CSCI 4360/6360 Data Science II

Kernel Methods

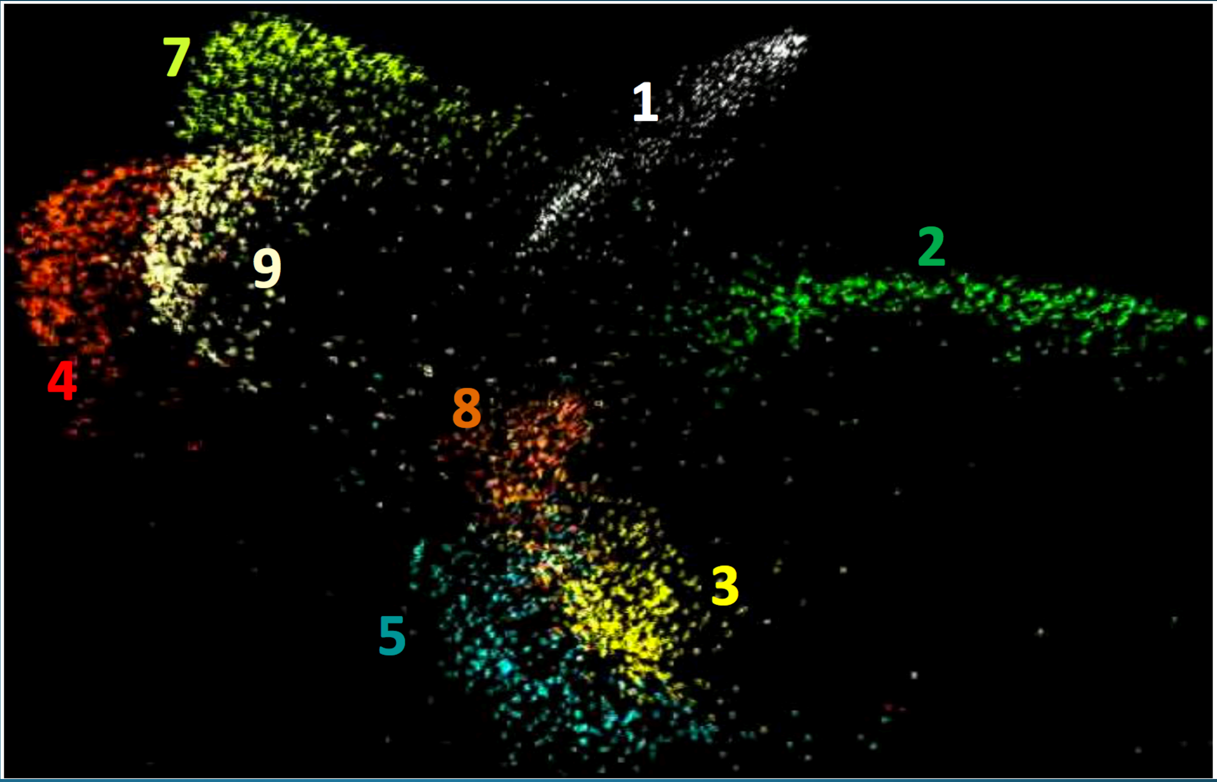
Parametric Statistics

- Assume some functional form (Gaussian, Bernoulli, Multinomial, logistic, linear) for
  - $P(X_i|Y)$ and $P(Y)$ as in Naïve Bayes
  - $P(Y|X)$ as in Logistic Regression
- Estimate parameters ($\mu, \sigma^2, \theta, w, \beta$) using MLE/MAP
  - Plug-n-chug

- **Advantages**: need relatively few data points to learn parameters
- **Drawbacks**: Strong assumptions rarely satisfied in practice

Embeddings

- Again!
- MNIST, projected into 2D embedding space
- What distribution do these follow?
- **Highly nonlinear**



Nonparametric Statistics

- Typically very few, if any, distributional assumptions
- Usually requires more data
- Let number of parameters scale with the data

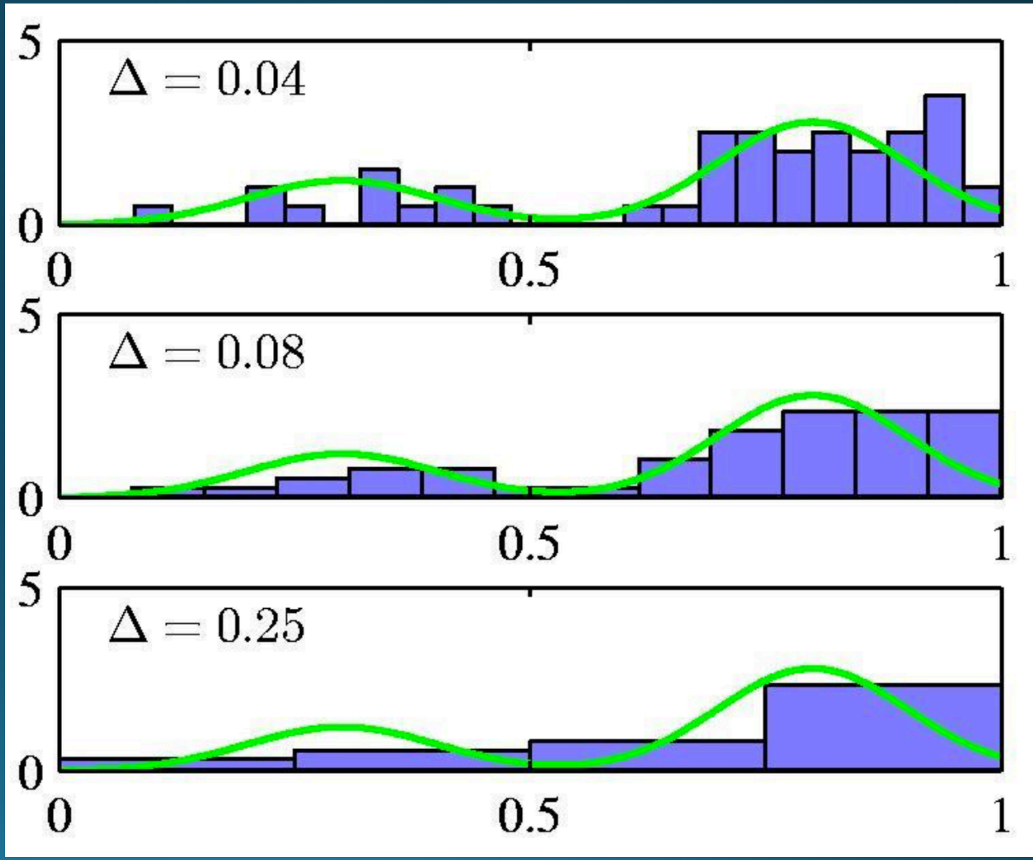
- **Today**
  - Kernel density estimation
  - K-nearest neighbors classification
  - Kernel regression

Density Estimation

- You've done this before—histograms!
- Partition feature space into distinct bins with specified widths and count number of observations n_i in each bin

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

- Same width is often used for all bins
- Bin width acts as **smoothing parameter**

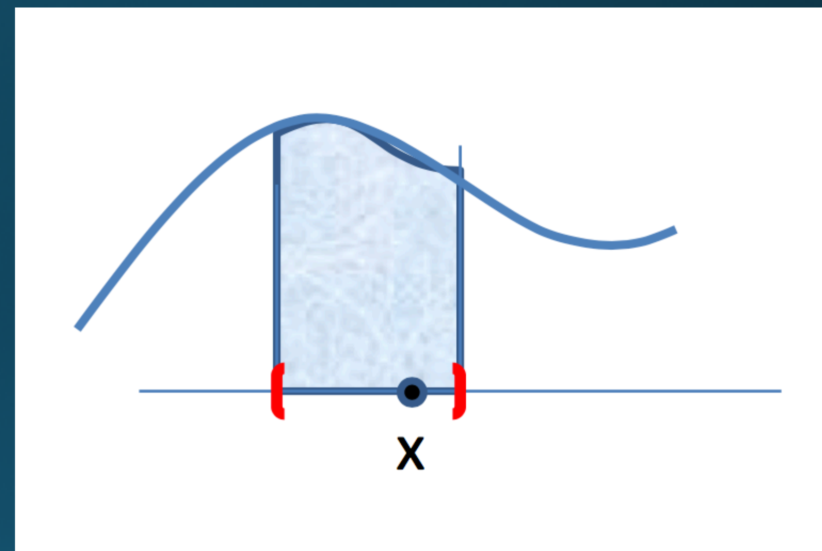


Effect of Δ

- # of bins = 1/Δ

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

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



- Bias of histogram density estimate

$$\mathbb{E}\left[\hat{p}(x)\right] = \frac{1}{\Delta}P(X \in \mathrm{Bin}_x) = \frac{1}{\Delta}\int_{z \in \mathrm{Bin}_x} p(z)dz \approx \frac{p(x)\Delta}{\Delta}$$

$$= p$$

Assuming density is roughly constant in each bin
(roughly true, if Δ is small)

