\mathbf{1}_{x \in \mathrm{Bin}_i}$$
- Kernel density est $$\widehat{p}(x) = \frac{n_x}{n\Delta}$$

Fix Δ, estimate number of points within Δ of x (n_i or n_x) from data

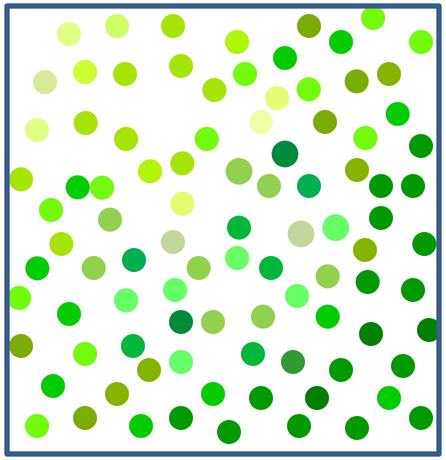
Fix $n_x = k$, estimate Δ from data (volume of ball around x that contains k training pts)

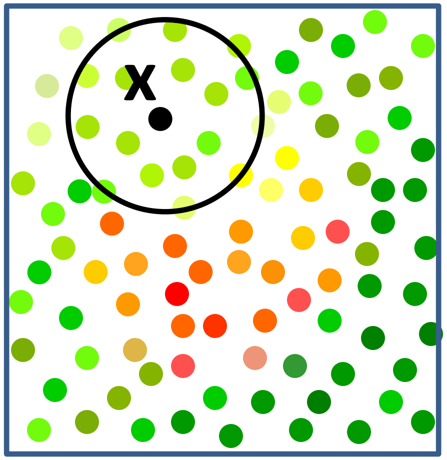
- k-NN density est $$\widehat{p}(x) = \frac{k}{n\Delta_{k,x}}$$

Local Kernel Regression

- What is the temperature in the room?

at location x?





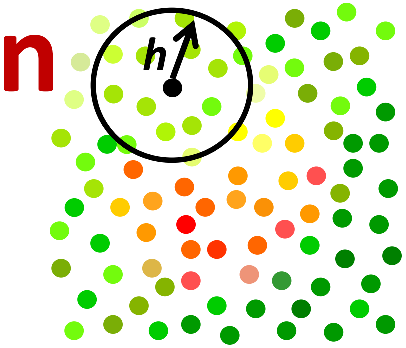
$$\widehat{T} = \frac{1}{n}\sum_{i=1}^{n} Y_i$$

$$\widehat{T}(x) = \frac{\sum_{i=1}^{n} Y_i \mathbf{1}_{||X_i - x|| \le h}}{\sum_{i=1}^{n} \mathbf{1}_{||X_i - x|| \le h}}$$

Average

"Local" Average

Local Kernel Regression



- Nonparametric estimator
- Nadaraya-Watson Kernel Estimator

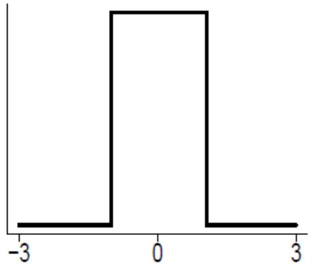
$$\widehat{f}_n(X) = \sum_{i=1}^{n} w_i Y_i \quad \text{Where} \quad w_i(X) = \frac{K\left(\frac{X-X_i}{h}\right)}{\sum_{i=1}^{n} K\left(\frac{X-X_i}{h}\right)}$$

- Weight each training point based on distance to test point
- Boxcar kernel yields

