Machine Learning
CSE 6363 (Fall 2019)

Lecture 10 Support Vector Machine

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History of SVM

- SVM is related to statistical learning theory [3]
- SVM was first introduced in 1992 [1]
- SVM becomes popular because of its success in handwritten digit recognition
  - 1.1% test error rate for SVM. This is the same as the error rates of a carefully constructed neural network
- SVM is now regarded as an important example of “kernel methods”, one of the key area in machine learning

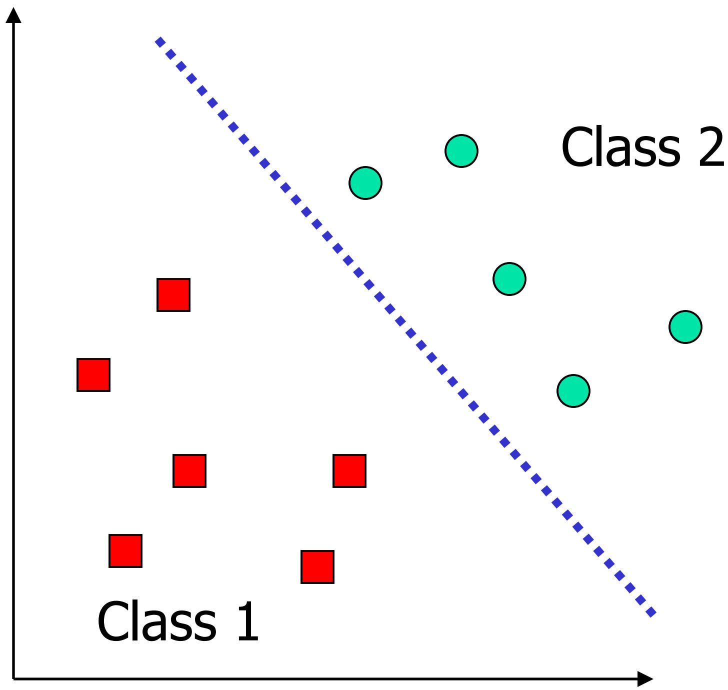
[1] B.E. Boser *et al*. A Training Algorithm for Optimal Margin Classifiers. Proceedings of the Fifth Annual Workshop on Computational Learning Theory 5 144-152, Pittsburgh, 1992.

[2] L. Bottou *et al*. Comparison of classifier methods: a case study in handwritten digit recognition. Proceedings of the 12th IAPR International Conference on Pattern Recognition, vol. 2, pp. 77-82.

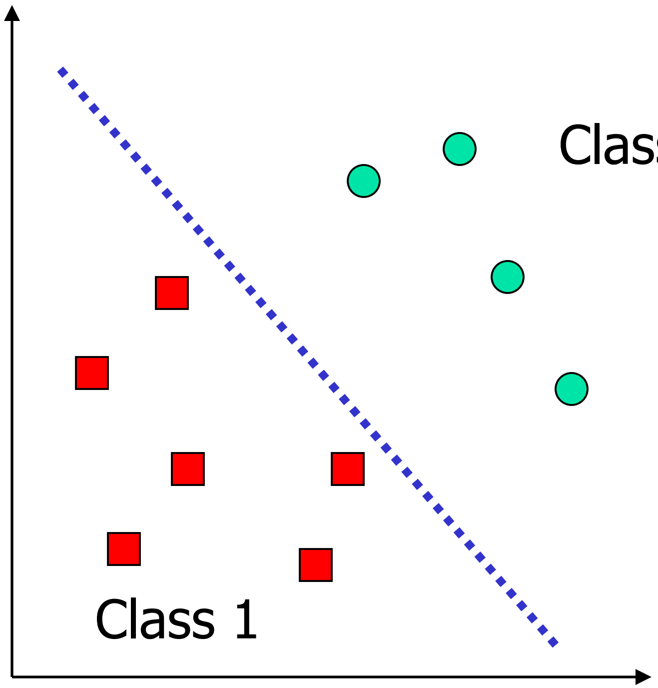
[3] V. Vapnik. The Nature of Statistical Learning Theory. 2nd edition, Springer, 1999.

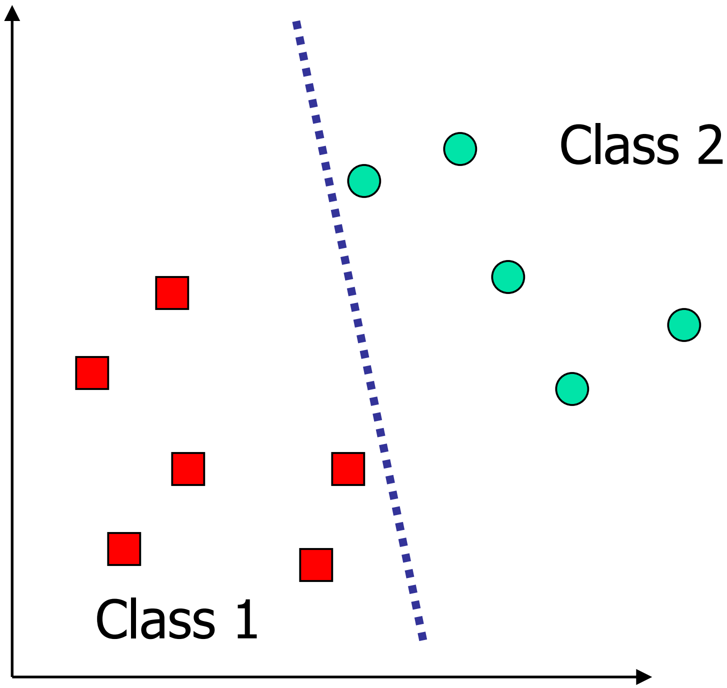
What is a good Decision Boundary?

- Consider a two-class, linearly separable classification problem
- Many decision boundaries!
  - The Perceptron algorithm can be used to find such a boundary
  - Different algorithms have been proposed
- Are all decision boundaries equally good?