Bias-Variance Trade-off

- Choice of # of bins
  - if Δ is small
  - if Δ is large

$$\mathbb{E}\left[\hat{p}(x)\right] \approx p(x)$$
$$\mathbb{E}\left[\hat{p}(x)\right] \approx \hat{p}(x)$$

p(x) approximately constant per bin

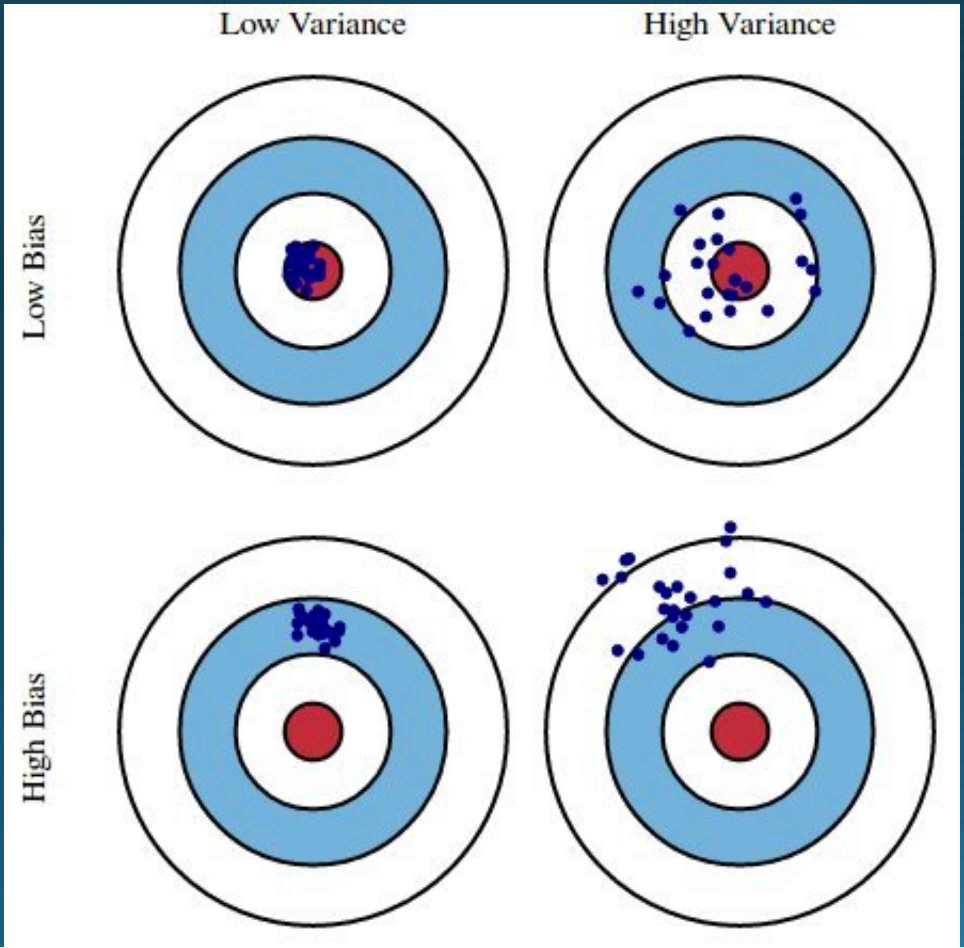
More data per bin stabilizes estimate

- **Bias**: how close is mean of estimate to the truth
- **Variance**: how much does estimate vary around the mean

Small Δ, large #bins ⟺ "**Small bias**, **Large variance**"

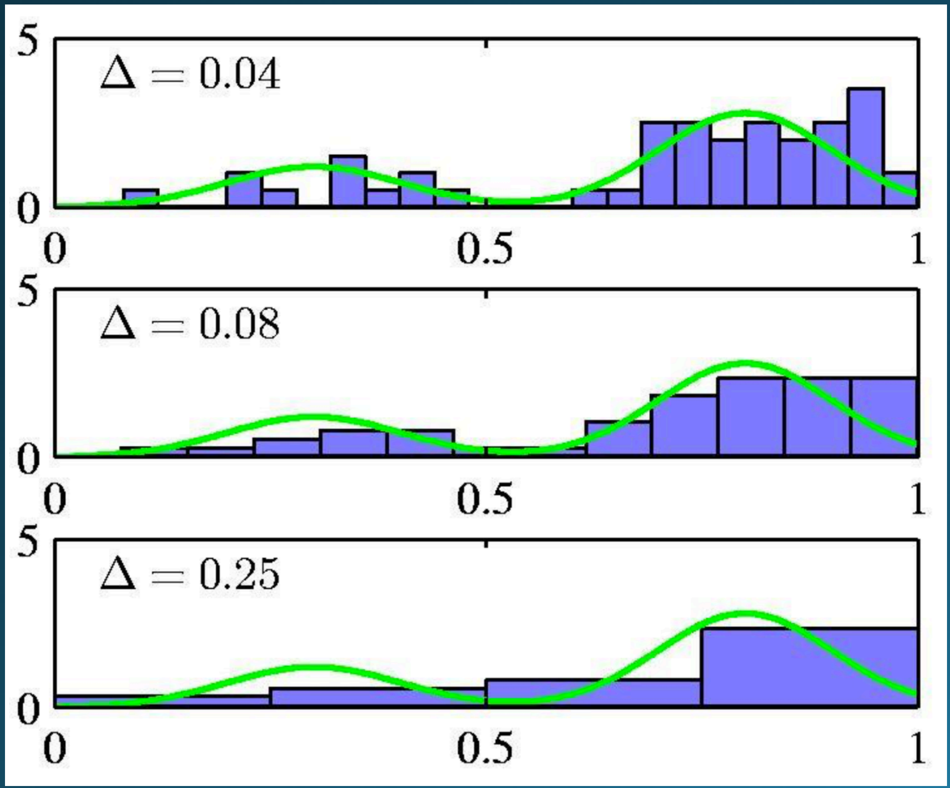
Large Δ, small #bins ⟺ "**Large bias**, **Small variance**"

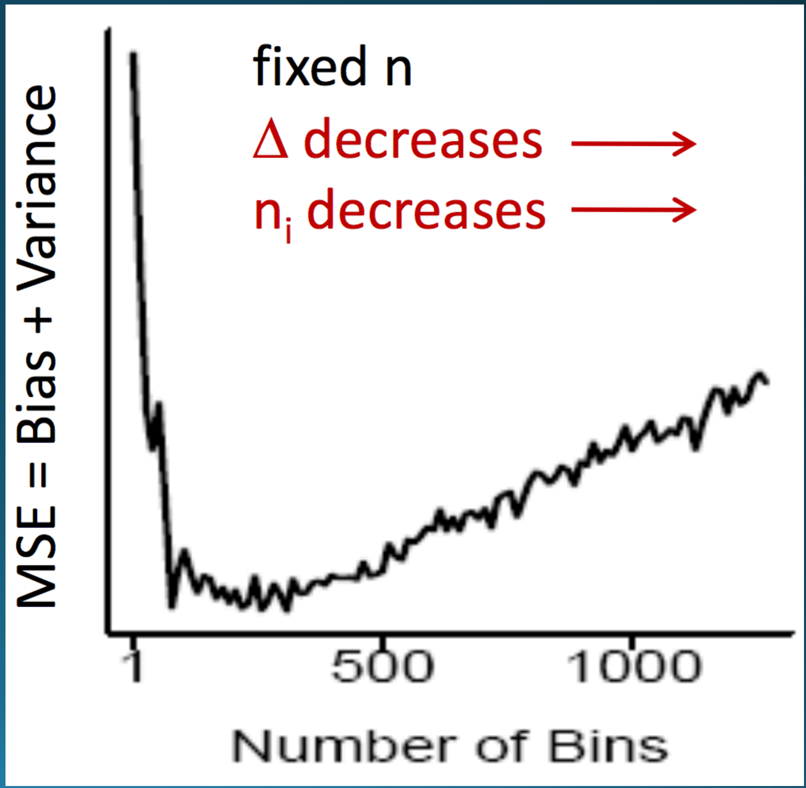
Bias-Variance Trade-off



Choice of number of bins

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

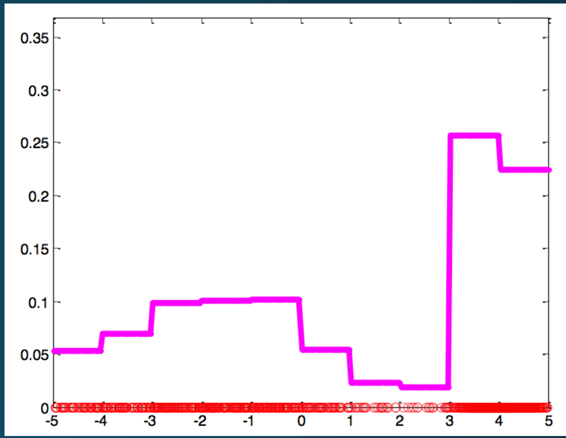




Kernel Density Estimation

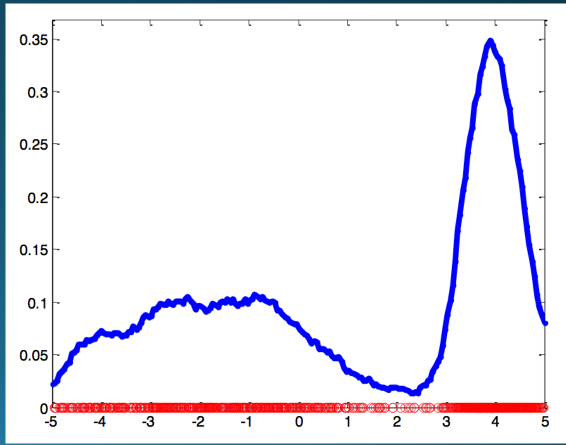
- Histograms are “blocky” estimates

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



- Kernel density estimate, aka “Parzen / moving window” method

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



Kernel Density Estimation

- More generally:

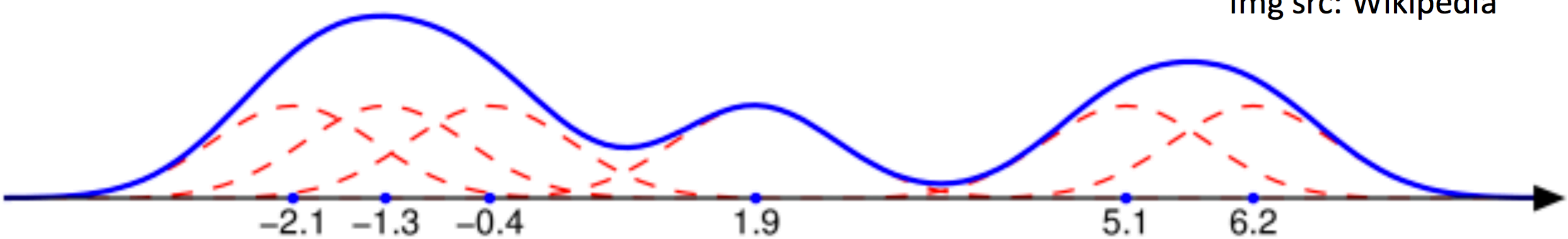
$$\hat{p}(x) = \frac{1}{\Delta} \frac{\sum_{j=1}^{n} K\left(\frac{X_j - x}{\Delta}\right)}{n}$$

- *K* is the kernel function (not to be confused with φ from Kernel PCA)
- Embodies any number of possible kernel functions

Kernel Density Estimation

- Places small "bumps" at each data point, determined by *K*
- Estimator itself consists of a [normalized] "sum of bumps"

Img src: Wikipedia



- Where points are denser, density estimate will be higher

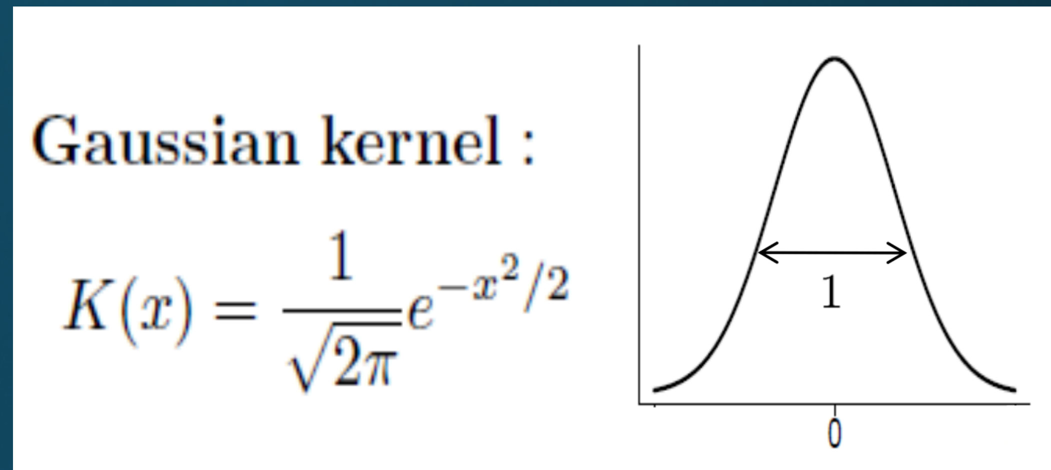
Kernels

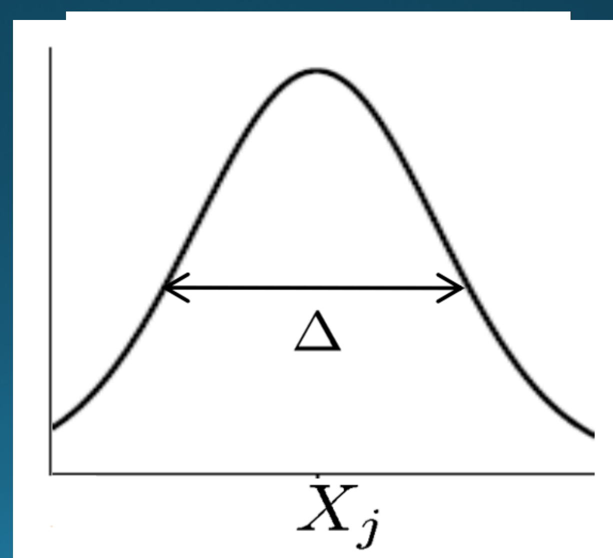
- Any function that satisfies

$$K(x) \geq 0$$

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

- SciPy has a **ton**
  - See “signal.get_window”

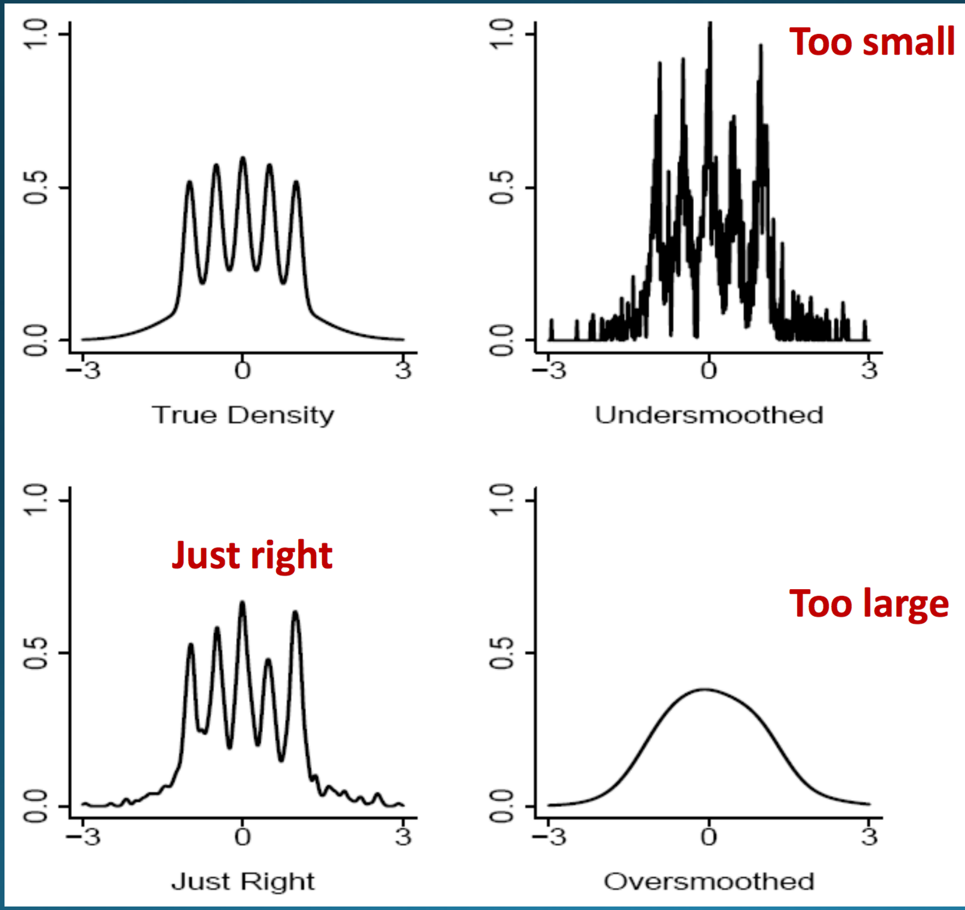




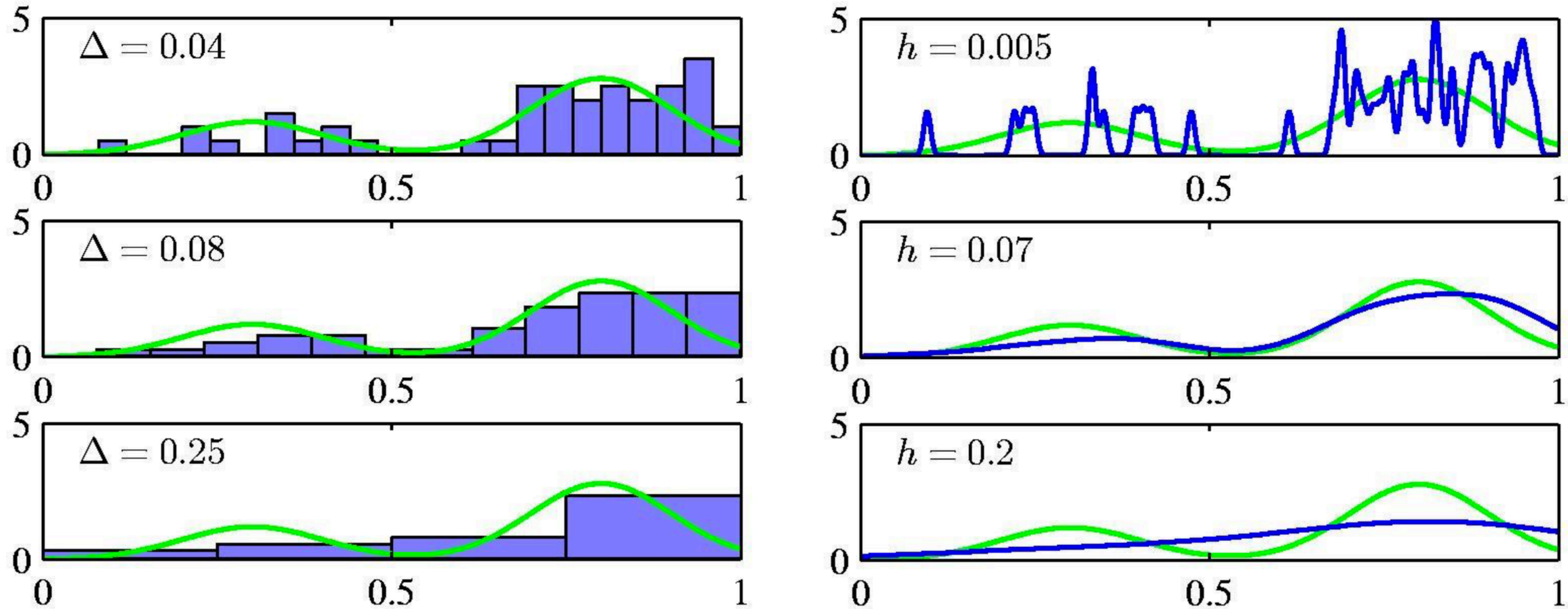
Infinite support: need all points to compute estimate. **But quite popular.**

