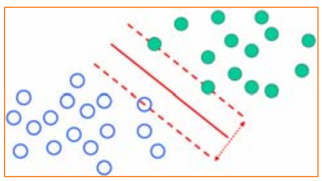
Machine Learning

10-701/15-781, Fall 2006

Support Vector Machines

Eric Xing



Lecture 8, October 5, 2006

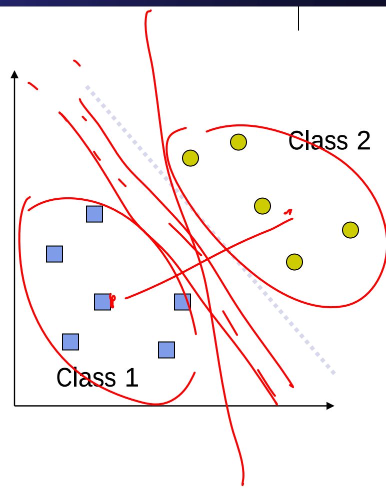
Reading: Chap. 6&7, C.B book

Outline

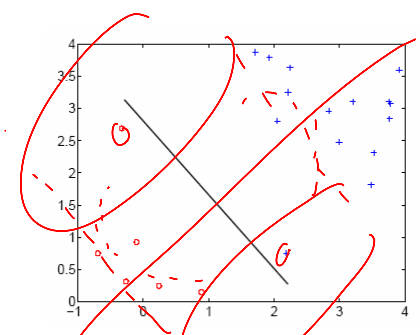
- Maximum margin classification
- Constrained optimization
- Lagrangian duality
- Kernel trick
- Non-separable cases

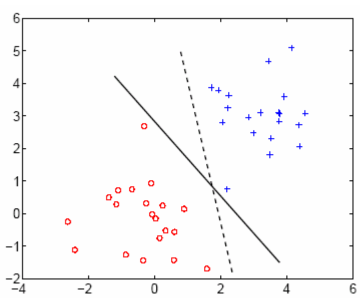
What is a good Decision Boundary?

- Consider a binary classification task with y = ±1 labels (not 0/1 as before).
- When the training examples are linearly separable, we can set the parameters of a linear classifier so that all the training examples are classified correctly
- Many decision boundaries!
  - Generative classifiers
  - Logistic regressions ...
- Are all decision boundaries equally good?



Examples of Bad Decision Boundaries



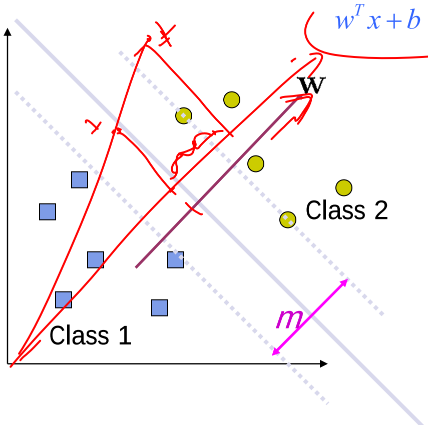


- Why we may have such boundaries?
  - Irregular distribution
  - Imbalanced training sizes
  - outliners

Classification and Margin

- Parameterzing decision boundary
  - Let w denote a vector orthogonal to the decision boundary, and b denote a scalar "offset" term, then we can write the decision boundary as:

$$w^T x + b = 0$$



- Margin

$w^T x+b > 0$ for all x in class 2

$w^T x+b < 0$ for all x in class 1

Or more compactly:

$$(w^T x_i+b)y_i > 0$$

The margin between two points

$\mathbf{m}=(w^T x_i+b)-(w^T x_j+b)=w^T(x_i-x_j)$

Maximum Margin Classification

- The margin is: $$m = w^T\left(x_{i^*} - x_{j^*}\right)$$
- It make sense to set constrains on W:
- Here is our Maximum Margin Classification problem:

$$\begin{aligned} &\max_{w,b} && m \\ &\text{s.t} && y_i(w^T x_i + b) \geq m, \quad \forall i \\ & && \|w\| = 1 \end{aligned}$$

- Equivalently, we can instead work on this:

$$\begin{aligned} &\max_{w,b} && \frac{m}{\|w\|} \\ &\text{s.t} && y_i(w^T x_i + b) \geq m, \quad \forall i \end{aligned}$$

Maximum Margin Classification, con'd.