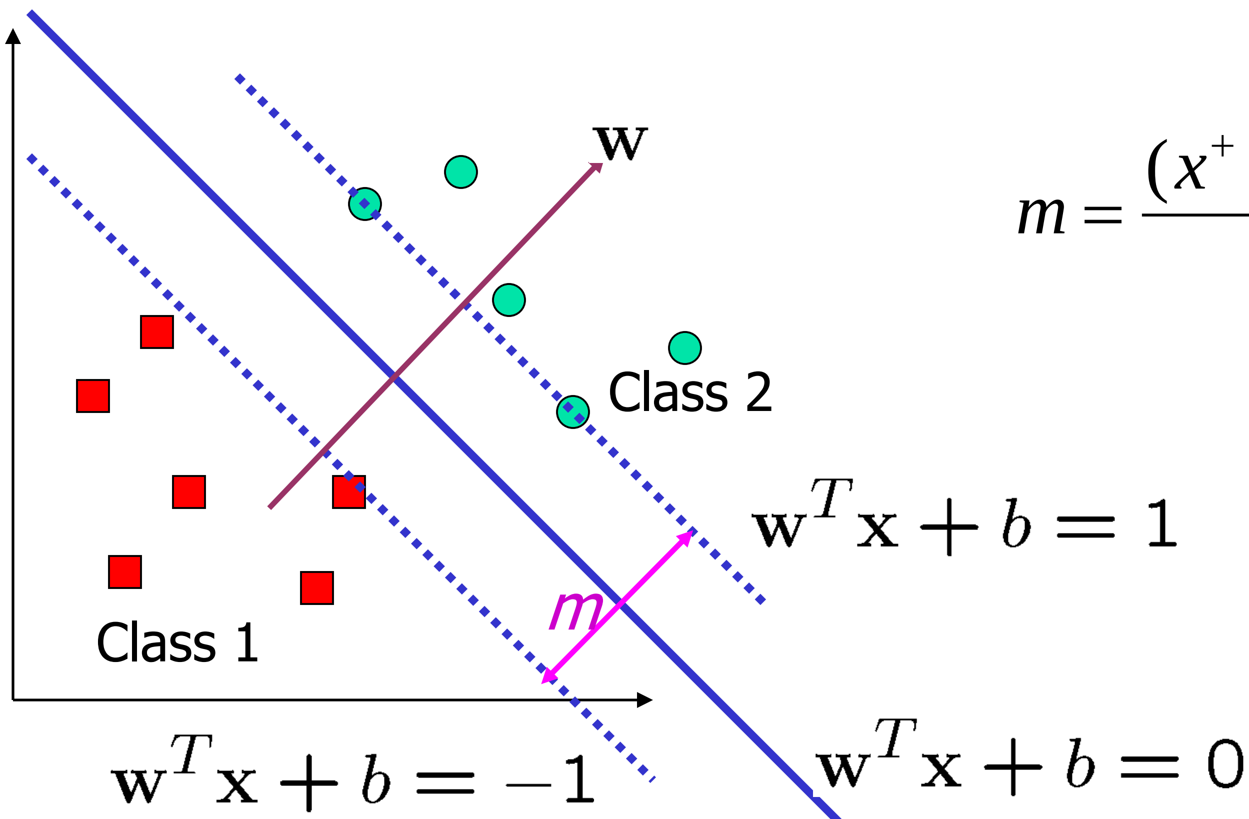
Examples of Bad Decision Boundaries





Large-margin Decision Boundary

- The decision boundary should be as far away from the data of both classes as possible
  - We should maximize the margin, *m*
  - Distance between the origin and the line $\mathbf{w}^t\mathbf{x}=k$ is $k/||\mathbf{w}||$



$$m = \frac{(x^+ - x^-)\cdot w}{|w|} = \frac{2}{|w|}$$

Finding the Decision Boundary

- Let $\{x_1, ..., x_n\}$ be our data set and let $y_i \in \{1,-1\}$ be the class label of x_i
- The decision boundary should classify all points correctly $\Rightarrow \quad y_i(\mathbf{w}^T\mathbf{x}_i + b) \geq 1, \qquad \forall i$
- The decision boundary can be found by solving the following constrained optimization problem

$$\text{Minimize } \frac{1}{2}||\mathbf{w}||^2$$
$$\text{subject to } y_i(\mathbf{w}^T\mathbf{x}_i + b) \geq 1 \qquad \forall i$$

- This is a constrained optimization problem. Solving it requires some new tools
  - Feel free to ignore the following several slides; what is important is the constrained optimization problem above

Recap of Constrained Optimization

- Suppose we want to: minimize f($\mathbf{x}$) subject to g($\mathbf{x}$) = 0
- A necessary condition for $\mathbf{x}_0$ to be a solution:

$$\begin{cases} \frac{\partial}{\partial \mathbf{x}}\Big(f(\mathbf{x}) + \alpha g(\mathbf{x})\Big)\Big|_{\mathbf{x}=\mathbf{x}_0} = \mathbf{0} \\ g(\mathbf{x}) = 0 \end{cases}$$

- α: the Lagrange multiplier
- For multiple constraints $g_i(\mathbf{x}) = 0$, i=1, …, m, we need a Lagrange multiplier α_i for each of the constraints

$$\begin{cases} \frac{\partial}{\partial \mathbf{x}}\Big(f(\mathbf{x}) + \sum_{i=1}^{n} \alpha_i g_i(\mathbf{x})\Big)\Big|_{\mathbf{x}=\mathbf{x}_0} = \mathbf{0} \\ g_i(\mathbf{x}) = 0 \qquad \text{for } i = 1, \ldots, m \end{cases}$$

Recap of Constrained Optimization

- The case for inequality constraint $g_i(\mathbf{x}) \leq 0$ is similar, except that the Lagrange multiplier α_i should be positive
- If $\mathbf{x}_0$ is a solution to the constrained optimization problem

$$\min_{\mathbf{x}} f(\mathbf{x}) \quad \text{subject to} \quad g_i(\mathbf{x}) \leq 0 \quad \text{for } i = 1, \ldots, m$$

- There must exist $\alpha_i \geq 0$ for i=1, …, m such that $\mathbf{x}_0$ satisfy

$$\begin{cases} \frac{\partial}{\partial \mathbf{x}} \left(f(\mathbf{x}) + \sum_i \alpha_i g_i(\mathbf{x}) \right) \Big|_{\mathbf{x}=jx_0} & = \mathbf{0} \\ g_i(\mathbf{x}) \leq 0 \quad \text{for } i = 1, \ldots, m \end{cases}$$

- The function $f(\mathbf{x}) + \sum_i \alpha_i g_i(\mathbf{x})$ is also known as the Lagrangrian; we want to set its gradient to **0**

