CMSC828G **Principles of Data Mining** Lecture #21

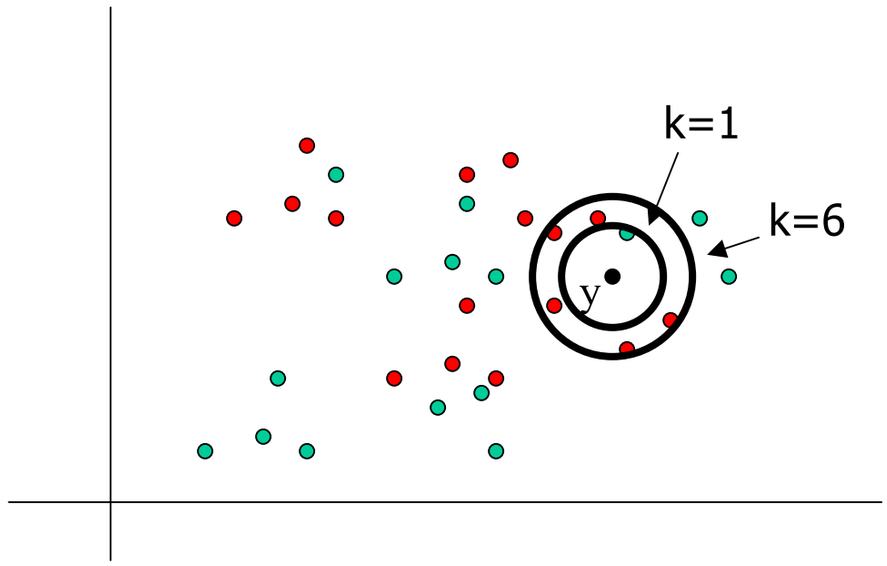
- Today's Reading:
  - HMS, 6.3, 7.3.1, 10

- Today's Lecture:
  - Predictive Modeling
    - bias and variance in KNN
    - SVMs
    - evaluating predictive models
    - feature selection
  - Finding Patterns

- Upcoming Due Dates:
  - H3 due thu

Nearest Neighbor Methods

- To classify a new input vector y, examine the k-closest training data points to y and assign the object to the most frequently occurring class



Issues

- Distance measure
  - Most common: euclidean
- Choosing k
  - Increasing k reduces variance, increases bias
- For high-dimensional space, problem that the nearest neighbor may not be very close at all!
- Memory-based technique. Must make a pass through the data for each classification. This can be prohibitive for large data sets.
- Indexing the data can help; for example KD trees

Bias and Variance in NN vs. Linear Regression

- NN – no assumptions about the model (low bias)
  prediction not stable (high variance)

$$\hat{y}(x) = \frac{1}{k} \sum_{x_i \in N_k(x)} y_i$$

- LR – strong assumptions about the model (high bias)
  prediction is stable (low variance)

$$\hat{y} = X^T \hat{\beta}$$

SVM Resources

- www.support-vector.net
- tutorials:
  - http://www.support-vector.net/icml-tutorial.pdf
  - C. J. C. Burges. A Tutorial on Support Vector Machines for Pattern Recognition. *Knowledge Discovery and Data Mining*, 2(2), 1998.
  - A. J. Smola and B. Schölkopf. A Tutorial on Support Vector Regression. NeuroCOLT Technical Report NC-TR-98-030, Royal Holloway College, University of London, UK, 1998.
- books:
  - Cristianini, N., Shawe-Taylor, J., *An Introduction to Support Vector Machines*, Cambridge University Press, (2000).
  - Schölkopf, S., Burges, C. J. C., Smola, A. J., *Advances in Kernel Methods: Support Vector Learning*, MIT Press, Cambridge, MA, (1999).