- The optimization problem:

$$\max_{w,b} \quad \frac{m}{\|w\|}$$
$$\text{s.t} \quad y_i(w^T x_i + b) \geq m, \quad \forall i$$

- But note that the magnitude of m merely scales w and b, and does not change the classification boundary at all!
- So we instead work on this cleaner problem:

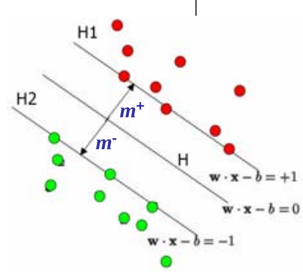
$$\max_{w,b} \quad \frac{1}{\|w\|}$$
$$\text{s.t} \quad y_i(w^T x_i + b) \geq 1, \quad \forall i$$

- The solution to this leads to the famous **Support Vector Machines** --- believed by many to be the best "off-the-shelf" supervised learning algorithm

Support vector machine

- A convex quadratic programming problem with linear constrains:

$$\max_{w,b} \quad \frac{1}{\|w\|}$$
$$\text{s.t} \quad y_i(w^T x_i + b) \geq 1, \quad \forall i$$



  - The attained margin is now given by $\frac{1}{\|w\|}$
  - Only a few of the classification constraints are relevant ➔ **support vectors**
- Constrained optimization
  - We can directly solve this using commercial quadratic programming (QP) code
  - But we want to take a more careful investigation of Lagrange duality, and the solution of the above is its dual form.
  - ➔ deeper insight: support vectors, kernels …
  - ➔ more efficient algorithm

Lagrangian Duality

- The Primal Problem

Primal:

$$\min_w \ f(w)$$
$$\text{s.t.} \quad g_i(w) \le 0, \ i = 1, \ldots, k$$
$$h_i(w) = 0, \ i = 1, \ldots, l$$

The generalized Lagrangian:

$$\mathcal{L}(w, \alpha, \beta) = f(w) + \sum_{i=1}^{k} \alpha_i g_i(w) + \sum_{i=1}^{l} \beta_i h_i(w)$$

the α's ($\alpha_i \geq 0$) and β's are called the Lagarangian multipliers

Lemma:

$$\max_{\alpha,\beta,\alpha_i \ge 0} \ \mathcal{L}(w,\alpha,\beta) = \begin{cases} f(w) & \text{if } w \text{ satisfies primal constraints} \\ \infty & \text{o/w} \end{cases}$$

A re-written Primal:

$$\min_w \max_{\alpha,\beta,\alpha_i \ge 0} \ \mathcal{L}(w,\alpha,\beta)$$

Lagrangian Duality, cont.

- Recall the Primal Problem:

$$\min_w \max_{\alpha,\beta,\alpha_i \ge 0} \ \mathcal{L}(w,\alpha,\beta)$$

- The Dual Problem:

$$\max_{\alpha,\beta,\alpha_i \ge 0} \min_w \ \mathcal{L}(w,\alpha,\beta)$$

- **Theorem (weak duality):**

$$d^* = \max_{\alpha,\beta,\alpha_i \ge 0} \min_w \mathcal{L}(w,\alpha,\beta) \ \le \ \min_w \max_{\alpha,\beta,\alpha_i \ge 0} \ \mathcal{L}(w,\alpha,\beta) = p^*$$