Back to the Original Problem

$$\text{Minimize } \frac{1}{2}||\mathbf{w}||^2$$

$$\text{subject to } 1 - y_i(\mathbf{w}^T\mathbf{x}_i + b) \leq 0 \qquad \text{for } i = 1, \ldots, n$$

- The Lagrangian is

$$\mathcal{L} = \frac{1}{2}\mathbf{w}^T\mathbf{w} + \sum_{i=1}^{n} \alpha_i \left(1 - y_i(\mathbf{w}^T\mathbf{x}_i + b)\right)$$

  - Note that $||\mathbf{w}||^2 = \mathbf{w}^T\mathbf{w}$

- Setting the gradient of $\mathcal{L}$ w.r.t. **w** and b to zero, we have

$$\mathbf{w} + \sum_{i=1}^{n} \alpha_i(-y_i)\mathbf{x}_i = \mathbf{0} \quad \Rightarrow \quad \mathbf{w} = \sum_{i=1}^{n} \alpha_i y_i \mathbf{x}_i$$

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

The Dual Problem

- If we substitute $\mathbf{w} = \sum_{i=1}^{n} \alpha_i y_i \mathbf{x}_i$ to $\mathcal{L}$, we have

$$\begin{aligned}\mathcal{L} &= \frac{1}{2} \sum_{i=1}^{n} \alpha_i y_i \mathbf{x}_i^T \sum_{j=1}^{n} \alpha_j y_j \mathbf{x}_j + \sum_{i=1}^{n} \alpha_i \left(1 - y_i(\sum_{j=1}^{n} \alpha_j y_j \mathbf{x}_j^T \mathbf{x}_i + b)\right) \\ &= \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_i \alpha_j y_i y_j \mathbf{x}_i^T \mathbf{x}_j + \sum_{i=1}^{n} \alpha_i - \sum_{i=1}^{n} \alpha_i y_i \sum_{j=1}^{n} \alpha_j y_j \mathbf{x}_j^T \mathbf{x}_i - b \sum_{i=1}^{n} \alpha_i y_i \\ &= -\frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_i \alpha_j y_i y_j \mathbf{x}_i^T \mathbf{x}_j + \sum_{i=1}^{n} \alpha_i\end{aligned}$$

- Note that $\sum_{i=1}^{n} \alpha_i y_i = 0$

- This is a function of α_i only

The Dual Problem

- The new objective function is in terms of α_i only
- It is known as the dual problem: if we know **w**, we know all α_i; if we know all α_i, we know **w**
- The original problem is known as the primal problem
- The objective function of the dual problem needs to be maximized!
- The dual problem is therefore:

$$\text{max.} \quad W(\boldsymbol{\alpha}) = \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i=1,j=1}^{n} \alpha_i \alpha_j y_i y_j \mathbf{x}_i^T \mathbf{x}_j$$

$$\text{subject to } \alpha_i \geq 0, \qquad \sum_{i=1}^{n} \alpha_i y_i = 0$$

Properties of α_i when we introduce the Lagrange multipliers

The result when we differentiate the original Lagrangian w.r.t. b

The Dual Problem

$$\text{max. } W(\boldsymbol{\alpha}) = \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i=1,j=1}^{n} \alpha_i \alpha_j y_i y_j \mathbf{x}_i^T \mathbf{x}_j$$

$$\text{subject to } \alpha_i \geq 0, \sum_{i=1}^{n} \alpha_i y_i = 0$$

- This is a quadratic programming (QP) problem
  - A global maximum of α_i can always be found
- **w** can be recovered by $\mathbf{w} = \sum_{i=1}^{n} \alpha_i y_i \mathbf{x}_i$

Characteristics of the Solution

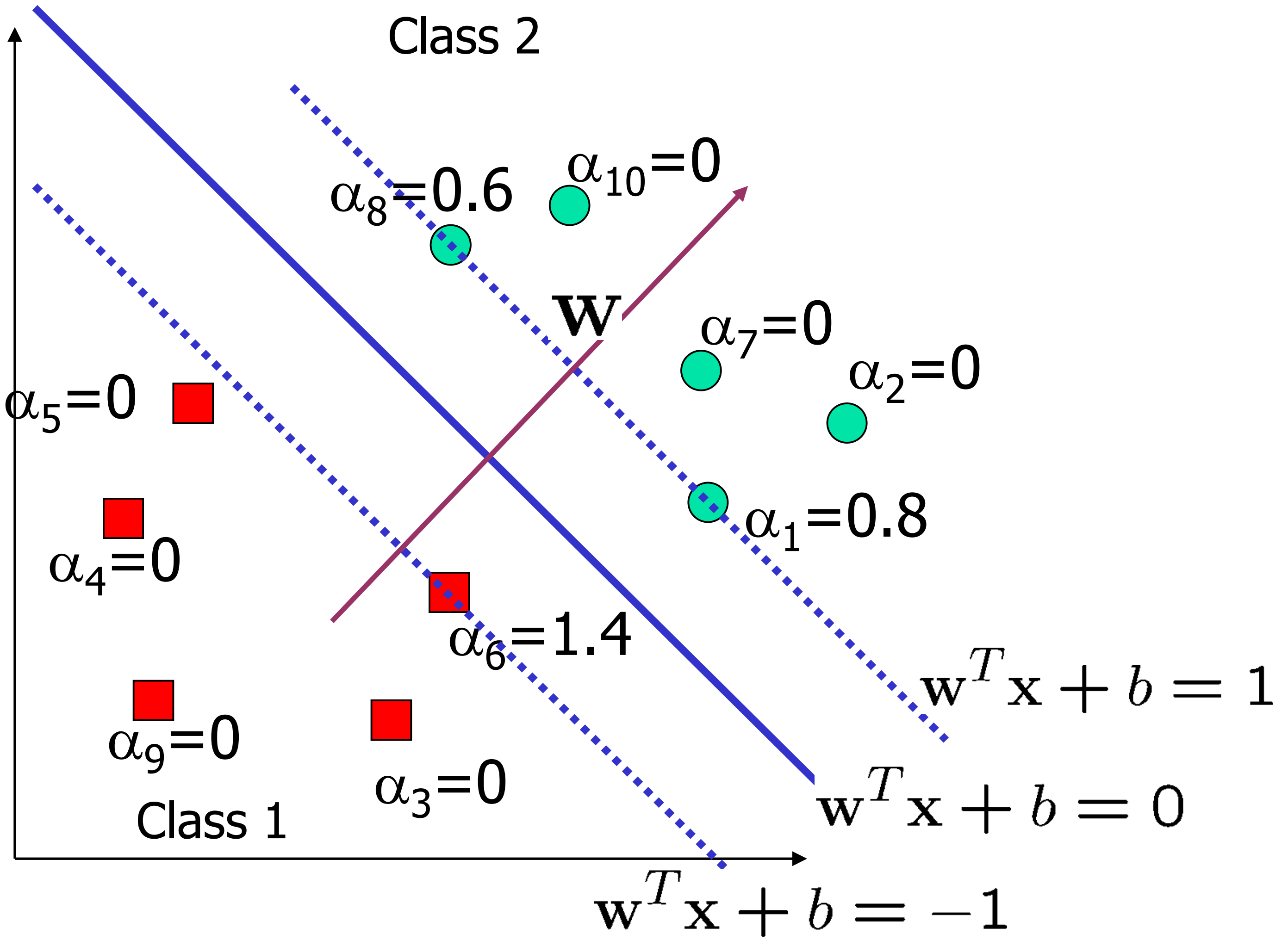
- Many of the α_i are zero
  - **w** is a linear combination of a small number of data points
- $\mathbf{x}_i$ with non-zero α_i are called support vectors (SV)
  - The decision boundary is determined only by the SV
  - Let t_j (j=1, ..., s) be the indices of the s support vectors. We can write $\mathbf{w} = \sum_{j=1}^{s} \alpha_{t_j} y_{t_j} \mathbf{x}_{t_j}$