Support Vector Machines (SVMs)

- currently the 'en vogue' approach to classification, regression
- successful applications in a wide variety of fields: bioinformatics, text, handwriting recognition, image processing
- draws people from machine learning, optimization, statistics, neural networks, functional analysis
- introduced by Bosner, Guyon and Vapnik, 1992
- Kernel Machines: SVMs are a particular instance

Basic Idea

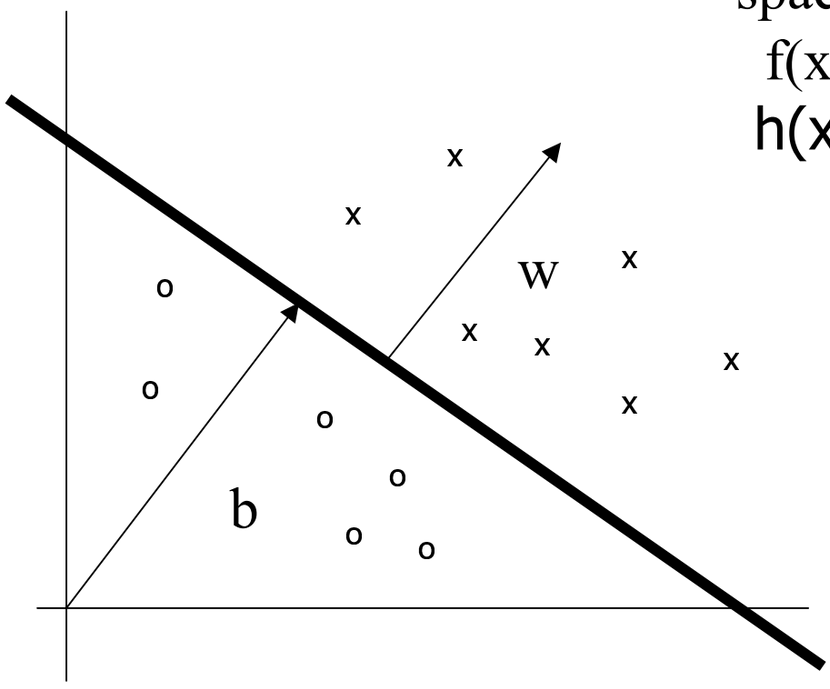
- For a given learning task, with a given finite amount of training data, the best generalization performance: balance between the accuracy on that particular training set and the "capacity" of the machine (ability of machine to learn any training set without error.
- botanist example (Burges)
  - **Too much capacity** is like a botanist with a photographic memory who, when presented with new tree, concludes that it is not a tree because it has a different number of leaves from anything seen before
  - **Too little capacity**: if it's green, it's a tree

… neither generalize well!

Linear SVMs

- Simplest case: classification using hyperplane in input space
- The Perceptron Algorithm (Rosenblatt, 57)
- Notation:
  - input space: $x \in X$
  - output space: $y \in Y = \{-1,+1\}$
  - hypothesis: $h \in H$
  - function: $f: X \to R$
  - training Set: $S = \{(x_1,y_1),\ldots,(x_m,y_m)\}$
  - test error: ε
  - dot product $\langle x,z \rangle$

Perceptron



Linear separation of the input space

$f(x) = \langle w,x \rangle + b$

$h(x)=\text{sign}(f(x))$

Update rule:

if $y_i \langle w_k,x_i \rangle + b <= 0$ then

$w_{k+1} = w_k + \eta y_i x_i$

$k++$

Observation

- Solution is linear combination of training points:

$$w = \sum \alpha_i y_i x_i, \quad \alpha_i \geq 0$$

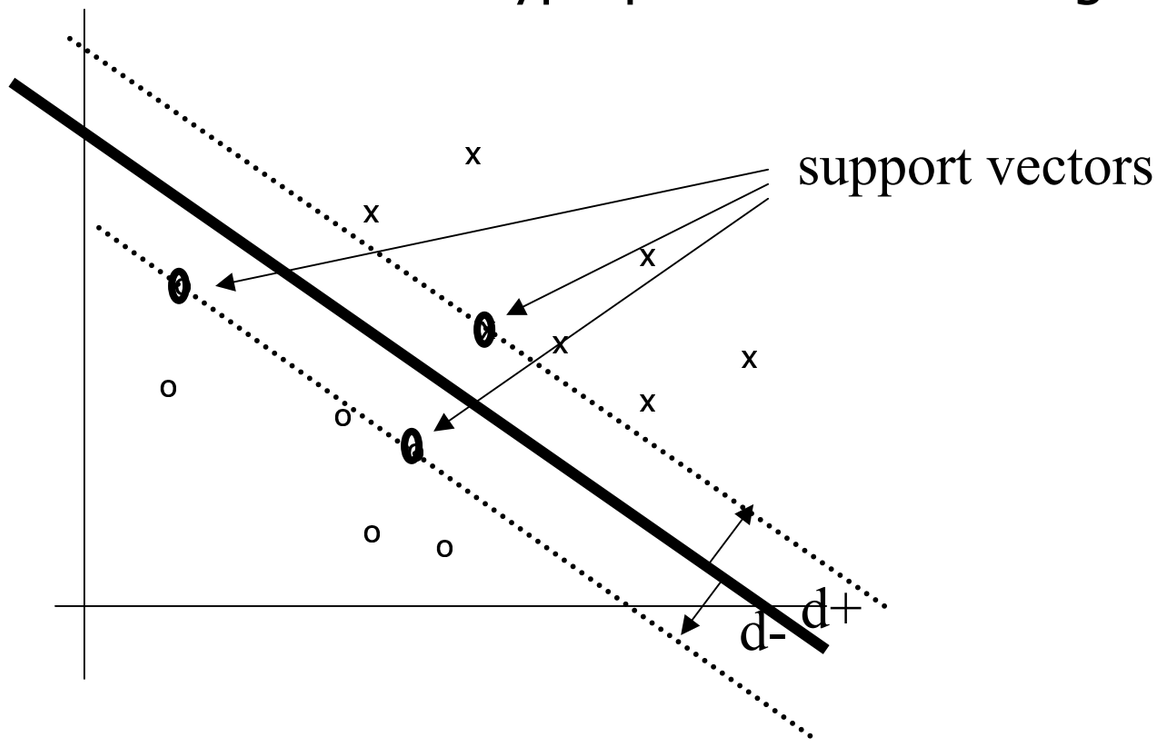
- Only used informative points (mistake driven)

- can represent in dual form:

$$f(x) = \langle w, x \rangle + b = \sum \alpha_i y_i \langle x_i, x \rangle + b$$

Linear Support Vector Machines

- d_+ distance to closest positive example, d_- distance to closest negative example.
- Define margin of separating hyperplane to be $d_+ + d_-$
- SVMs look for hyperplane with the largest margin



Constrained Optimization

$$x_i \cdot w + b \geq +1 \text{ for } y_i = +1 \qquad (1)$$

$$x_i \cdot w + b \leq -1 \text{ for } y_i = -1 \qquad (2)$$

combine: $y_i(x_i \cdot w + b) - 1 \geq 0 \quad \forall i$

for points for which equality (1) hold, lie on hyperplane H_1:

$$H_1 : x_i \cdot w + b = 1$$

with normal w and perpendicular distance from the origin $\frac{|1-b|}{\|w\|}$

for points for which equality (2) hold, lie on hyperplane H_2:

$$H_2 : x_i \cdot w + b = -1$$

with normal w and perpendicular distance from the origin $\frac{|-1-b|}{\|w\|}$

$$d_+ = d_- = \frac{1}{\|w\|}$$

margin $\frac{2}{\|w\|}$; can maximize margine by minimizing $\|w\|^2$ subject to constraints

Lagrangian

- Introduce Lagrange multipliers α_I

$$L_P \equiv \frac{1}{2}\|w\|^2 - \sum_{i=1}^{l} \alpha_i y_i (x_i \cdot w + b) + \sum_{i=1}^{l} \alpha_i$$

- Minimize L_P with respect to w, b and $\alpha_I >= 0$
- convex programming problem

•can equivalently solve the dual problem L_D

$$L_D = \sum_{i=1}^{l} \alpha_i - \frac{1}{2} \sum_{i,j} \alpha_i \alpha_j y_i y_j x_i \cdot x_j$$