- **Theorem (strong duality):**

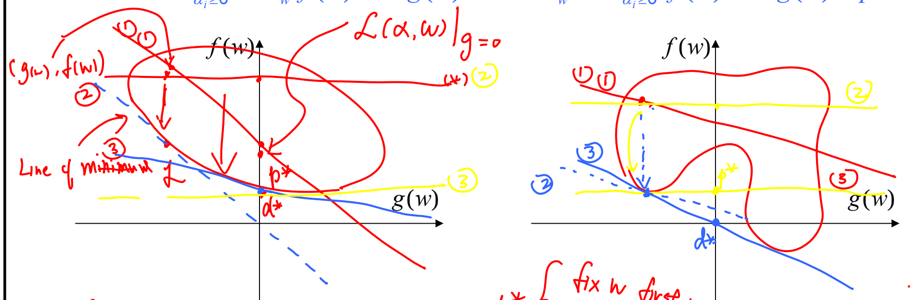
Iff there exist a saddle point of $\mathcal{L}(w,\alpha,\beta)$, we have

$$d^* = p^*$$

A sketch of strong and weak duality

- Now, ignoring $h(x)$ for simplicity, let's look at what's happening graphically in the duality theorems.

$$d^* = \max_{\alpha_i \geq 0} \min_w f(w) + \alpha^T g(w) \;\leq\; \min_w \max_{\alpha_i \geq 0} f(w) + \alpha^T g(w) = p^*$$



d^* { fix α first: (slope)
then minimize w: → shift line down
then ~~minimize~~ max α: → get the largest intercept on $f(w)$

p^* { fix w first:
the max α: → hold (f, g) fixed and change the slope to max intercept. (*)
then min over w: → shift the line to min intercept (**)

The KKT conditions

- If there exists some saddle point of $\mathcal{L}$, then the saddle point satisfies the following "Karush-Kuhn-Tucker" (KKT) conditions:

$$\frac{\partial}{\partial w_i}\mathcal{L}(w,\alpha,\beta) = 0, \quad i = 1,\ldots,n$$

$$\frac{\partial}{\partial \beta_i}\mathcal{L}(w,\alpha,\beta) = 0, \quad i = 1,\ldots,l$$

$$\alpha_i g_i(w) = 0, \quad i = 1,\ldots,k$$

$$g_i(w) \leq 0, \quad i = 1,\ldots,k$$

$$\alpha_i \geq 0, \quad i = 1,\ldots,k$$

- **Theorem**: If w^*, α^* and β^* satisfy the KKT condition, then it is also a solution to the primal and the dual problems.

Solving optimal margin classifier

- Recall our opt problem:

$$\begin{aligned} \max_{w,b} \quad & \frac{1}{\|w\|} \\ \text{s.t} \quad & y_i(w^T x_i + b) \geq 1, \quad \forall i \end{aligned}$$

- This is equivalent to

$$\begin{aligned} \min_{w,b} \quad & \frac{1}{2} w^T w \\ \text{s.t} \quad & 1 - y_i(w^T x_i + b) \leq 0, \quad \forall i \end{aligned} \qquad (*)$$

- Write the Lagrangian:

$$\mathcal{L}(w,b,\alpha) = \frac{1}{2} w^T w - \sum_{i=1}^{m} \alpha_i \left[y_i(w^T x_i + b) - 1 \right]$$

  - Recall that (*) can be reformulated as $\min_{w,b} \max_{\alpha_i \geq 0} \mathcal{L}(w,b,\alpha)$
    Now we solve its **dual problem**: $\max_{\alpha_i \geq 0} \min_{w,b} \mathcal{L}(w,b,\alpha)$

The Dual Problem

$$\max_{\alpha_i \geq 0} \min_{w,b} \mathcal{L}(w,b,\alpha)$$

- We minimize $\mathcal{L}$ with respect to w and b first:

$$\nabla_w \mathcal{L}(w,b,\alpha) = w - \sum_{i=1}^{m} \alpha_i y_i x_i = 0, \qquad (*)$$

$$\nabla_b \mathcal{L}(w,b,\alpha) = \sum_{i=1}^{m} \alpha_i y_i = 0, \qquad (**)$$

Note that **(*)** implies:

$$w = \sum_{i=1}^{m} \alpha_i y_i x_i \qquad (***)$$

- Plus (***) back to $\mathcal{L}$, and using (**), we have:

$$\mathcal{L}(w,b,\alpha) = \sum_{i=1}^{m} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{m} \alpha_i \alpha_j y_i y_j (\mathbf{x}_i^T \mathbf{x}_j)$$

The Dual problem, cont.