- For testing with a new data **z**
  - Compute $\mathbf{w}^T\mathbf{z} + b = \sum_{j=1}^{s} \alpha_{t_j} y_{t_j} (\mathbf{x}_{t_j}^T \mathbf{z}) + b$ and classify **z** as class 1 if the sum is positive, and class 2 otherwise
  - Note: **w** need not be formed explicitly

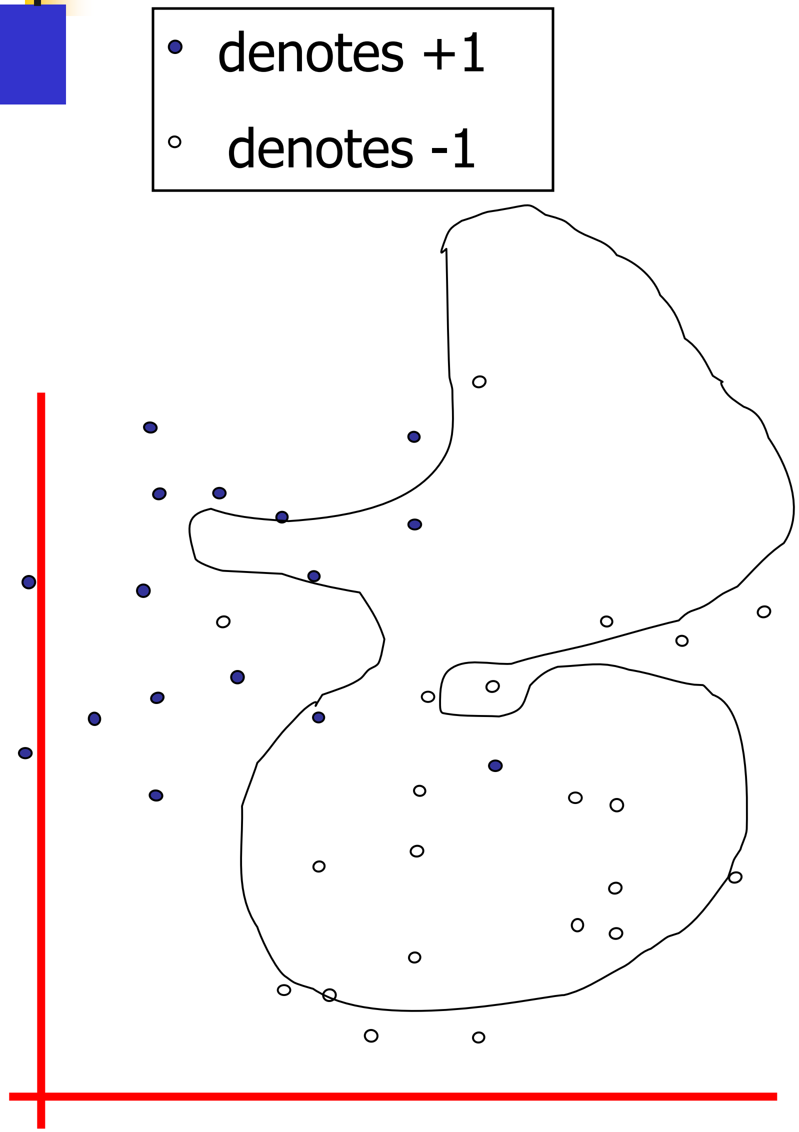
The Quadratic Programming Problem

- Many approaches have been proposed
  - Loqo, cplex, etc. (see http://www.numerical.rl.ac.uk/qp/qp.html)
- Most are “interior-point” methods
  - Start with an initial solution that can violate the constraints
  - Improve this solution by optimizing the objective function and/or reducing the amount of constraint violation
- For SVM, sequential minimal optimization (SMO) seems to be the most popular
  - A QP with two variables is trivial to solve
  - Each iteration of SMO picks a pair of (α_i,α_j) and solve the QP with these two variables; repeat until convergence
- In practice, we can just regard the QP solver as a “black-box” without bothering how it works