Choice of kernel bandwidth

The **Bart-Simpson Density**



Histograms versus KDE

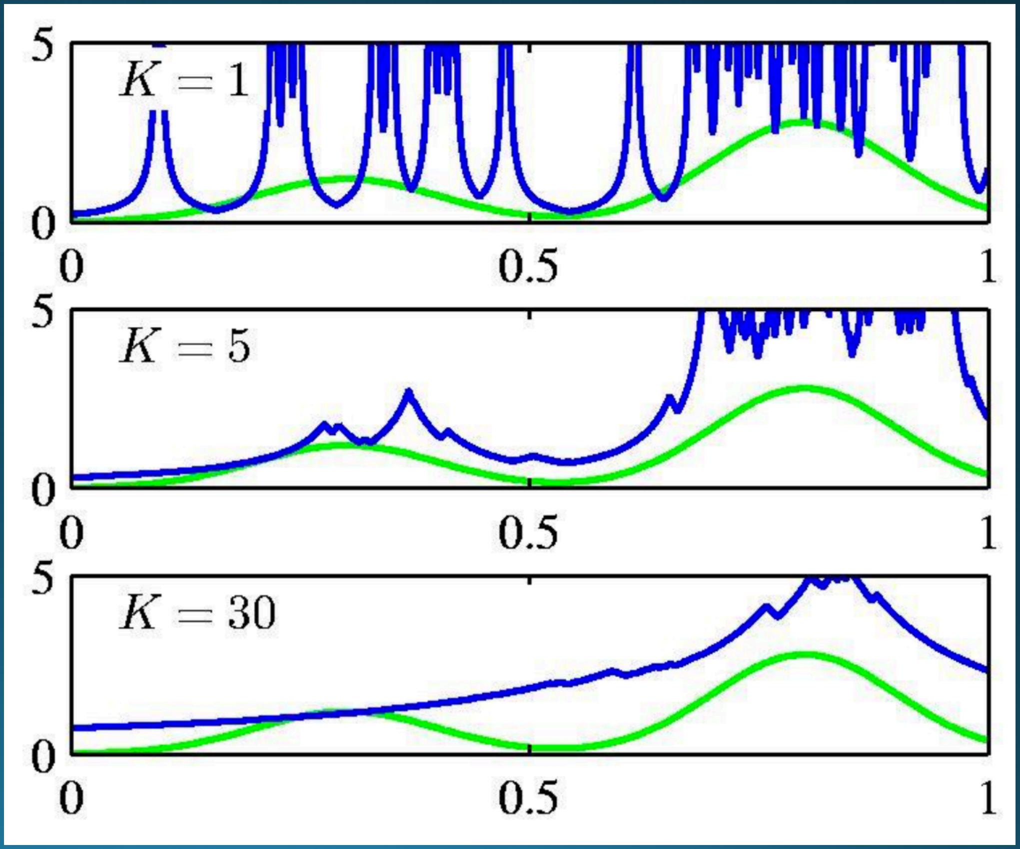


KNN Density Estimation

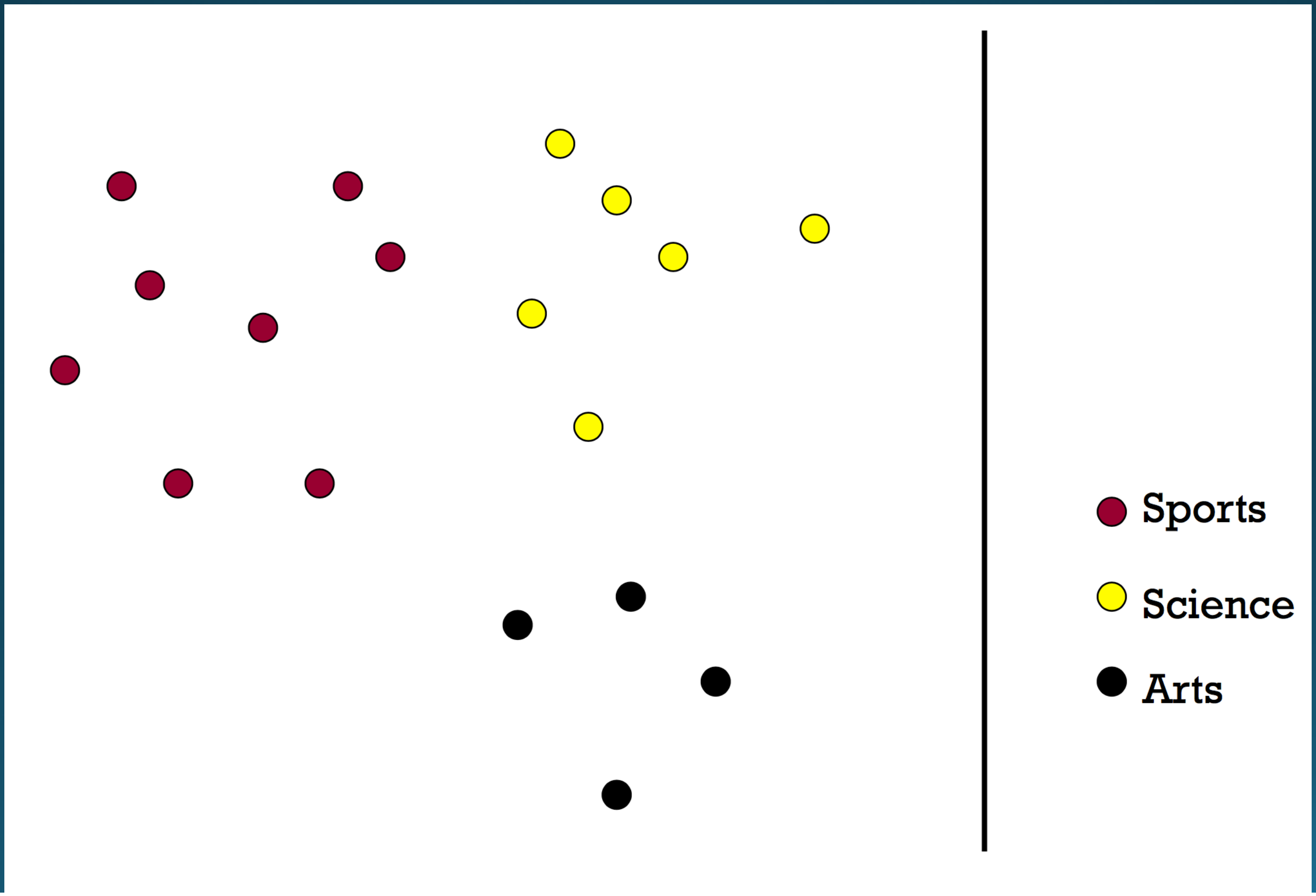
- Recall
  - Histograms $$\hat{p}(x) = \frac{n_i}{n\Delta}\mathbf{1}_{x \in \text{Bin}_i}$$
  - KDE $$\hat{p}(x) = \frac{n_x}{n\Delta}$$
- Fix Δ, estimate number of points within Δ of x (n_i or n_x) from the data
- Fix $n_x = k$, estimate Δ from data (volume of ball around x with k data points)
- **KNN Density Estimation** $$\hat{p}(x) = \frac{k}{n\Delta_{k,x}}$$

KNN Density Estimation

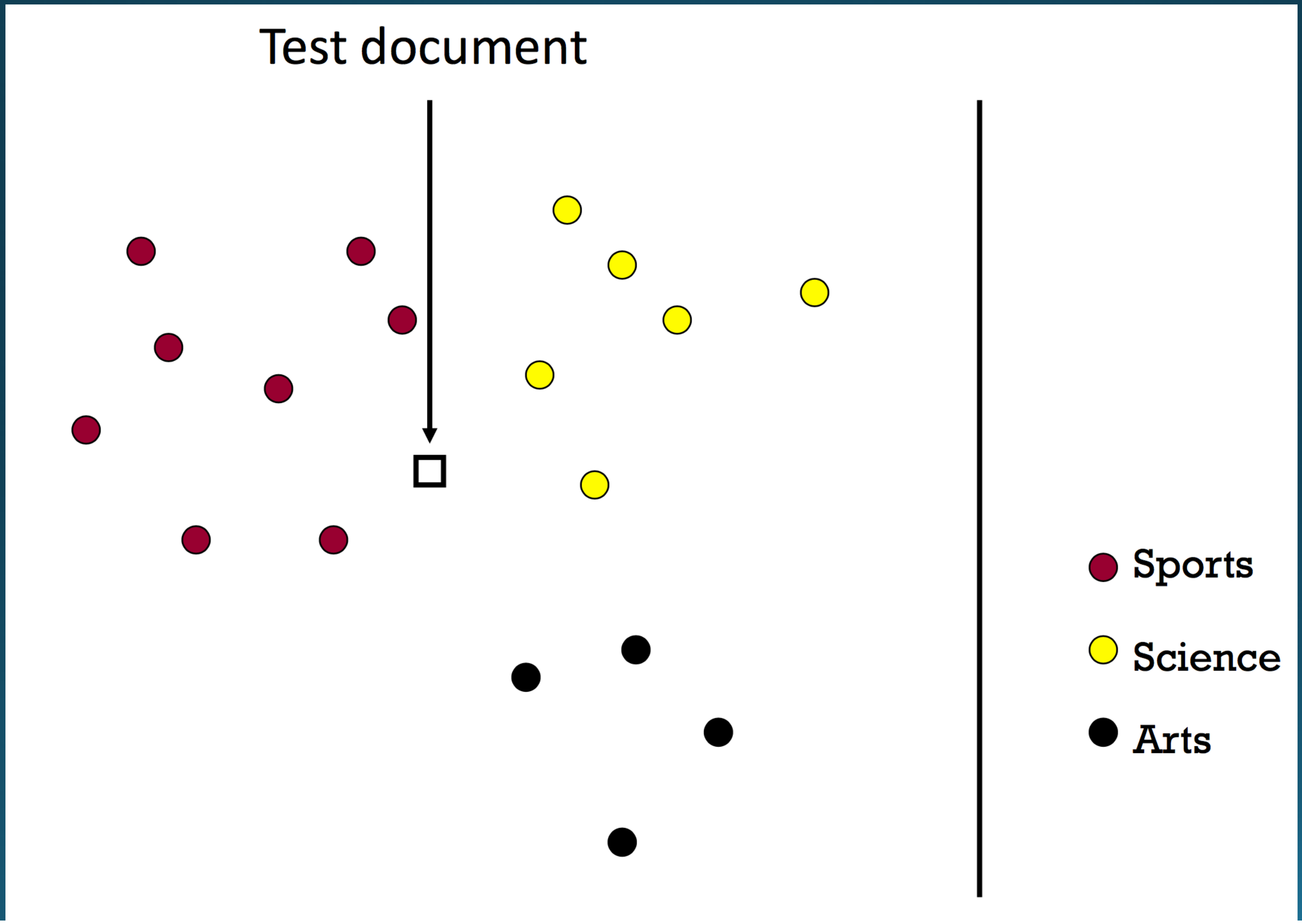
- *k* acts as a smoother
- Not very popular for density estimation
  - Computationally expensive
  - Estimates are poor
- **But related version for classification is very popular**



