Instance-Based Learning

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Many Slides from Pedro Domingos

Instance-Based Learning

Key idea: Just store all training examples $\langle x_i, f(x_i) \rangle$

Nearest neighbor:

- Given query instance x_q, first locate nearest training example x_n, then estimate $\hat{f}(x_q) \leftarrow f(x_n)$

k-Nearest neighbor:

- Given x_q, take vote among its k nearest neighbors (if discrete-valued target function)
- Take mean of f values of k nearest neighbors (if real-valued)

$$\hat{f}(x_q) \leftarrow \frac{1}{k} \sum_{i=1}^{k} f(x_i)$$

Advantages and Disadvantages

Advantages:

- Training is very fast
- Learn complex target functions easily
- Don't lose information

Disadvantages:

- Slow at query time
- Lots of storage
- Easily fooled by irrelevant attributes

Distance Measures

- **Numeric features:**
  - Euclidean, Manhattan, L^n-norm:

    $$L^n(\mathbf{x}_1, \mathbf{x}_2) = \sqrt[n]{\sum_{i=1}^{\#\text{dim}} |\mathbf{x}_{1,i} - \mathbf{x}_{2,i}|^n}$$

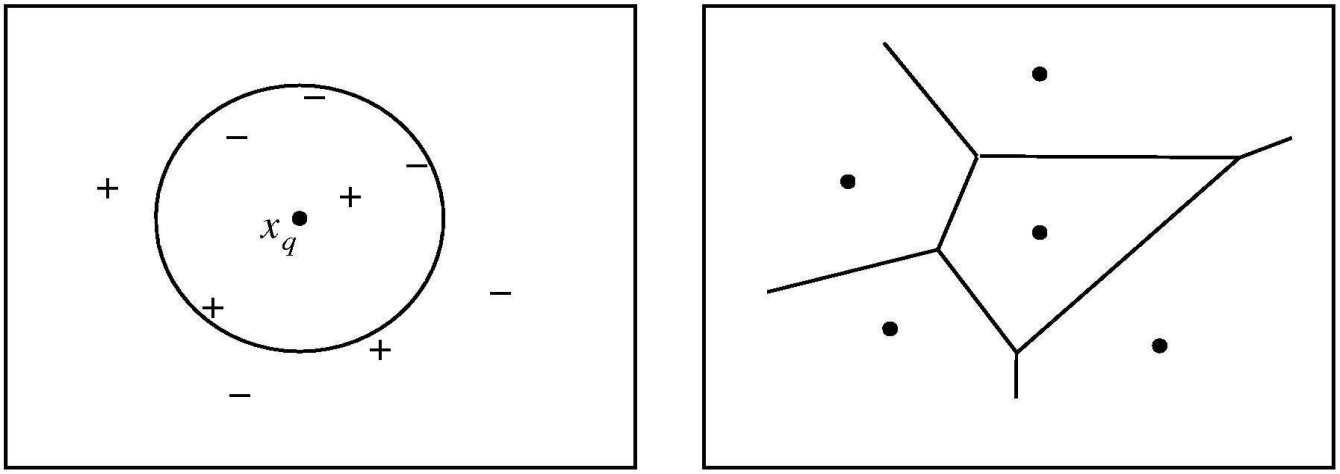
  - Normalized by: range, std. deviation

- **Symbolic features:**
  - Hamming/overlap
  - Value difference measure (VDM):

    $$\delta(val_i, val_j) = \sum_{h=1}^{\#\text{classes}} |P(c_h|val_i) - P(c_h|val_j)|^n$$

- **In general:** arbitrary, encode knowledge

Voronoi Diagram



S: Training set

Voronoi cell of $\mathbf{x} \in S$:
All points closer to $\mathbf{x}$ than to any other instance in S

Region of class C:
Union of Voronoi cells of instances of C in S

Distance-Weighted k-NN

Might want to weight nearer neighbors more heavily ...

$$\hat{f}(x_q) \leftarrow \frac{\sum_{i=1}^{k} w_i f(x_i)}{\sum_{i=1}^{k} w_i}$$

where

$$w_i \equiv \frac{1}{d(x_q, x_i)^2}$$

and $d(x_q, x_i)$ is distance between x_q and x_i

Notice that now it makes sense to use *all* training examples instead of just k

Curse of Dimensionality

- Imagine instances described by 20 attributes, but only 2 are relevant to target function
- **Curse of dimensionality**:
  - Nearest neighbor is easily misled when hi-dim X
  - Easy problems in low-dim are hard in hi-dim
  - Low-dim intuitions don't apply in hi-dim
- **Examples:**
  - Normal distribution
  - Uniform distribution on hypercube
  - Points on hypergrid
  - Approximation of sphere by cube
  - Volume of hypersphere