A Geometrical Interpretation



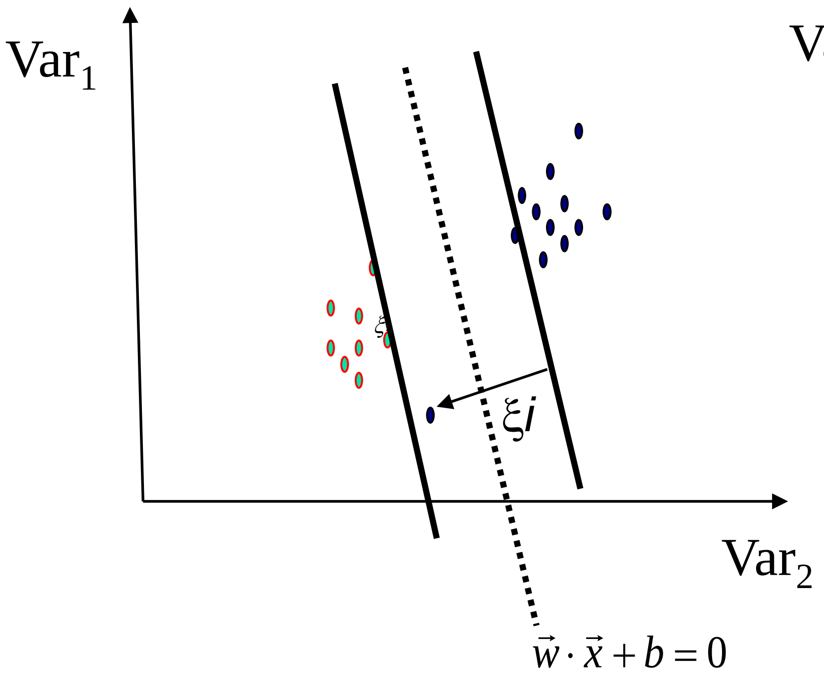
Dataset with Noise



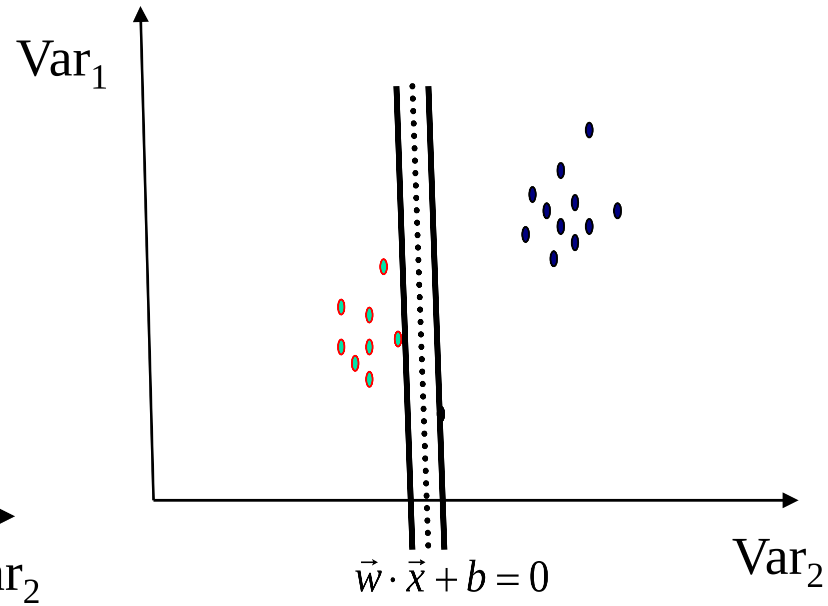
- **Hard Margin:** So far we require all data points be classified correctly
  - No training error
- What if the training set is noisy?
  - Solution 1: use very powerful kernels

OVERFITTING!

Robustness of Soft vs Hard Margin SVMs



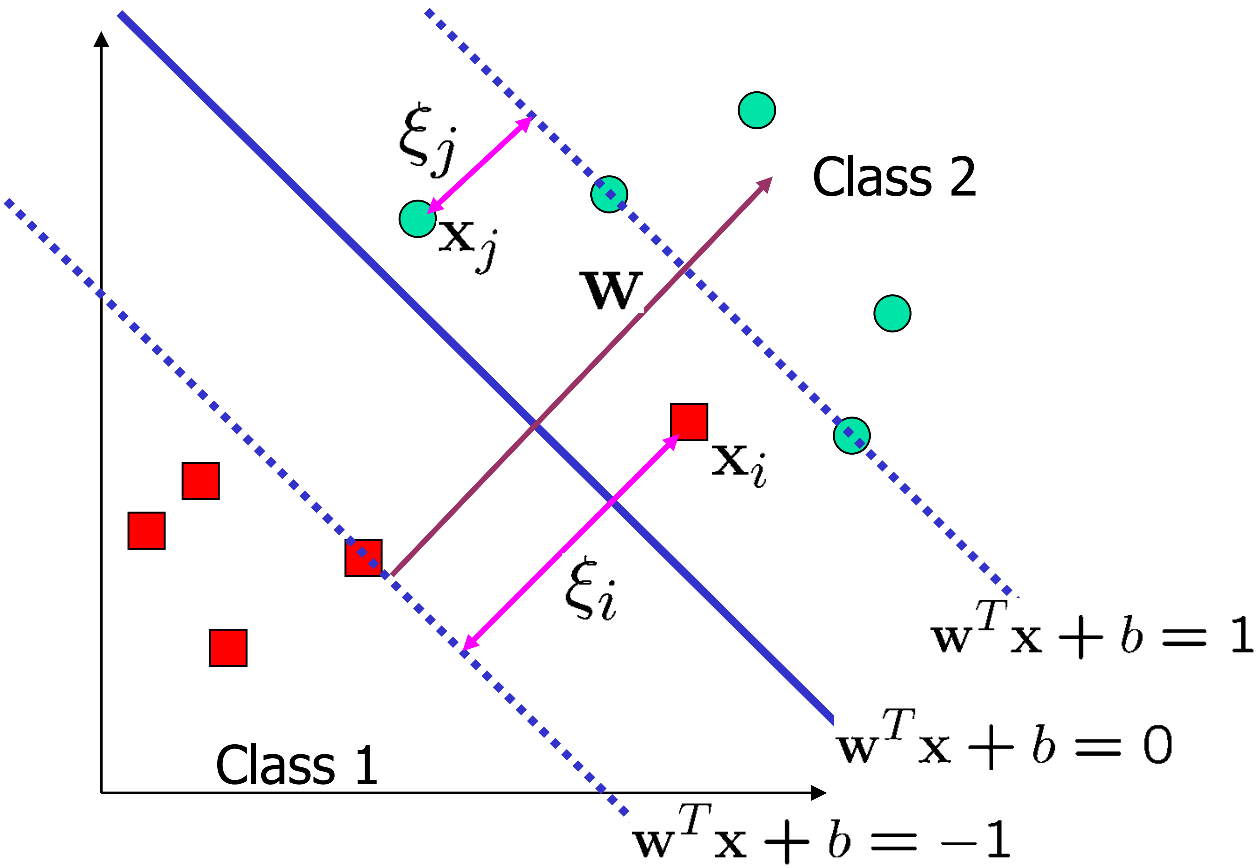
Soft Margin SVN



Hard Margin SVN

Non-linearly Separable Problems

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



Soft Margin Hyperplane

- If we minimize $\sum_i \xi_i$, ξ_i can be computed by

$$\begin{cases} \mathbf{w}^T\mathbf{x}_i + b \geq 1 - \xi_i & y_i = 1 \\ \mathbf{w}^T\mathbf{x}_i + b \leq -1 + \xi_i & y_i = -1 \\ \xi_i \geq 0 & \forall i \end{cases}$$