KNN Classification

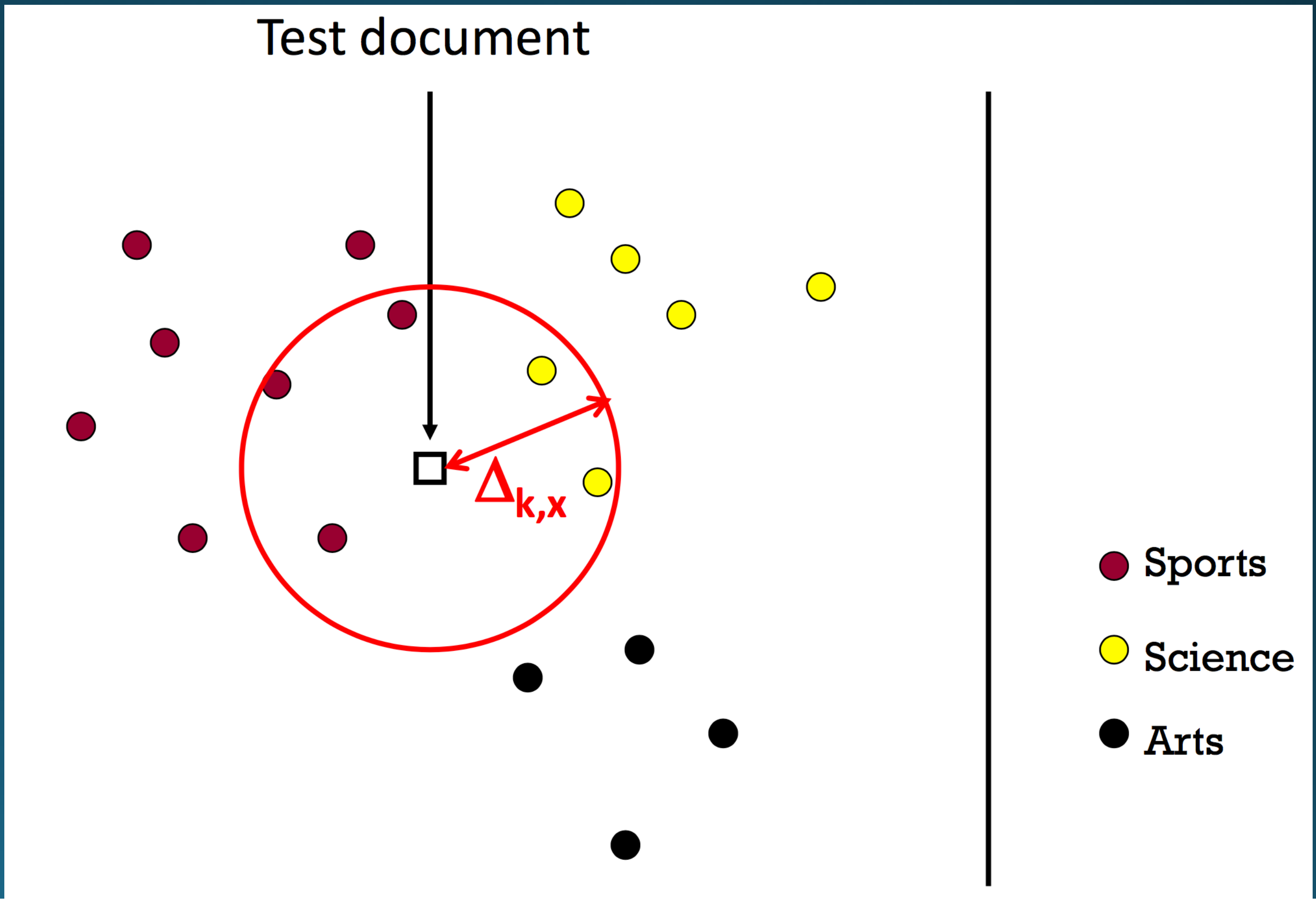


KNN Classification



KNN Classification

- $k = 4$
- What should we predict?
- Average? Majority? **Why?**



KNN Classification

- Optimal classifier

$$f^*(x) = \arg\max_y P(y|x) = \arg\max_y P(x|y)P(y)$$

- KNN classifier

$$\hat{f}_{kNN}(x) = \arg\max_y \hat{p}_{kNN}(x|y)\hat{P}(y) = \arg\max_y k_y$$

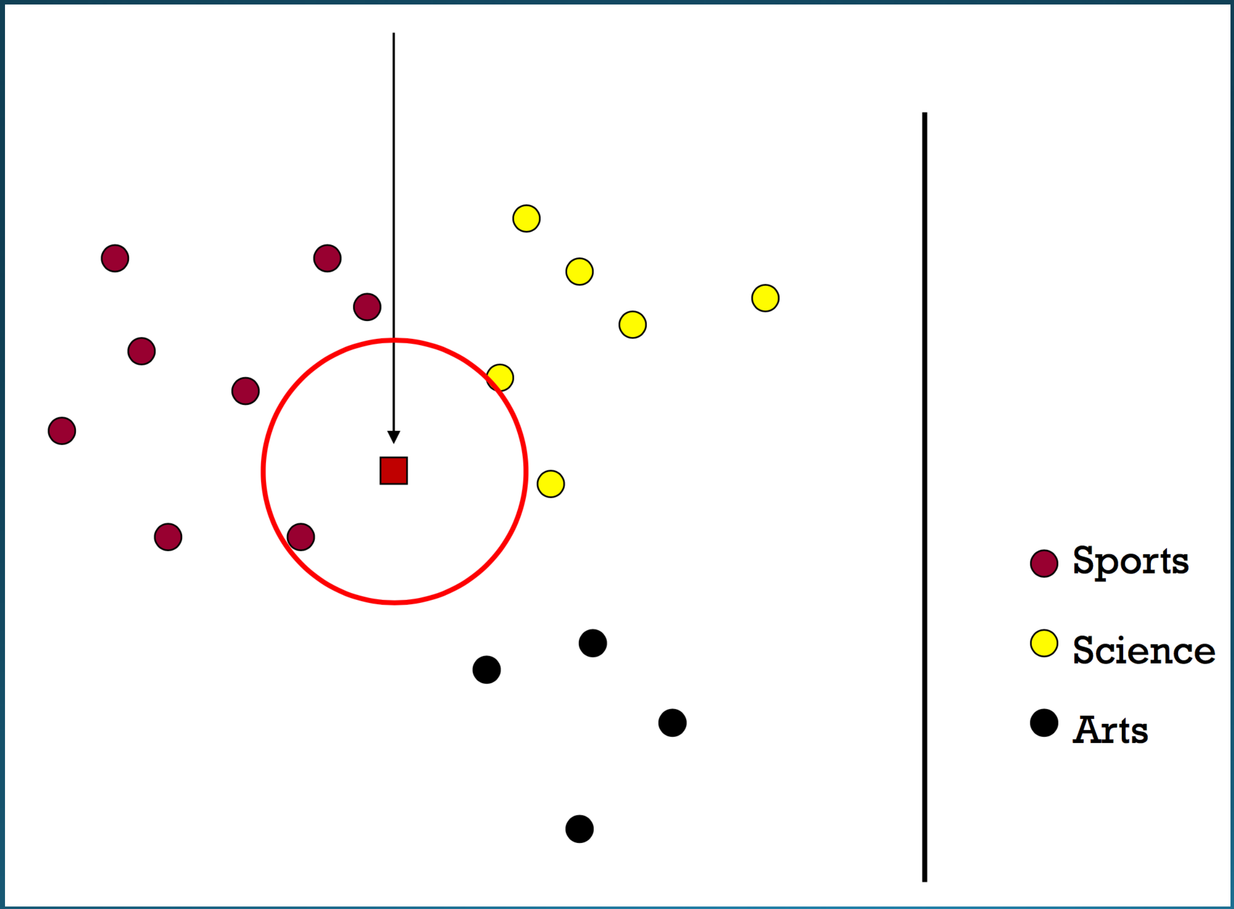
# of training points in class *y*

$$\hat{p}_{kNN}(x|y) = \frac{k_y}{n_y \Delta_{k,x}}$$

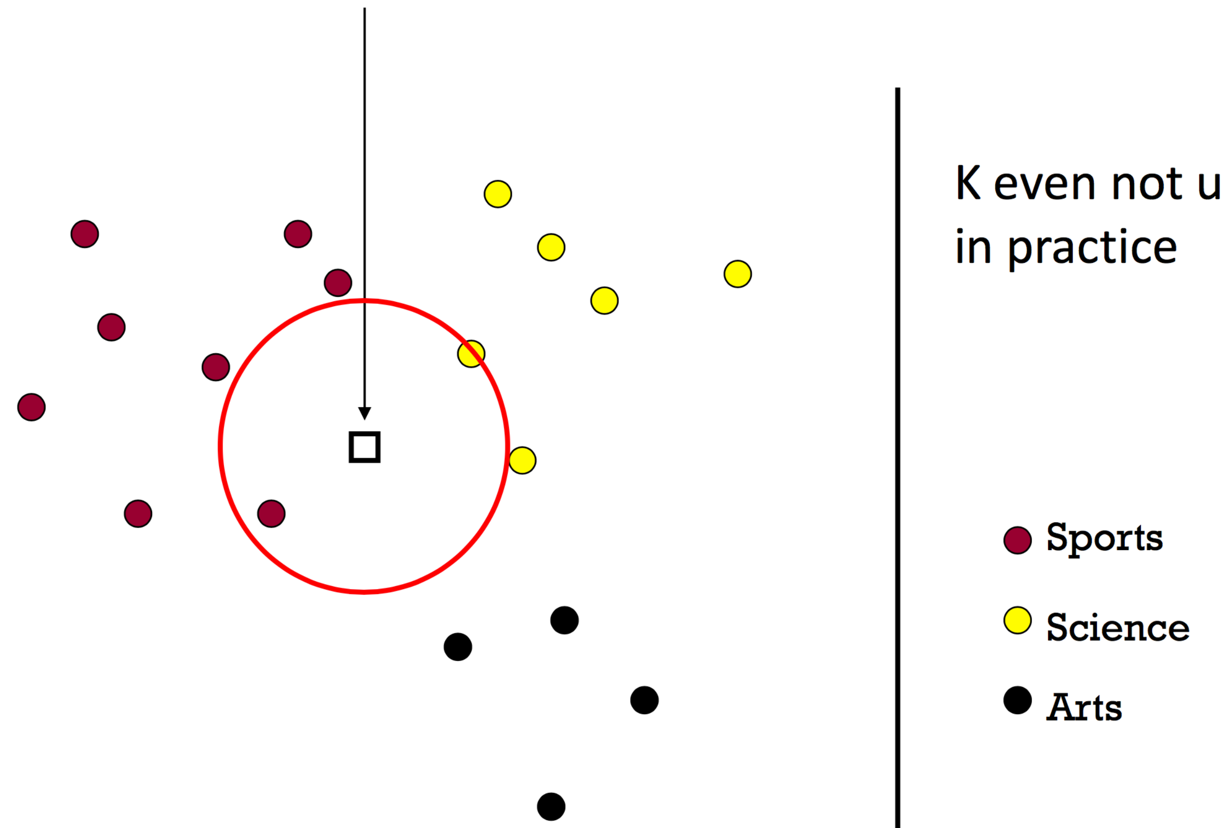
# of training points in class *y* that lie within Δ_k ball