- Now we have the following dual opt problem:

$$\max_\alpha \mathcal{J}(\alpha) = \sum_{i=1}^{m} \alpha_i - \frac{1}{2}\sum_{i,j=1}^{m} \alpha_i \alpha_j y_i y_j (\mathbf{x}_i^T \mathbf{x}_j)$$

$$\text{s.t.} \quad \alpha_i \geq 0, \quad i = 1, \ldots, k$$

$$\sum_{i=1}^{m} \alpha_i y_i = 0.$$

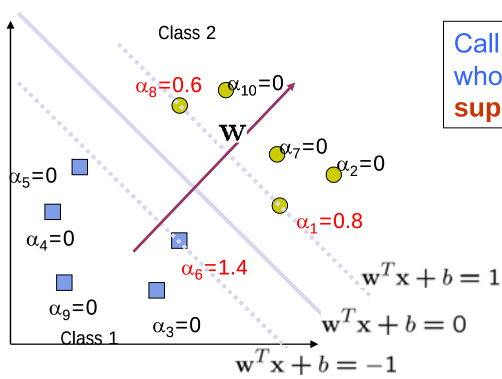
- This is, (again,) a **quadratic programming** problem.
  - A global maximum of α_i can always be found.
  - But what's the big deal??
  - Note two things:

1. w can be recovered by $w = \sum_{i=1}^{m} \alpha_i y_i \mathbf{x}_i$ See next …
2. The "kernel" $\mathbf{x}_i^T \mathbf{x}_j$ More later …

Support vectors

- Note the KKT condition --- only a few α_i's can be nonzero!!

$$\alpha_i g_i(w) = 0, \quad i = 1, \ldots, k$$



Call the training data points whose α_i's are nonzero the **support vectors** (SV)

Support vector machines

- Once we have the Lagrange multipliers $\{\alpha_i\}$, we can reconstruct the parameter vector w as a weighted combination of the training examples:

$$w = \sum_{i \in SV} \alpha_i y_i \mathbf{x}_i$$

- For testing with a new data z
  - Compute

$$w^T z + b = \sum_{i \in SV} \alpha_i y_i \left(\mathbf{x}_i^T z\right) + b$$

    and classify z as class 1 if the sum is positive, and class 2 otherwise
  - Note: w need not be formed explicitly

Interpretation of support vector machines

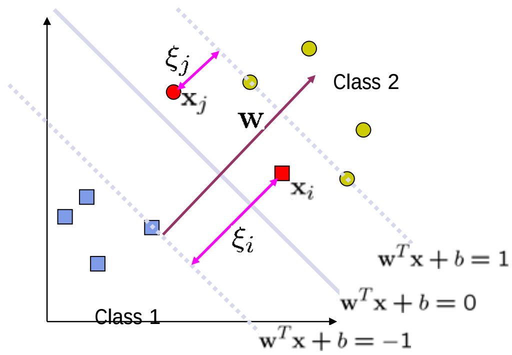
- The optimal w is a linear combination of a small number of data points. This "sparse" representation can be viewed as data compression as in the construction of kNN classifier

- To compute the weights $\{\alpha_i\}$, and to use support vector machines we need to specify only the inner products (or kernel) between the examples $\mathbf{x}_i^T \mathbf{x}_j$

- We make decisions by comparing each new example z with only the support vectors:

$$y^* = \operatorname{sign}\left(\sum_{i \in SV} \alpha_i y_i \left(\mathbf{x}_i^T z\right) + b\right)$$

Non-linearly Separable Problems



- We allow "error" ξ_i in classification; it is based on the output of the discriminant function $\boldsymbol{w}^T\boldsymbol{x}+b$
- ξ_i approximates the number of misclassified samples

Soft Margin Hyperplane

- Now we have a slightly different opt problem:

$$\min_{w,b} \quad \frac{1}{2}w^T w + C\sum_{i=1}^{m}\xi_i$$

$$\text{s.t} \quad \begin{array}{l} y_i(w^T x_i + b) \geq 1 - \xi_i, \quad \forall i \\ \xi_i \geq 0, \quad \forall i \end{array}$$