  - 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
- We want to minimize $\frac{1}{2}||\mathbf{w}||^2 + C\sum_{i=1}^{n}\xi_i$
  - C : tradeoff parameter between error and margin
- The optimization problem becomes

$$\text{Minimize } \frac{1}{2}||\mathbf{w}||^2 + C\sum_{i=1}^{n}\xi_i$$
$$\text{subject to } y_i(\mathbf{w}^T\mathbf{x}_i + b) \geq 1 - \xi_i, \quad \xi_i \geq 0$$

The Optimization Problem

- The dual of this new constrained optimization problem is

$$\text{max.}\ W(\boldsymbol{\alpha}) = \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i=1,j=1}^{n} \alpha_i \alpha_j y_i y_j \mathbf{x}_i^T \mathbf{x}_j$$

See Bishop: 7.22-7.32

$$\text{subject to } C \geq \alpha_i \geq 0, \sum_{i=1}^{n} \alpha_i y_i = 0$$

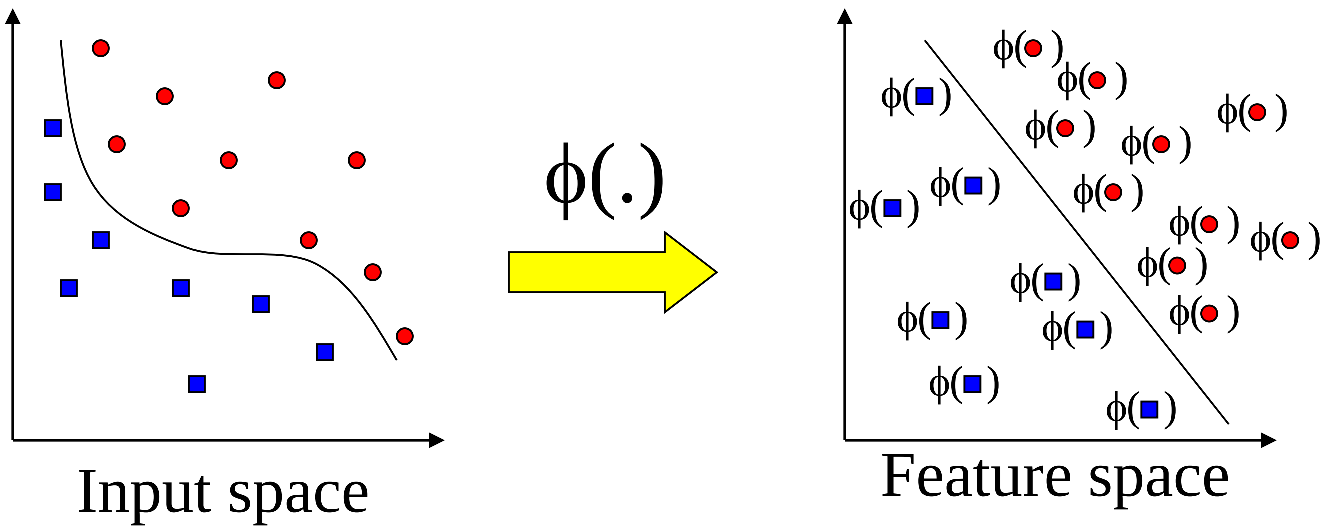
- **w** is recovered as $\mathbf{w} = \sum_{j=1}^{s} \alpha_{t_j} y_{t_j} \mathbf{x}_{t_j}$

- 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 $x_1 x_2$ make the problem linearly separable

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

$$\text{max. } W(\boldsymbol{\alpha}) = \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i=1,j=1}^{n} \alpha_i \alpha_j y_i y_j \mathbf{x}_i^T \mathbf{x}_j$$

$$\text{subject to } C \geq \alpha_i \geq 0, \sum_{i=1}^{n} \alpha_i y_i = 0$$

- 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 $\phi(.)$ and $K(.,.)$

- Suppose $\phi(.)$ is given as follows

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

- An inner product in the feature space is

$$\langle\phi(\left[\begin{smallmatrix} x_1 \\ x_2 \end{smallmatrix}\right]), \phi(\left[\begin{smallmatrix} y_1 \\ y_2 \end{smallmatrix}\right])\rangle = (1 + x_1y_1 + x_2y_2)^2$$

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

$$K(\mathbf{x}, \mathbf{y}) = (1 + x_1y_1 + x_2y_2)^2$$

- This use of kernel function to avoid carrying out $\phi(.)$ explicitly is known as the kernel trick

Kernel Functions

- In practical use of SVM, the user specifies the kernel function; the transformation $\phi(.)$ is not explicitly stated
- Given a kernel function $K(\mathbf{x}_i, \mathbf{x}_j)$, the transformation $\phi(.)$ is given by its eigenfunctions (a concept in functional analysis)
  - Eigenfunctions can be difficult to construct explicitly
  - This is why people only specify the kernel function without worrying about the exact transformation
- Another view: kernel function, being an inner product, is really a similarity measure between the objects