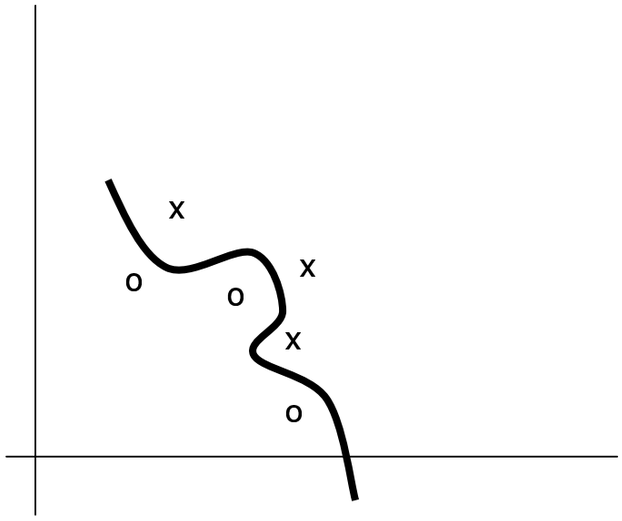
•maximize L_D with respect to constraints on w, b and $\alpha_I >= 0$

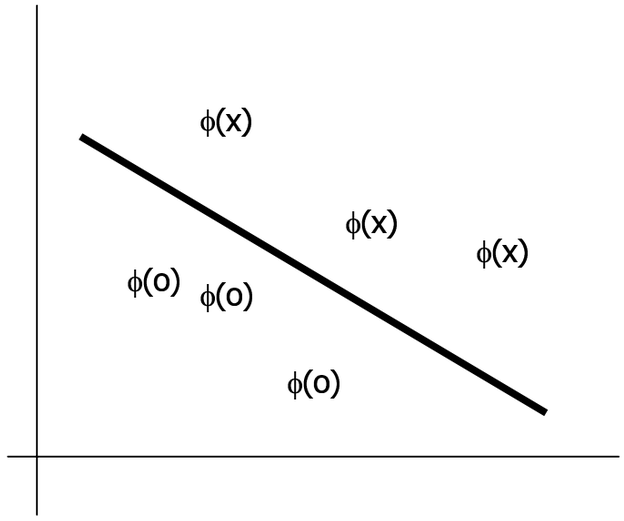
Limitations of LSVMs

- Linear classifiers cannot deal with
  - nonlinearly separable data
  - noisy data
- One solution: network of simple linear classifiers: Neural Network
- Other solution: map data into a richer feature space which includes non-linear features, then use a linear classifier

SVMs cont.

- Map data into feature space where they are linearly separable $x \rightarrow \phi(x)$





SVMs cont.

- In dual representation, the data points only appear inside dot products:

$$f(x) = \sum \alpha_i y_i \langle \phi(x_i), \phi(x) \rangle + b$$

- Introduce Kernels
- function that returns the value of the dot product between the images of the two arguments

$$K(x_1, x_2) = \langle (x_1), \phi(x_2) \rangle$$

- solves computational problem of working in high dimensional space

SVMs summary

- Properties: duality, kernels, margin, convexity
- based on statistical learning theory; connections to VC-dimension
- very general and rich class of pattern recognition methods

Evaluating and Comparing Classifiers

- estimating true future error rate
- reclassify the training data and see the proportion that is misclassified. Called the *apparent* or *resubstitution* error rate. This is typically **underestimate** of future proportion and is ill-advised.
- Estimate future error by calculating error on new sample, the **test set**
- If data set is small, use cross-validation: leave some proportion of the data and evaluate on
  - leave-one-out

Cross-validation

- If data set is small, use cross-validation: leave out some proportion of the data when classifier is constructed and evaluate on left out portion. Repeat, with different parts of the data being omitted.
  - leave-one-out: leave out one point at a time
  - bootstrap methods:
    - Introduced by Efron, 1979, to calculate confidence intervals for parameters when sample size is small
    - at a high-level:
      - Observations randomly re-assigned and estimates are recomputed; treated as repeated experiments

Feature Selection

- classification in high dimensions--Too many variables!
- Not all variables may be necessary for accurate discrimination
- varialbe selection:
- select subset p’ of original p variables.
  - part of algorithm, e.g. tree inducer
  - wrapper: external loop that systimatically adds and removes variables from the current set
- variable transformation
  - pca, etc.
  - disadvantage: not necessarily matched for optimizing classification performance

References

- *Principles of Data Mining*, Hand, Mannila, Smyth. MIT Press, 2001.
- *Data Mining*, Witten and Eibe. Academic Press, 2000.
- *Machine Learning*, T. Mitchell. McGraw-Hill, 1997.
- Nello Cristianini's ICML 2001 tutorial, http://www.support-vector.net/icml-tutorial.pdf
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