SUPPORT VECTOR MACHINES

Today

- Reading
  - AIMA 18.9
- Goals
  - Finish Backpropagation
  - Introduce support vector machines (SVMs)
- A month for final projects
  - Should have found a group and starting on data collection
  - Progress reports start April 23rd!

Backpropagation

1. Begin with randomly initialized weights
2. Apply the neural network to each training example (each pass through examples is called an epoch)
3. If it misclassifies an example **modify the weights**
4. Continue until the neural network classifies all training examples correctly

(Derive gradient-descent update rule)

Backpropagation

```
function BACK-PROP-LEARNING(examples, network) returns a neural network
  inputs: examples, a set of examples, each with input vector x and output vector y
          network, a multilayer network with L layers, weights w_{i,j}, activation function g
  local variables: Δ, a vector of errors, indexed by network node

  repeat
     for each weight w_{i,j} in network do
        w_{i,j} ← a small random number
     for each example (x, y) in examples do
        /* Propagate the inputs forward to compute the outputs */
        for each node i in the input layer do
           a_i ← x_i
        for ℓ = 2 to L do
           for each node j in layer ℓ do
              in_j ← Σ_i w_{i,j} a_i
              a_j ← g(in_j)
        /* Propagate deltas backward from output layer to input layer */
        for each node j in the output layer do
           Δ[j] ← g'(in_j) × (y_j − a_j)
        for ℓ = L − 1 to 1 do
           for each node i in layer ℓ do
              Δ[i] ← g'(in_i) Σ_j w_{i,j} Δ[j]
        /* Update every weight in network using deltas */
        for each weight w_{i,j} in network do
           w_{i,j} ← w_{i,j} + α × a_i × Δ[j]
  until some stopping criterion is satisfied
  return network
```

Figure 18.24 The back-propagation algorithm for learning in multilayer networks.

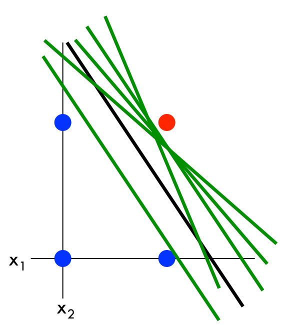
Support Vector Machines (SVMs)

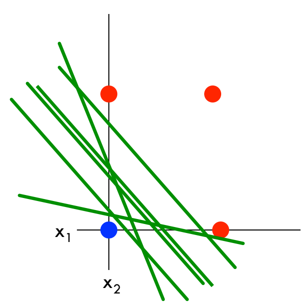
- SVMs are probably the most popular off-the-shelf classifier!
- Software Packages
  - LIBSVM (LIBLINEAR) – on the Resources page
  - SVM-Light

Linearly Separable

x_1	x_2	x_1 **and** x_2
0	0	0
0	1	0
1	0	0
1	1	1

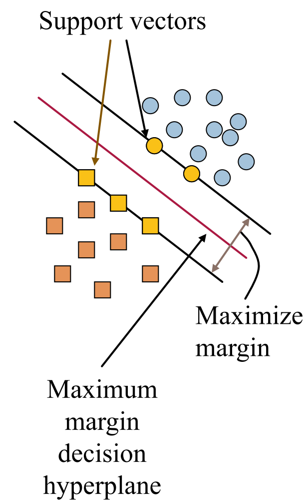
x_1	x_2	x_1 **or** x_2
0	0	0
0	1	1
1	0	1
1	1	1





Support Vector Machines

- A support vector machine (SVM) is a linear classifier that finds the decision boundary btw. two classes that is *maximally far from any point in the training set*
- The margin is the distance from the decision boundary to the closest data point
- The support vectors are a subset of the training examples that fully determine the decision boundary



Basic Linear Algebra Notes (on board)

- Length of a vector
- Unit vector
- Dot product
- Hyperplane
- Given this knowledge, how do we find the hyperplane with the maximum margin?

Solving the Optimization Problem

$$\min_{w,b} \frac{1}{2}||w||^2 \text{ such that } y^{(i)}\left(w^\intercal x^{(i)} + b\right) \geq 1 \quad \forall i$$

- Need to optimize a *quadratic* function subject to *linear* constraints
- Quadratic optimization problems are a well-known class of mathematical programming problem and many algorithms exist for solving them
- The solution involves constructing a *dual problem* where a *Lagrange multiplier* (a scalar value) is associated with every constraint in the primary problem

Solving the Optimization Problem

$$\min_{w,b} \frac{1}{2}||w||^2 \text{ such that } y^{(i)}\left(w^\intercal x^{(i)} + b\right) \geq 1 \quad \forall i$$

$$\max_\alpha \min_{w,b} \frac{1}{2}||w||^2 - \sum_{i=1}^{N} \alpha_i \left[y^{(i)}\left(w^\intercal x^{(i)} + b\right) - 1\right]$$

Dual

Lagrange multipliers

$$\max_\alpha \sum_{i=1}^{N} \alpha_i - \frac{1}{2} \sum_i \sum_j \alpha_i \alpha_j y^{(i)} y^{(j)} x^{(i)} x^{(j)}$$

$$\text{subject to } \alpha_i \geq 0 \text{ and } \sum_i \alpha_i y^{(i)} = 0$$

Solving the Optimization Problem

- The solution has the form:

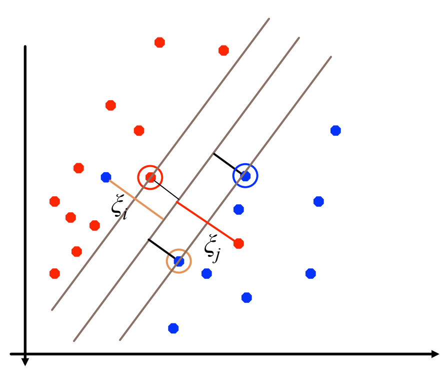
$$w = \sum_{i=1}^{N} \alpha_i y^{(i)} x^{(i)} \text{ and } b = y^{(i)} - w^\intercal x^{(i)} \text{ for any } x^{(i)} \text{ s.t. } \alpha_i \neq 0$$

- Each non-zero alpha indicates corresponding x_i is a *support vector*
- The classifying function has the form: $g(x_i) = \text{sign}\left(\sum_i \alpha_i y^{(i)} x^{(i)} x + b\right)$
- Relies on an inner product between the test point x and the support vectors x_i

Soft-margin Classification

If the training data is not linearly separable, *slack variables* ξ_i can be added to allow misclassification of difficult or noisy examples.

Still, try to minimize training set errors, and to place hyperplane “far” from each class (large margin)



How many support vectors?

- Determined by alphas in optimization
- Typically only a small proportion of the training data
- The number of support vectors determines the run time for prediction

How fast are SVMs?

Training

- Time for training is dominated by the time for solving the underlying quadratic programming problem
- Slower than Naïve Bayes
- Non-linear SVMs are worse

Testing (Prediction)

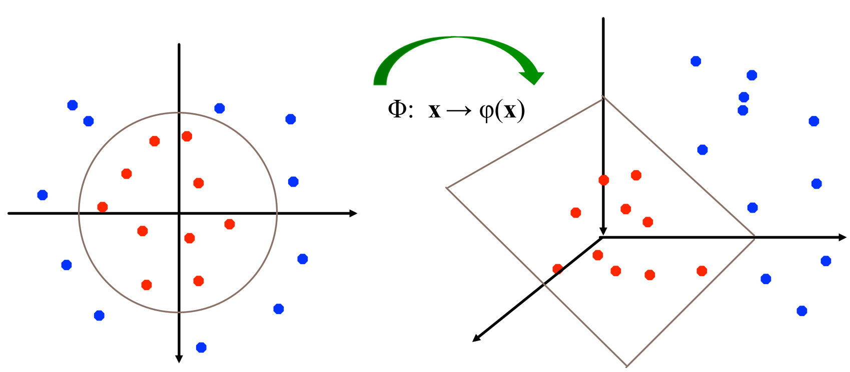
- Fast - as long as we don't have too many support vectors

Multi-label classification

- SVMs are inherently two-class classifiers
- Given C classes, common techniques are:
  - One-versus-all
    - Train C different SVMs where each SVM learns one class versus all the other classes
  - One-versus-one
    - Train C(C-1)/2 SVMs where each SVM learns to distinguish one class from another
- Multi-class SVMs
- Transductive SVMs

Non-linear SVMs

- General idea: the original feature space can always be mapped to some higher-dimensional feature space where the training set is separable:



The "Kernel" trick

- The linear classifier relies on an inner product between vectors $x_i^T x_j$

$$g(x_i) = \text{sign}\left(\sum_i \alpha_i y^{(i)} x^{(i)} x + b\right)$$

- If every example is mapped into a high-dimensional space via some transformation Φ: $\mathbf{x} \rightarrow \varphi(\mathbf{x})$ then the inner product becomes:

$$g(x_i) = \text{sign}\left(\sum_i \alpha_i y^{(i)} \varphi(x^{(i)})^\intercal \varphi(x) + b\right)$$

- A kernel function is some function that corresponds to a dot product in some transformed feature space:

$$K(\mathbf{x}_i,\mathbf{x}_j) = \varphi(\mathbf{x}_i)^T \varphi(\mathbf{x}_j)$$

The "Kernel" trick

- The kernel K may be cheaper to compute then the transformation φ
  - Implictly do the transformation

$$\phi(x) = \begin{bmatrix} x_1x_1 \\ x_1x_2 \\ x_1x_3 \\ x_2x_1 \\ x_2x_2 \\ x_2x_3 \\ x_3x_1 \\ x_3x_2 \\ x_3x_3 \end{bmatrix}$$

$$\begin{aligned} K(x,z) &= \left(\sum_{i=1}^n x_i z_i\right)\left(\sum_{j=1}^n x_i z_i\right) \\ &= \sum_{i=1}^n \sum_{j=1}^n x_i x_j z_i z_j \\ &= \sum_{i,j=1}^n (x_i x_j)(z_i z_j) \end{aligned}$$

*

Kernels

Why use kernels?

- Make non-separable problem separable.
- Map data into better representational space

Common kernels

- Linear
- Polynomial $\mathbf{K(x,z) = (1+x^Tz)^d}$
- Radial basis function (infinite dimensional space)

$$K(\mathbf{x}_i, \mathbf{x}_j) = e^{-\|\mathbf{x}_i - \mathbf{x}_j\|^2/2\sigma^2}$$

Summary

- Support Vector Machines (SVMs)
  - Choose hyperplane based on support vectors
  - Support vectors are critical points close to the decision boundary
  - Often among the best performing classifiers

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