Examples of Kernel Functions

- Polynomial kernel with degree *d*

$$K(\mathbf{x},\mathbf{y}) = (\mathbf{x}^T\mathbf{y} + 1)^d$$

- Radial basis function kernel with width σ

$$K(\mathbf{x},\mathbf{y}) = \exp(-||\mathbf{x}-\mathbf{y}||^2/(2\sigma^2))$$

  - Closely related to radial basis function neural networks
  - The feature space is infinite-dimensional
- Sigmoid with parameter κ and θ

$$K(\mathbf{x},\mathbf{y}) = \tanh(\kappa\mathbf{x}^T\mathbf{y} + \theta)$$

  - It does not satisfy the Mercer condition on all κ and θ

Modification Due to Kernel Function

- Change all inner products to kernel functions
- For training,

Original

$$\max.\ W(\boldsymbol{\alpha}) = \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i=1,j=1}^{n} \alpha_i \alpha_j y_i y_j \mathbf{x}_i^T \mathbf{x}_j$$

$$\text{subject to } C \geq \alpha_i \geq 0, \sum_{i=1}^{n} \alpha_i y_i = 0$$

With kernel function

$$\max.\ W(\boldsymbol{\alpha}) = \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i=1,j=1}^{n} \alpha_i \alpha_j y_i y_j K(\mathbf{x}_i, \mathbf{x}_j)$$

$$\text{subject to } C \geq \alpha_i \geq 0, \sum_{i=1}^{n} \alpha_i y_i = 0$$

Modification Due to Kernel Function

- For testing, the new data **z** is classified as class 1 if $f \geq 0$, and as class 2 if $f < 0$

Original

$$\mathbf{w} = \sum_{j=1}^{s} \alpha_{t_j} y_{t_j} \mathbf{x}_{t_j}$$

$$f = \mathbf{w}^T \mathbf{z} + b = \sum_{j=1}^{s} \alpha_{t_j} y_{t_j} \mathbf{x}_{t_j}^T \mathbf{z} + b$$

With kernel function

$$\mathbf{w} = \sum_{j=1}^{s} \alpha_{t_j} y_{t_j} \phi(\mathbf{x}_{t_j})$$

$$f = \langle \mathbf{w}, \phi(\mathbf{z}) \rangle + b = \sum_{j=1}^{s} \alpha_{t_j} y_{t_j} K(\mathbf{x}_{t_j}, \mathbf{z}) + b$$

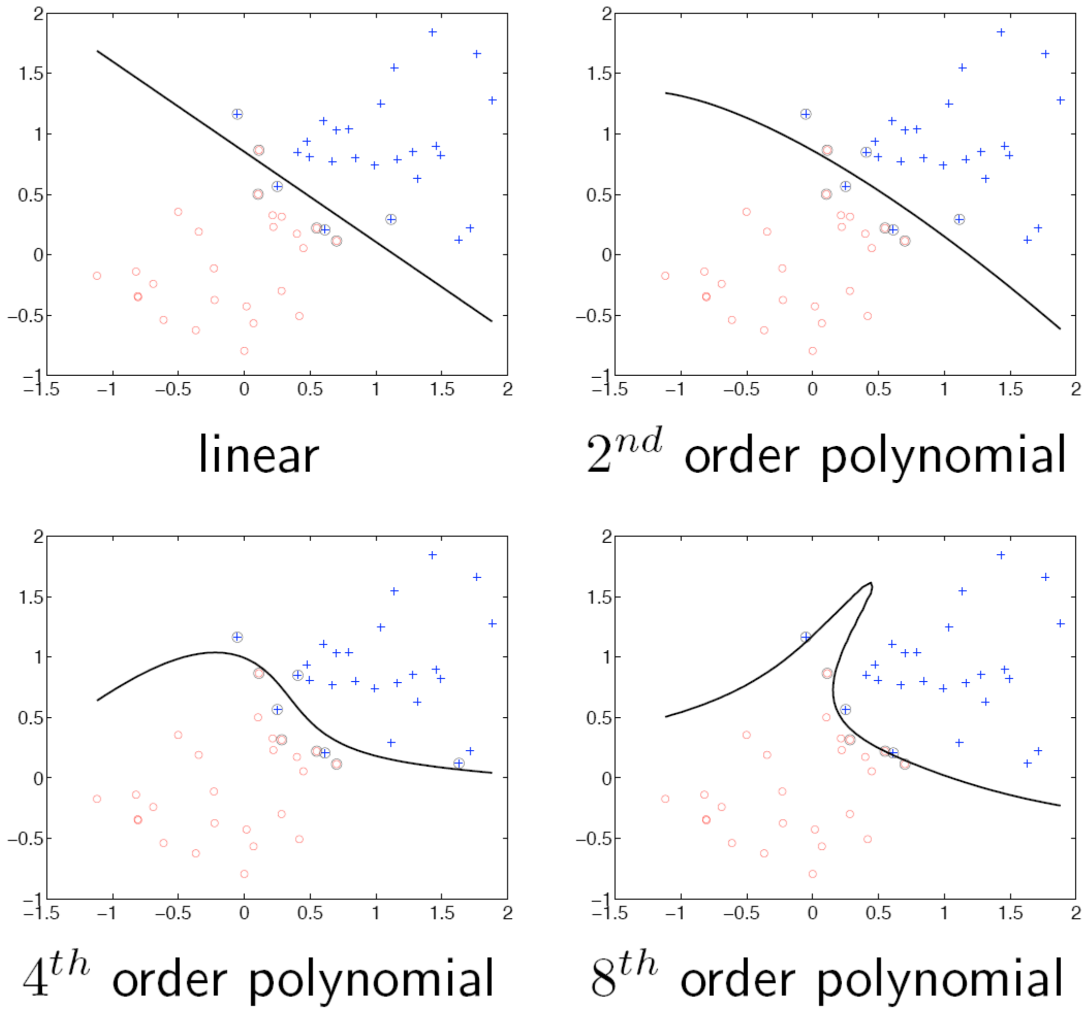
More on Kernel Functions

- Since the training of SVM only requires the value of $K(\mathbf{x}_i, \mathbf{x}_j)$, there is no restriction of the form of $\mathbf{x}_i$ and $\mathbf{x}_j$
  - $\mathbf{x}_i$ can be a sequence or a tree, instead of a feature vector
- $K(\mathbf{x}_i, \mathbf{x}_j)$ is just a similarity measure comparing $\mathbf{x}_i$ and $\mathbf{x}_j$
- For a test object $\mathbf{z}$, the discrimiant function essentially is a weighted sum of the similarity between z and a pre-selected set of objects (the support vectors)

$$f(\mathbf{z}) = \sum_{\mathbf{x}_i \in \mathcal{S}} \alpha_i y_i K(\mathbf{z}, \mathbf{x}_i) + b$$