$$\sum_y k_y = k \qquad \hat{P}(y) = \frac{n_y}{n}$$

1-NN

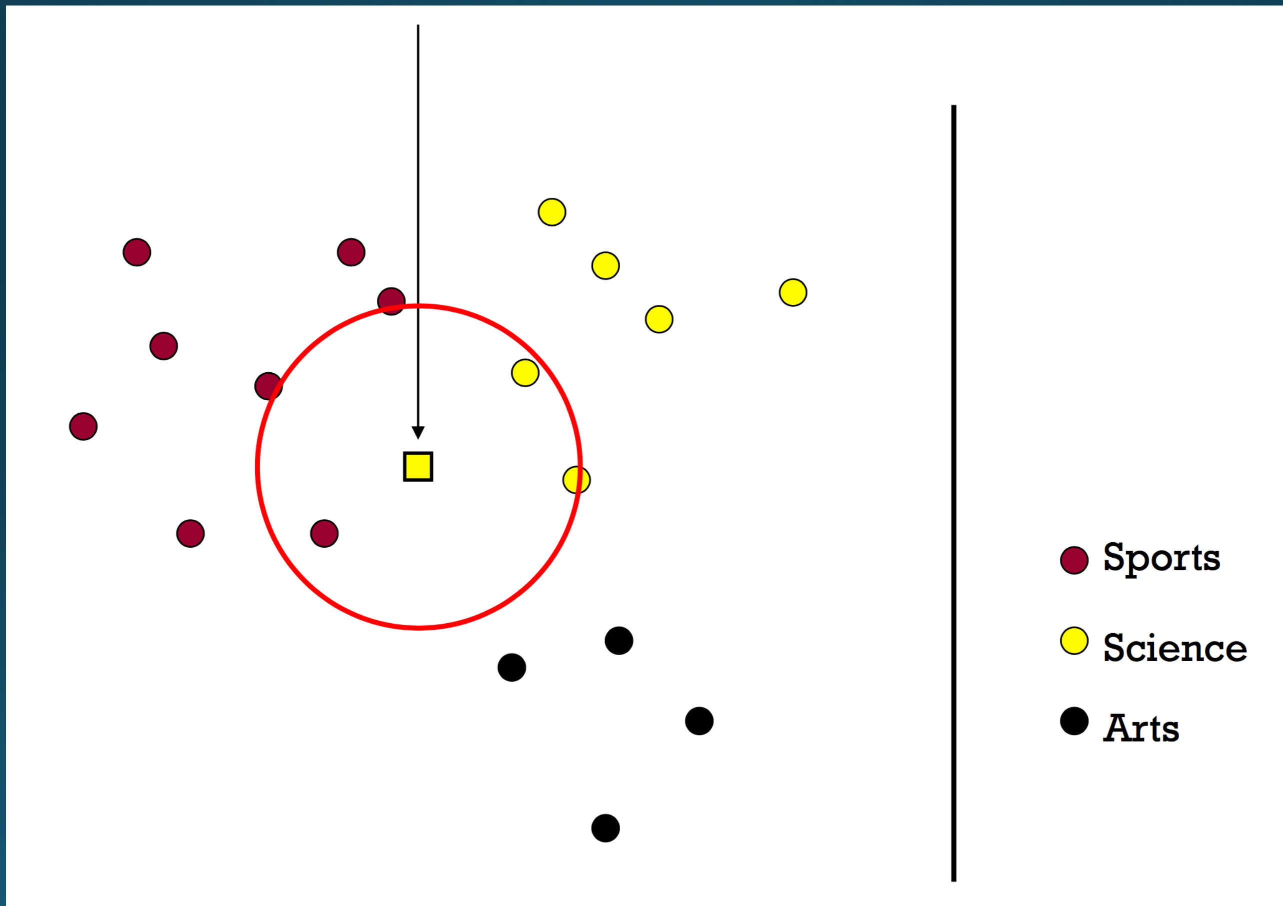


2-NN

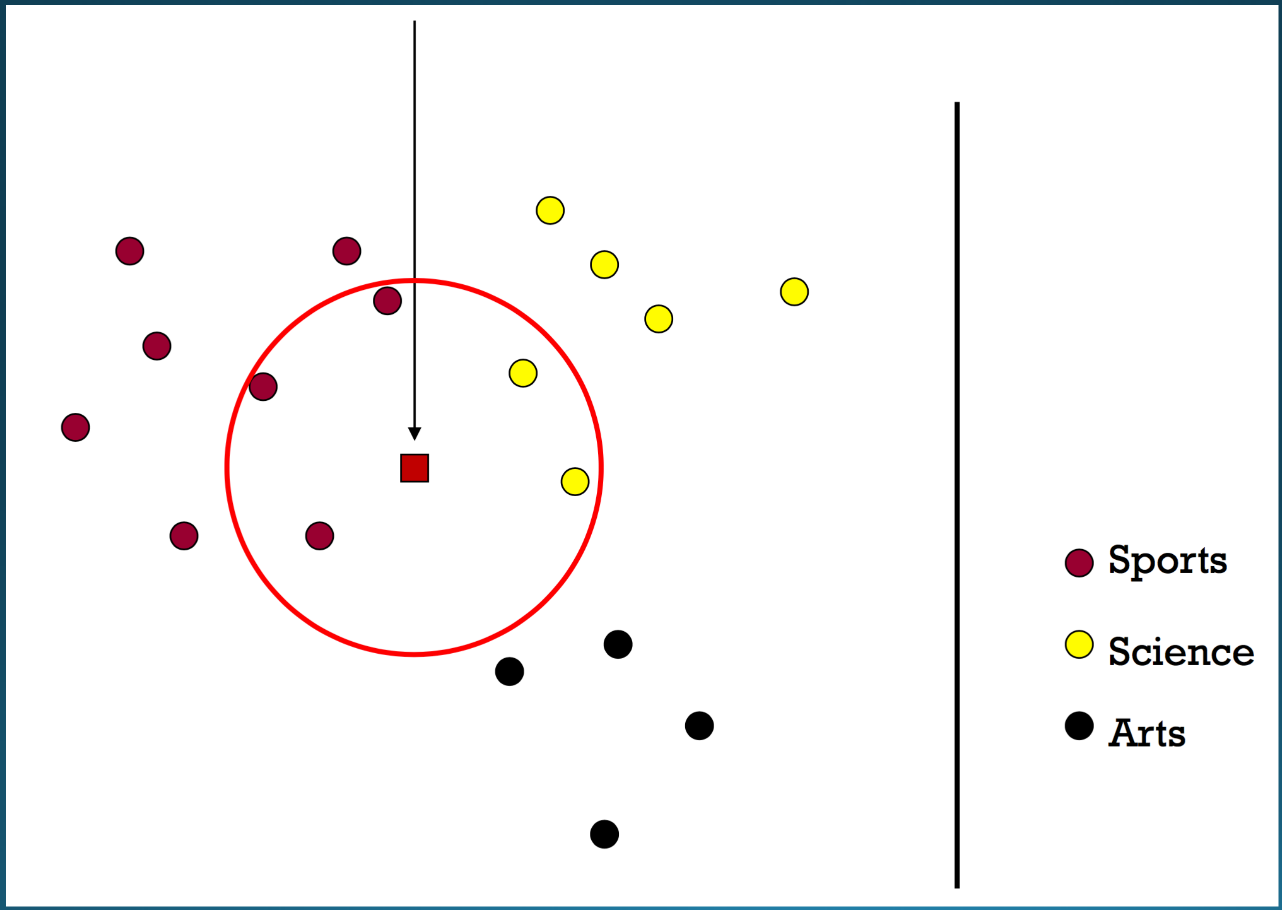


K even not used in practice

3-NN



5-NN



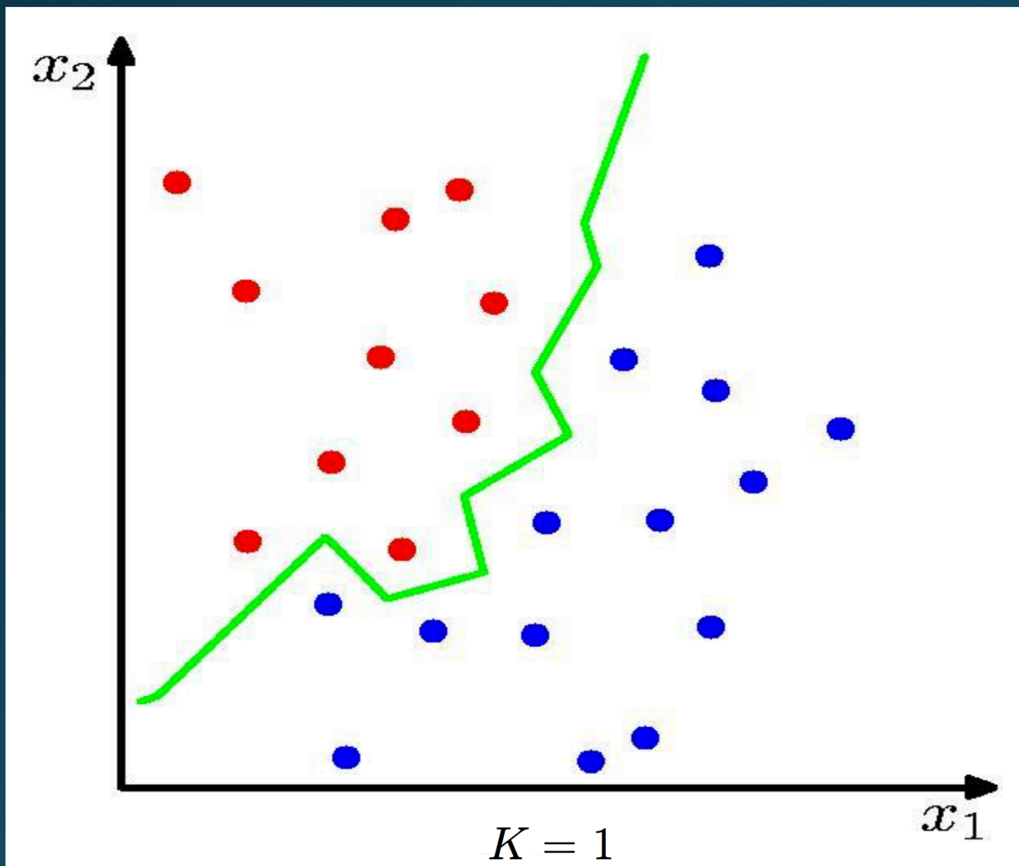
What is the best *k*?

- Bias-variance trade-off

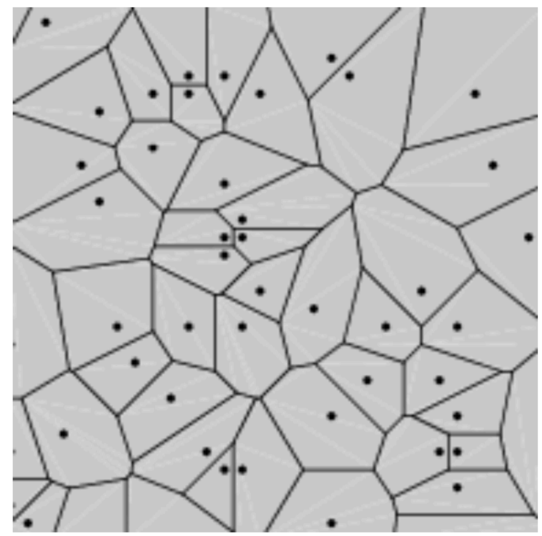
- **Large *k*** = predicted label is more stable
- **Small *k*** = predicted label is more accurate

- **Similar to density estimation**

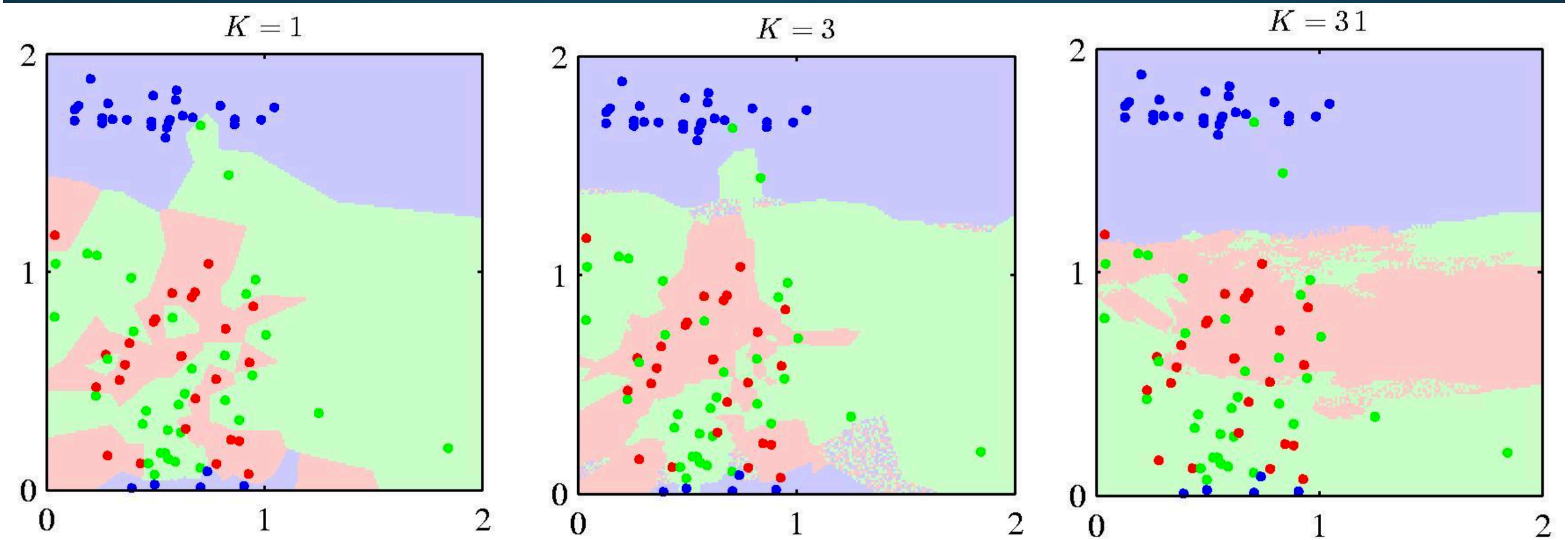
1-NN Decision Boundary



Voronoi
Diagram



KNN Decision Boundaries



- **Guarantee:** For $n \to \infty$, error rate of 1-NN is never more than 2x optimal error rate

Case Study: Newsgroups Classification

- 20 Newsgroups
- 61,118 words
- 18,774 documents
- Class label descriptions

comp.graphics comp.os.ms-windows.misc comp.sys.ibm.pc.hardware comp.sys.mac.hardware comp.windows.x	rec.autos rec.motorcycles rec.sport.baseball rec.sport.hockey	sci.crypt sci.electronics sci.med sci.space
misc.forsale	talk.politics.misc talk.politics.guns talk.politics.mideast	talk.religion.misc alt.atheism soc.religion.christian