  - ξ_i are "slack variables" in optimization
  - Note that ξ_i=0 if there is no error for $\mathbf{x}_i$
  - ξ_i is an upper bound of the number of errors
  - C : tradeoff parameter between error and margin

The Optimization Problem

- The dual of this new constrained optimization problem is

$$\max_\alpha \quad \mathcal{J}(\alpha) = \sum_{i=1}^{m} \alpha_i - \frac{1}{2}\sum_{i,j=1}^{m} \alpha_i \alpha_j y_i y_j (\mathbf{x}_i^T \mathbf{x}_j)$$

$$\text{s.t.} \quad 0 \le \alpha_i \le C, \quad i = 1, \ldots, k$$

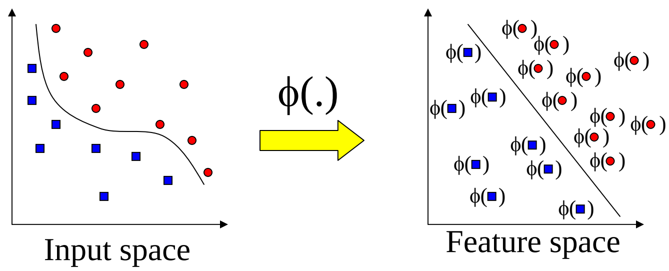
$$\sum_{i=1}^{m} \alpha_i y_i = 0.$$

- This is very similar to the optimization problem in the linear separable case, except that there is an upper bound C on α_i now
- Once again, a QP solver can be used to find α_i

Extension to Non-linear Decision Boundary

- So far, we have only considered large-margin classifier with a linear decision boundary
- How to generalize it to become nonlinear?
- Key idea: transform $\mathbf{x}_i$ to a higher dimensional space to "make life easier"
  - Input space: the space the point $\mathbf{x}_i$ are located
  - Feature space: the space of $\phi(\mathbf{x}_i)$ after transformation
- Why transform?
  - Linear operation in the feature space is equivalent to non-linear operation in input space
  - Classification can become easier with a proper transformation. In the XOR problem, for example, adding a new feature of x_1x_2 make the problem linearly separable (homework)

Transforming the Data



Note: feature space is of higher dimension than the input space in practice

- Computation in the feature space can be costly because it is high dimensional
  - The feature space is typically infinite-dimensional!
- The kernel trick comes to rescue

The Kernel Trick

- Recall the SVM optimization problem

$$\max_{\alpha} \quad \mathcal{J}(\alpha) = \sum_{i=1}^{m} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{m} \alpha_i \alpha_j y_i y_j (\mathbf{x}_i^T \mathbf{x}_j)$$

$$\text{s.t.} \quad 0 \le \alpha_i \le C, \quad i = 1, \ldots, k$$

$$\sum_{i=1}^{m} \alpha_i y_i = 0.$$

- The data points only appear as inner product
- As long as we can calculate the inner product in the feature space, we do not need the mapping explicitly
- Many common geometric operations (angles, distances) can be expressed by inner products
- Define the kernel function K by $K(\mathbf{x}_i, \mathbf{x}_j) = \phi(\mathbf{x}_i)^T \phi(\mathbf{x}_j)$

An Example for feature mapping and kernels

- Consider an input $\mathbf{x}=[x_1,x_2]$
- Suppose $\phi(.)$ is given as follows

$$\phi\left(\begin{bmatrix} x_1 \\ x_2 \end{bmatrix}\right) = 1, \sqrt{2}x_1, \sqrt{2}x_2, x_1^2, x_2^2, \sqrt{2}x_1x_2$$

- An inner product in the feature space is

$$\left\langle \phi\left(\begin{bmatrix} x_1 \\ x_2 \end{bmatrix}\right), \phi\left(\begin{bmatrix} x_1' \\ x_2' \end{bmatrix}\right) \right\rangle =$$