$\mathcal{S}$: the set of support vectors

SVM Examples



Example

- Suppose we have 5 1D data points
  - $x_1=1$, $x_2=2$, $x_3=4$, $x_4=5$, $x_5=6$, with 1, 2, 6 as class 1 and 4, 5 as class 2 $\Rightarrow$ $y_1=1$, $y_2=1$, $y_3=-1$, $y_4=-1$, $y_5=1$
- We use the polynomial kernel of degree 2
  - $K(x,y) = (xy+1)^2$
  - C is set to 100
- We first find α_i ($i=1, \ldots, 5$) by

$$\text{max.} \quad \sum_{i=1}^{5} \alpha_i - \frac{1}{2} \sum_{i=1}^{5} \sum_{j=1}^{5} \alpha_i \alpha_j y_i y_j (x_i x_j + 1)^2$$

$$\text{subject to } 100 \geq \alpha_i \geq 0, \sum_{i=1}^{5} \alpha_i y_i = 0$$

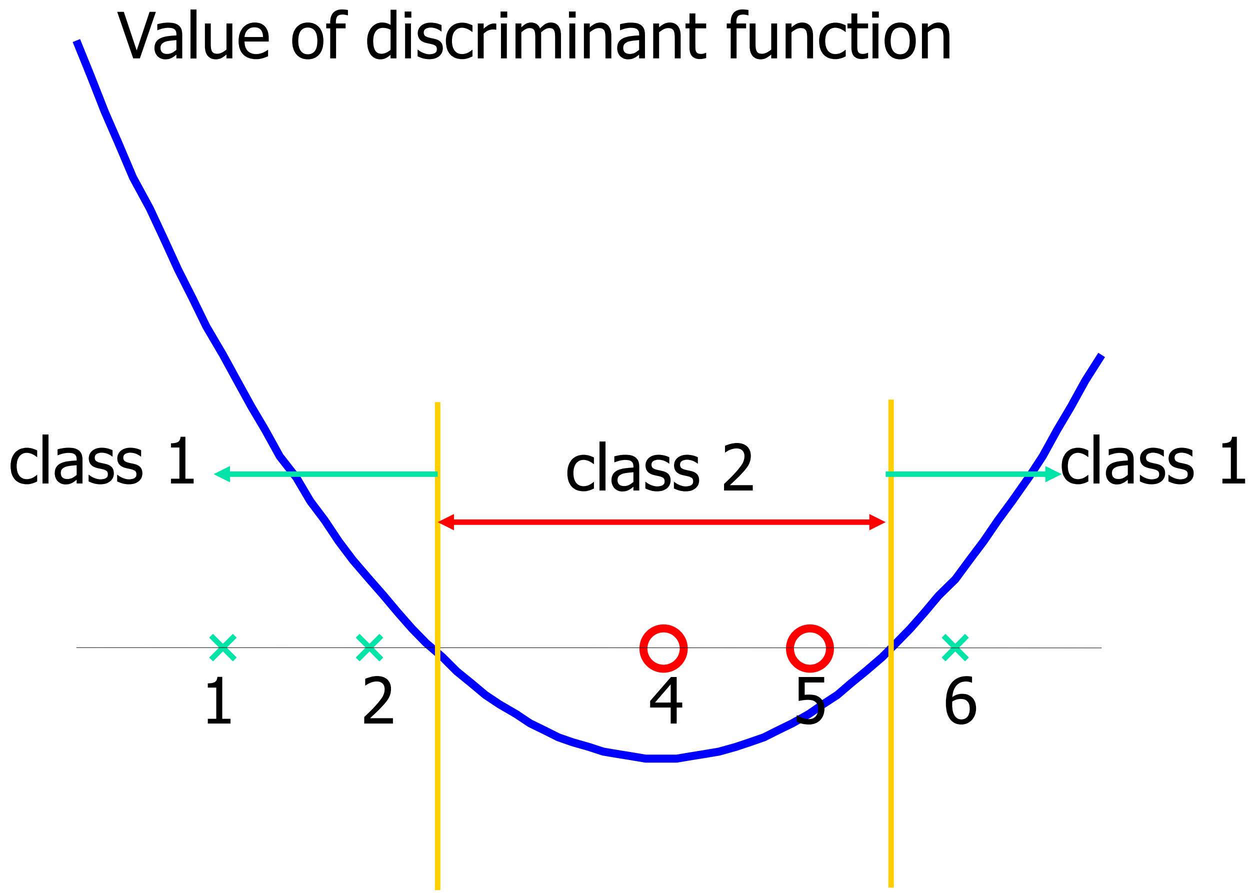
Example

- By using a QP solver, we get
  - $\alpha_1=0$, $\alpha_2=2.5$, $\alpha_3=0$, $\alpha_4=7.333$, $\alpha_5=4.833$
  - Note that the constraints are indeed satisfied
  - The support vectors are $\{x_2=2, x_4=5, x_5=6\}$
- The discriminant function is

$$
\begin{aligned}
& f(z) \\
&= 2.5(1)(2z+1)^2 + 7.333(-1)(5z+1)^2 + \overbrace{4.833}^{\alpha_5}\overbrace{(1)}^{y_5}\overbrace{(6z+1)^2}^{K(z,x_5)} + b \\
&= 0.6667z^2 - 5.333z + b
\end{aligned}
$$

- *b* is recovered by solving f(2)=1 or by f(5)=-1 or by f(6)=1, as x_2 and x_5 lie on the line $\phi(\mathbf{w})^T\phi(\mathbf{x}) + b = 1$ and x_4 lies on the line $\phi(\mathbf{w})^T\phi(\mathbf{x}) + b = -1$
- All three give b=9 $\Longrightarrow$ $f(z) = 0.6667z^2 - 5.333z + 9$

Example



Value of discriminant function
class 1
class 2
class 1
1
2
4
5
6

Choosing the Kernel Function

- Probably the most tricky part of using SVM.
- The kernel function is important because it creates the kernel matrix, which summarizes all the data
- Many principles have been proposed (diffusion kernel, Fisher kernel, string kernel, …)
- There is even research to estimate the kernel matrix from available information

- In practice, a low degree polynomial kernel or RBF kernel with a reasonable width is a good initial try
- Note that SVM with RBF kernel is closely related to RBF neural networks, with the centers of the radial basis functions automatically chosen for SVM

Strengths and Weaknesses of SVM

- Strengths
  - Training is relatively easy
    - No local optimal, unlike in neural networks
  - It scales relatively well to high dimensional data
  - Tradeoff between classifier complexity and error can be controlled explicitly
  - Non-traditional data like strings and trees can be used as input to SVM, instead of feature vectors
- Weaknesses
  - Need to choose a “good” kernel function.