Things Get Weird in High Dimensions

» High-Dimensional Spheres look like porcupines instead of balls

» Distances between points in high dimensions are all about the same

Things Get Weird in High Dimensions

» High-Dimensional Spheres

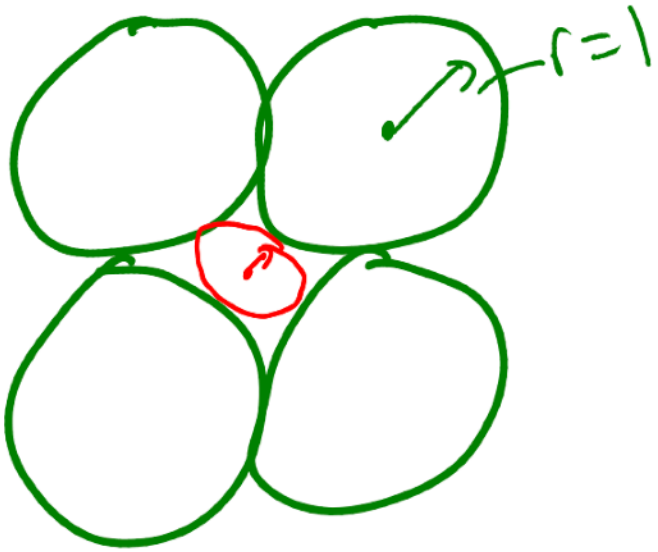


Figure 3.16: 2d spheres in spheres

$$D = 2$$

Pythagorean theorem says:

$$1^2 + 1^2 = (1 + r)^2$$

$$r = \sqrt{2} - 1 \approx 0.41$$

Inside the unit square

Things Get Weird in High Dimensions

» High-Dimensional Spheres

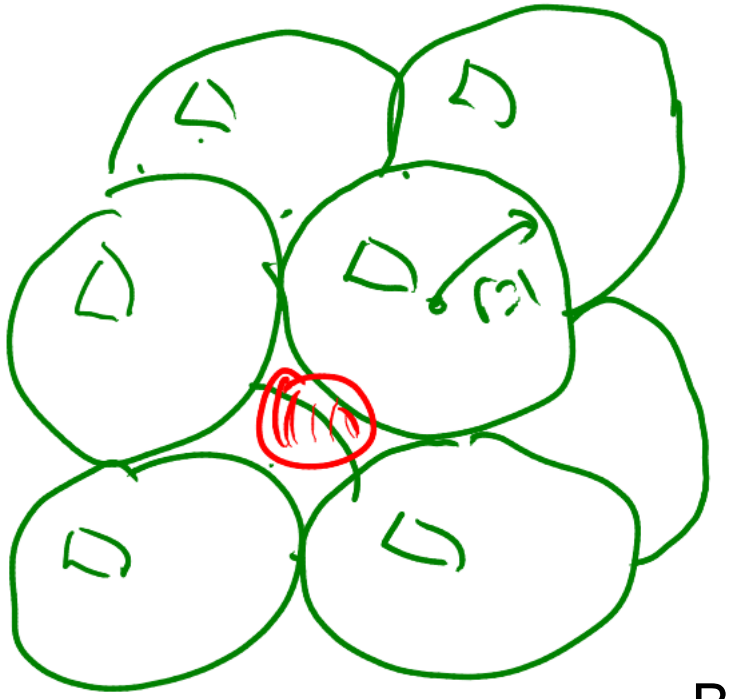
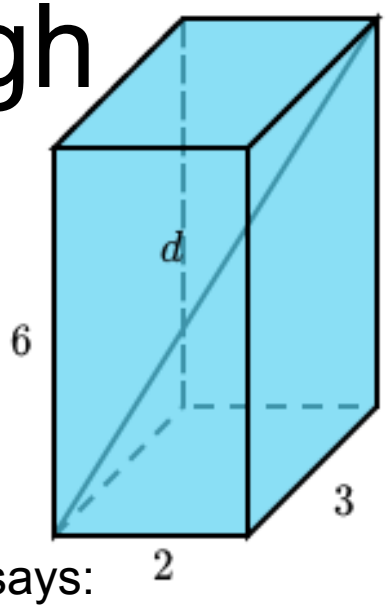


Figure 3.17: 3d spheres in spheres

$$D = 3$$



3d Pythagorean theorem says:

$$1^2 + 1^2 + 1^2 = (1 + r)^2$$

$$r = \sqrt{3} - 1 \approx 0.73$$

Bigger, but still inside the unit cube

Things Get Weird in High Dimensions

» High-Dimensional Spheres

$$D = N$$

?