- So, if we define the **kernel function** as follows, there is no need to carry out $\phi(.)$ explicitly

$$K(\mathbf{x},\mathbf{x}') = \left(1 + \mathbf{x}^T\mathbf{x}'\right)^2$$

More examples of kernel functions

- Linear kernel (we've seen it)

$$K(\mathbf{x},\mathbf{x}') = \mathbf{x}^T\mathbf{x}'$$

- Polynomial kernel (we just saw an example)

$$K(\mathbf{x},\mathbf{x}') = \left(1 + \mathbf{x}^T\mathbf{x}'\right)^p$$

where p = 2, 3, … To get the feature vectors we concatenate all pth order polynomial terms of the components of x (weighted appropriately)

- Radial basis kernel

$$K(\mathbf{x},\mathbf{x}') = \exp\left(-\frac{1}{2}\left\|\mathbf{x}-\mathbf{x}'\right\|^2\right)$$

In this case the feature space consists of functions and results in a non-parametric classifier.

Kernelized SVM

- Training:

$$\max_\alpha \quad \mathcal{J}(\alpha) = \sum_{i=1}^{m} \alpha_i - \frac{1}{2}\sum_{i,j=1}^{m} \alpha_i \alpha_j y_i y_j K(\mathbf{x}_i, \mathbf{x}_j)$$

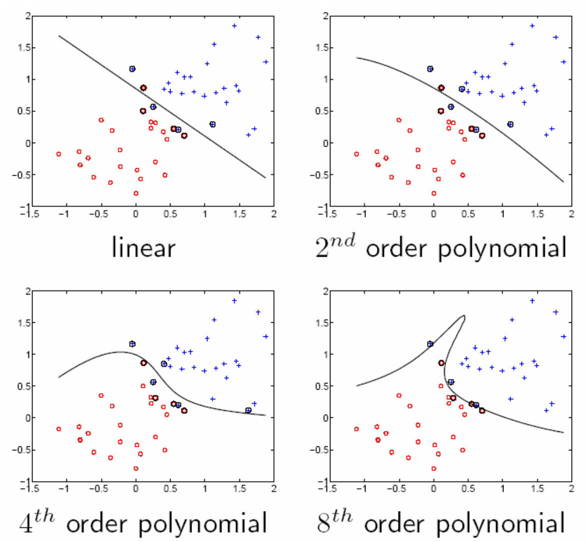
$$\text{s.t.} \quad 0 \le \alpha_i \le C, \quad i = 1, \ldots, k$$

$$\sum_{i=1}^{m} \alpha_i y_i = 0.$$

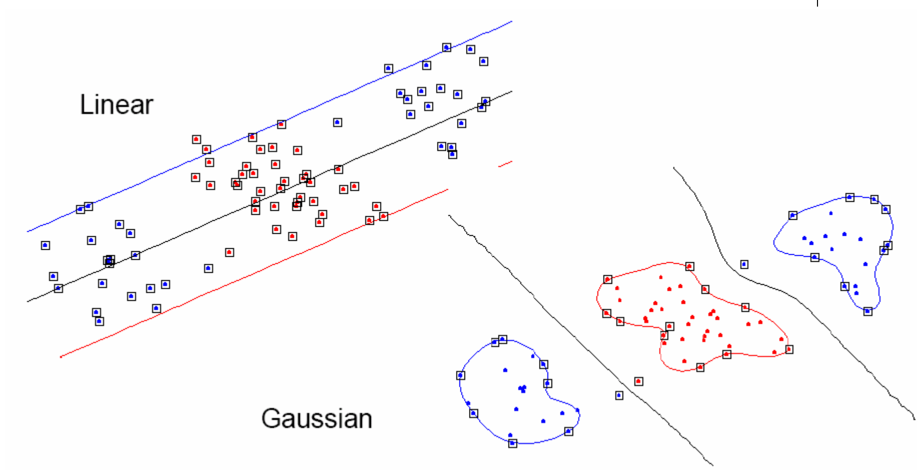
- Using:

$$y^* = \text{sign}\left(\sum_{i \in SV} \alpha_i y_i K(\mathbf{x}_i, z) + b \right)$$

SVM examples



Examples for Non Linear SVMs – Gaussian Kernel



Cross-validation error

- The leave-one-out cross-validation error does not depend on the dimensionality of the feature space but only on the # of support vectors!

$$\text{Leave-one-out CV error} = \frac{\#\,\text{support vectors}}{\#\,\text{of training examples}}$$