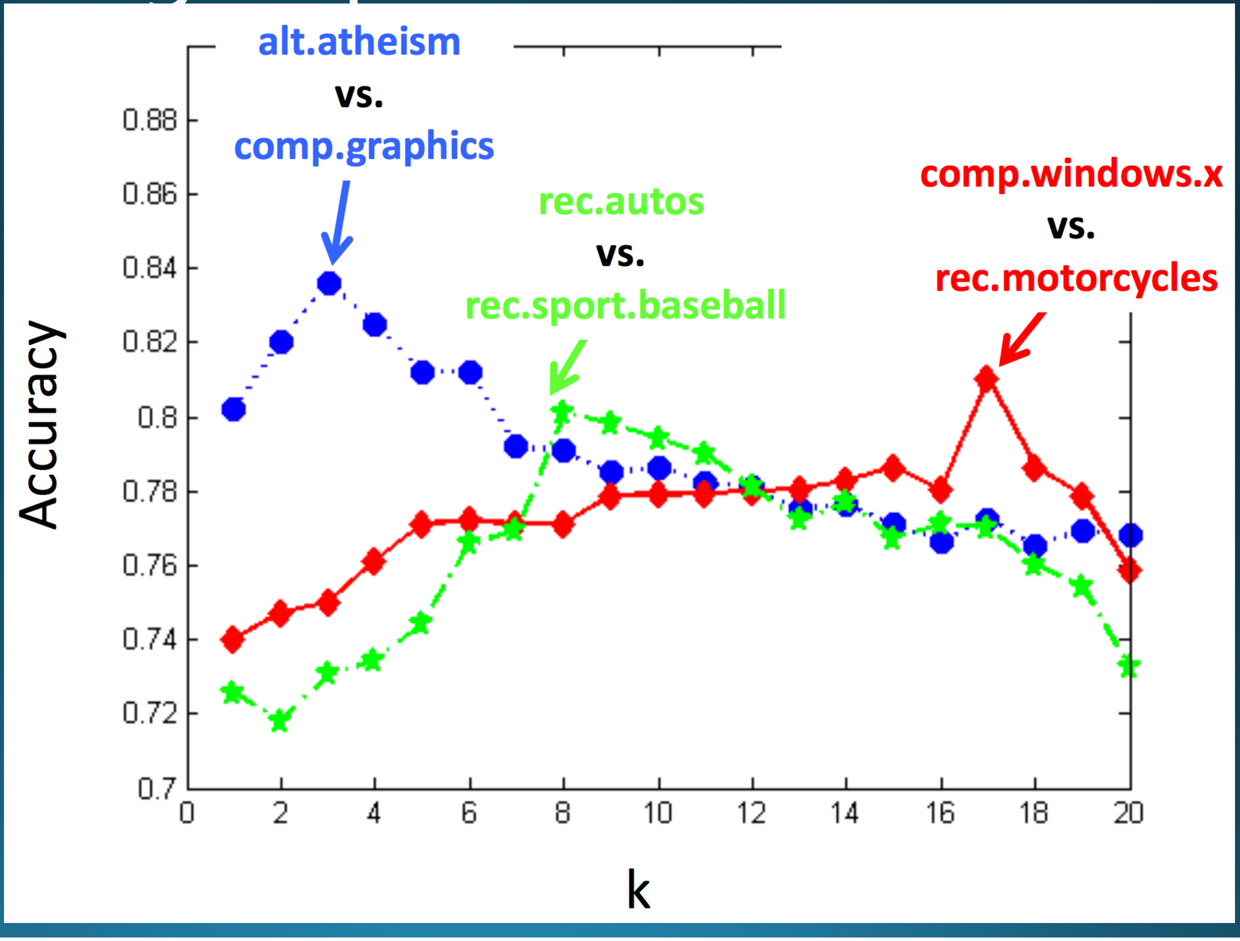
Case Study: Newsgroups Classification

- Training/Testing
  - 50%-50% randomly split
  - 10 runs
  - Report average results
- Evaluation Criteria

$$Accuracy = \frac{\sum_{i \in test\ set} \mathrm{I}(predict_i == true\ label_i)}{\#\ of\ test\ samples}$$

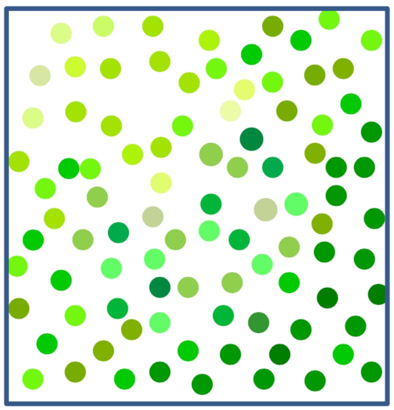
Case Study: Newsgroups Classification

- Results in binary class comparisons



Temperature Sensing

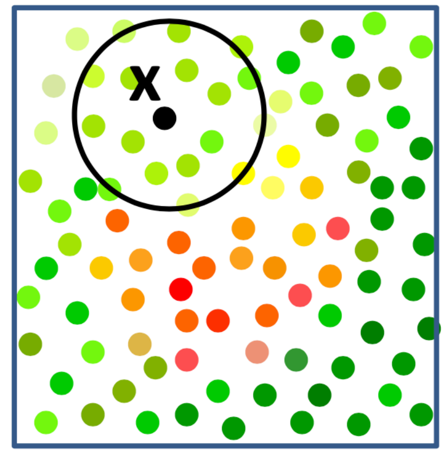
- What is the temperature in the room?



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

Average

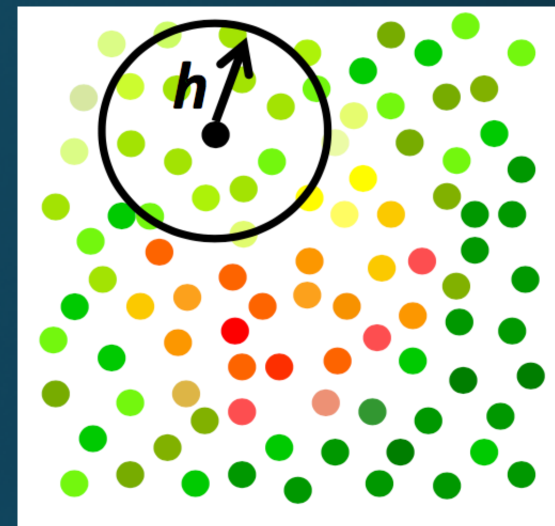
at location x?



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

"Local" Average

Kernel Regression

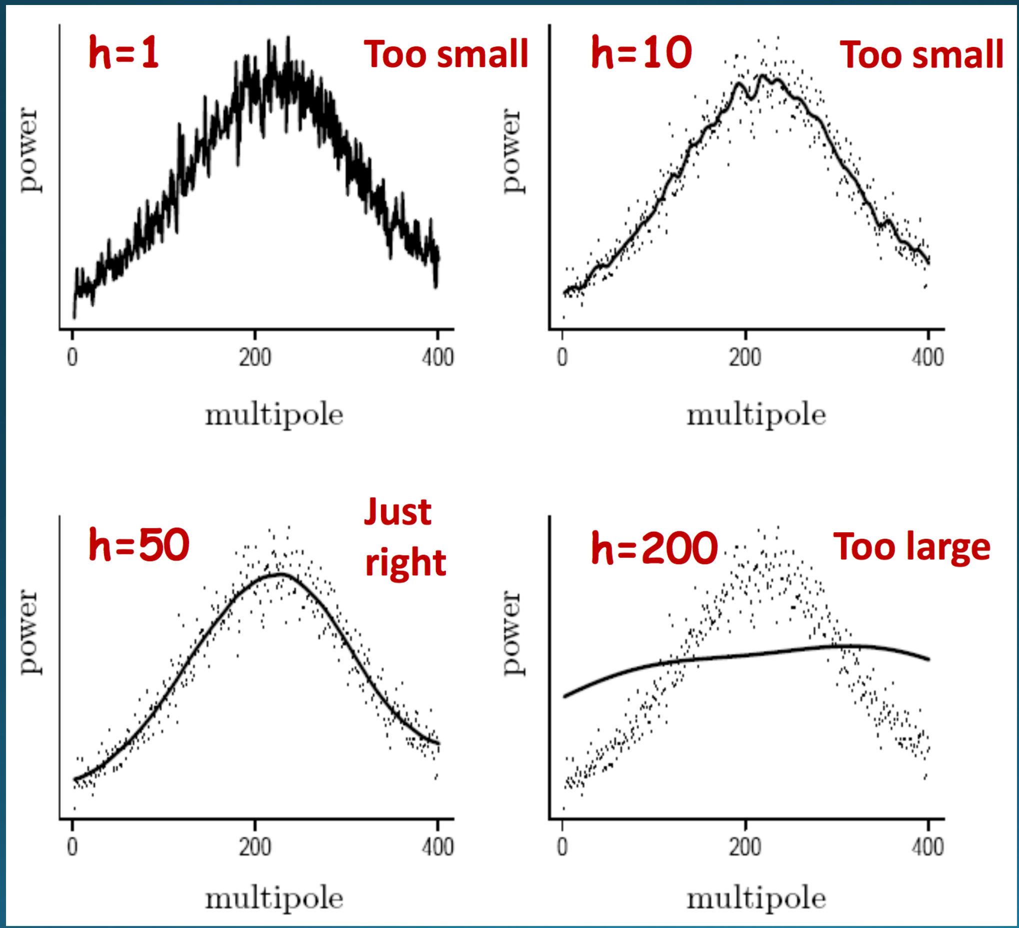


- Or "local" regression
- Nadaraya-Watson Kernel Estimator

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

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

Choice of kernel bandwidth



Choice of *kernel* is not terribly important!

Kernel Regression as WLS

- Weighted Least Squares (WLS) has the form

$$\min_f \sum_{i=1}^{n} w_i (f(X_i) - Y_i)^2$$

- Compare to Nadaraya-Watson form

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

- **Kernel regression corresponds to locally constant estimator obtained from [locally] weighted least squares**

- **Set** $f(X_i) = \beta$ **where** $\boldsymbol{\beta}$ **is constant**

Kernel Regression as WLS

$$\min_{\beta} \sum_{i=1}^{n} w_i(\beta - Y_i)^2$$

A constant value

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

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

Individual weights have to sum to 1

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

Summary

- Nonparametric places mild assumptions on data; good models for complex data
  - Usually requires storing & computing with full dataset
- Parametric models rely on very strong, simplistic assumptions
  - Once fitted, they are much more efficient with storage and computation
- Effects of bin width & kernel bandwidth
  - Bias-variance trade-off
- KNN classifier
  - Non-linear decision boundaries
- Kernel regression
  - Comparison to weighted least squares

Questions?

Course Details

- Assignment 5 coming out **now**
  - Pushed everything back a week
- Projects start imminently
- Neural networks next!

References

- “All of Nonparametric Statistics”, http://www.stat.cmu.edu/~larry/all-of-nonpar/index.html