$$r = \sqrt{N} - 1$$

N = 1000 -> r = 30.6

Radius of the middle hypersphere
extends way beyond the unit hypercube

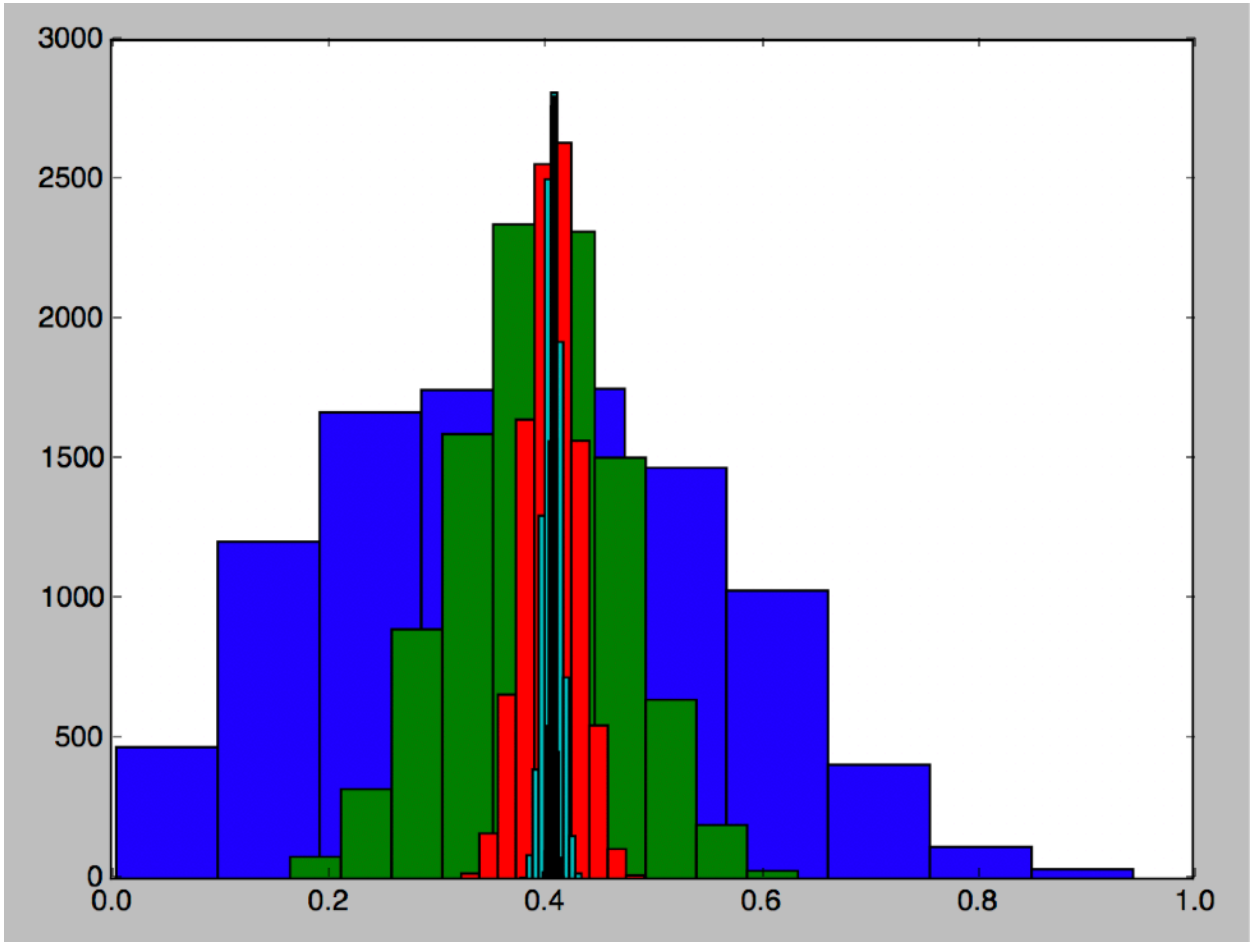
Things Get Weird in High Dimensions

- Distances between points
  - Maximum Distance between any two points in a unit hypercube grows as $\sqrt{D}$
  - But can show that variance is constant (independet of D): $\frac{1}{\sqrt{18}}$
  - Effective variance behaves as: $\frac{1}{\sqrt{18D}}$