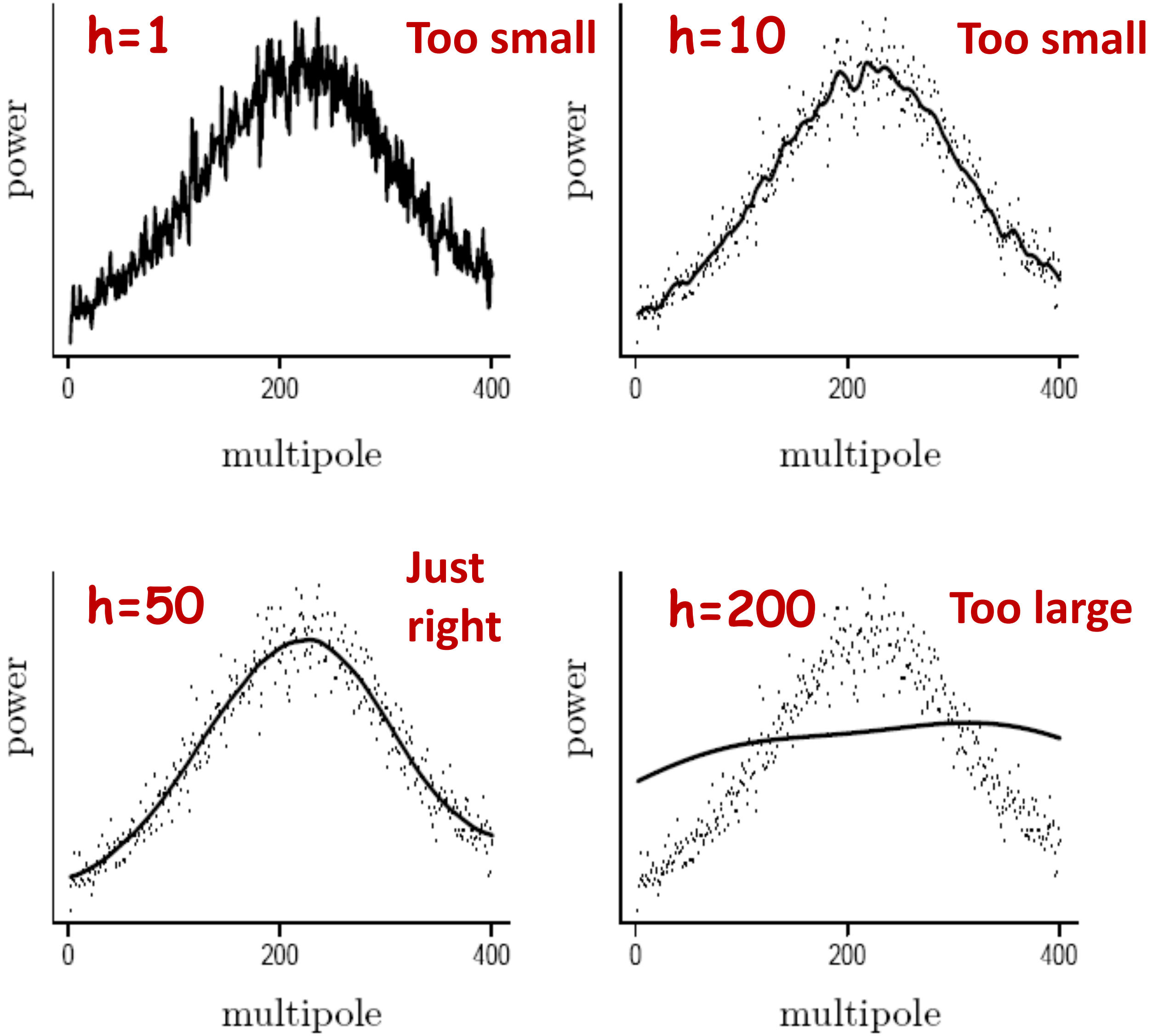
  local average

boxcar kernel :

$$K(x) = \frac{1}{2} I(x),$$



Choice of kernel bandwidth h



h=1 Too small

h=10 Too small

h=50 Just right

h=200 Too large

Image Source: Larry’s book – All of Nonparametric Statistics

Kernel Regression as Weighted Least Squares

$$\min_f \sum_{i=1}^{n} w_i(f(X_i) - Y_i)^2 \qquad w_i(X) = \frac{K\left(\frac{X-X_i}{h}\right)}{\sum_{i=1}^{n} K\left(\frac{X-X_i}{h}\right)}$$

Weighted Least Squares

Kernel regression corresponds to locally constant estimator obtained from (locally) weighted least squares

i.e. set $f(X_i) = \beta$ (a constant)

Kernel Regression as Weighted Least Squares

set $f(X_i) = \beta$ (a constant)

$$\min_{\beta} \sum_{i=1}^{n} w_i(\underset{\substack{\big\downarrow \\ \text{constant}}}{\beta} - Y_i)^2$$

$$w_i(X) = \frac{K\left(\frac{X-X_i}{h}\right)}{\sum_{i=1}^{n} K\left(\frac{X-X_i}{h}\right)}$$

$$\frac{\partial J(\beta)}{\partial \beta} = 2\sum_{i=1}^{n} w_i(\beta - Y_i) = 0$$

Notice that $\sum_{i=1}^{n} w_i = 1$

$$\Rightarrow \widehat{f}_n(X) = \widehat{\beta} = \sum_{i=1}^{n} w_i Y_i$$

Local Linear/Polynomial Regression

$$\min_{f} \sum_{i=1}^{n} w_i (f(X_i) - Y_i)^2 \qquad w_i(X) = \frac{K\left(\frac{X - X_i}{h}\right)}{\sum_{i=1}^{n} K\left(\frac{X - X_i}{h}\right)}$$

Weighted Least Squares

Local Polynomial regression corresponds to locally polynomial estimator obtained from (locally) weighted least squares

i.e. set $f(X_i) = \beta_0 + \beta_1 (X_i - X) + \frac{\beta_2}{2!}(X_i - X)^2 + \cdots + \frac{\beta_p}{p!}(X_i - X)^p$

(local polynomial of degree p around X)

Summary

- Non-parametric approaches

Four things make a nonparametric/memory/instance based/lazy learner:

1. *A distance metric, dist(x,X_i)*

   Euclidean (and many more)

2. *How many nearby neighbors/radius to look at?*

   k, Δ/h

3. *A weighting function (optional)*

   W based on kernel K

4. *How to fit with the local points?*

   Average, Majority vote, Weighted average, Poly fit

Summary

- Parametric vs Nonparametric approaches

  - Nonparametric models place very mild assumptions on the data distribution and provide good models for complex data

    Parametric models rely on very strong (simplistic) distributional assumptions

  - Nonparametric models (not histograms) requires storing and computing with the entire data set.

    Parametric models, once fitted, are much more efficient in terms of storage and computation.