Things Get Weird in High Dimensions

```
import numpy as np
import matplotlib.pyplot as plt
import sys
import math

N = 100

def DistancesBetweenRandomPoints(D):
    data = np.random.random((N,D))

    dsum = 0.0
    dlist = []
    for i in range(N):
        for j in range(N):
            if i != j:
                dlist += [np.linalg.norm(data[i,:] - data[j,:])]       #Euclidean distance between rows i and j
                count += 1
    return dlist

plt.hist([(x / math.sqrt(2)) for x in DistancesBetweenRandomPoints(2)])
plt.hist([(x / math.sqrt(10)) for x in DistancesBetweenRandomPoints(10)])
plt.hist([(x / math.sqrt(100)) for x in DistancesBetweenRandomPoints(100)])
plt.hist([(x / math.sqrt(1000)) for x in DistancesBetweenRandomPoints(1000)])
plt.hist([(x / math.sqrt(10000)) for x in DistancesBetweenRandomPoints(10000)])
plt.show()
```

Things Get Weird in High Dimensions



Feature Selection

- **Filter approach:**
  Pre-select features individually
  - E.g., by info gain
- **Wrapper approach:**
  Run learner with different combinations of features
  - Forward selection
  - Backward elimination
  - Etc.

FORWARD_SELECTION(FS)

    FS: Set of features used to describe examples

Let $SS = \emptyset$

Let $BestEval = 0$

Repeat

    Let $BestF = None$

    For each feature F in FS and not in SS

        Let $SS' = SS \cup \{F\}$

        If $Eval(SS') > BestEval$

            Then Let $BestF = F$

                Let $BestEval = Eval(SS')$

    If $BestF \neq None$

        Then Let $SS = SS \cup \{BestF\}$

Until $BestF = None$ or $SS = FS$

Return SS

BACKWARD_ELIMINATION(FS)
    FS: Set of features used to describe examples
Let $SS = FS$
Let $BestEval = Eval(SS)$
Repeat
    Let $WorstF = None$.
    For each feature F in SS
        Let $SS' = SS - \{F\}$
        If $Eval(SS') \geq BestEval$
            Then Let $WorstF = F$
                Let $BestEval = Eval(SS')$
    If $WorstF \neq None$
        Then Let $SS = SS - \{WorstF\}$
Until $WorstF = None$ or $SS = \emptyset$
Return SS

Reducing Computational Cost

- Efficient retrieval: k-D trees
  (only work in low dimensions)
- Efficient similarity comparison:
  - Use cheap approx. to weed out most instances
  - Use expensive measure on remainder
- Form prototypes
- Edited k-NN:
  Remove instances that don't affect frontier

Overfitting Avoidance

- Set k by cross-validation
- Form prototypes
- Remove noisy instances
  - E.g., remove $\mathbf{x}$ if all of $\mathbf{x}$'s k nearest neighbors are of another class

Collaborative Filtering

(AKA Recommender Systems)

- **Problem:**
  Predict whether someone will like a Web page, newsgroup posting, movie, book, CD, etc.
- **Previous approach:**
  Look at content
- **Collaborative filtering:**
  - Look at what similar users liked
  - Similar users = Similar likes & dislikes

Collaborative Filtering

- Represent each user by vector of ratings
- Two types:
  - Yes/No
  - Explicit ratings (e.g., 0 – * * * * *)
- Predict rating:

$$\hat{R}_{ik} = \overline{R}_i + \alpha \sum_{X_j \in \mathbf{N}_i} W_{ij}(R_{jk} - \overline{R}_j)$$

- Similarity (Pearson coefficient):

$$W_{ij} = \frac{\sum_k (R_{ik} - \overline{R}_i)(R_{jk} - \overline{R}_j)}{\sqrt{\sum_k (R_{ik} - \overline{R}_i)^2} \sqrt{\sum_k (R_{jk} - \bar{R}_j)^2}}$$

Fine Points

- Primitive version:

$$\hat{R}_{ik} = \alpha \sum_{X_j \in \mathbf{N}_i} W_{ij} R_{jk}$$

- $\alpha = (\sum |W_{ij}|)^{-1}$
- $\mathbf{N}_i$ can be whole database, or only k nearest neighbors
- R_{jk} = Rating of user j on item k
- $\overline{R}_j$ = Average of all of user j's ratings
- Summation in Pearson coefficient is over all items rated by *both* users
- In principle, any prediction method can be used for collaborative filtering

Example

	R_1	R_2	R_3	R_4	R_5	R_6
Alice	2	-	4	4	-	5
Bob	1	5	4	-	3	4
Chris	5	2	-	2	1	-
Diana	3	-	2	2	-	4