COMP/EECE 7/8745 Machine Learning

Topics:

Supervised learning

- Support Vector Machine (SVM)
- Kernelization approaches
- Applications of SVM

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History of SVM (Support Vector Machines)

- 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, LeNet 4.
    - See Section 5.11 in [2] or the discussion in [3] for details
- SVM is now regarded as an important example of **"kernel methods", one of the key area in machine learning**
  - Note: the meaning of "kernel" is different from the "kernel" function for Parzen windows

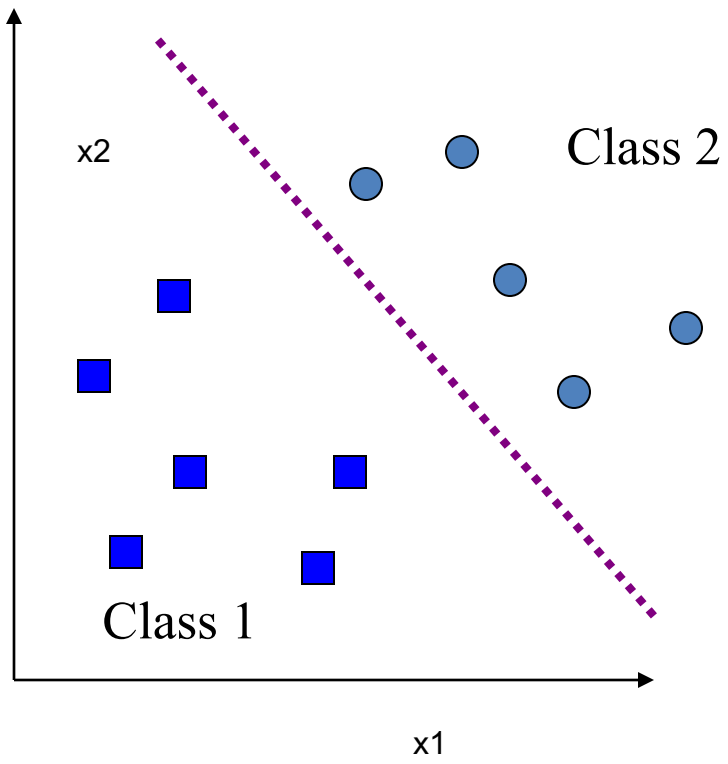
[1] B.E. Boser *et al*. A Training Algorithm for Optimal Margin Classifiers. Proceedings of the Fifth Annual Workshop on Computational Learning Theory 5 144-152, Pittsburgh, 1992.

[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.

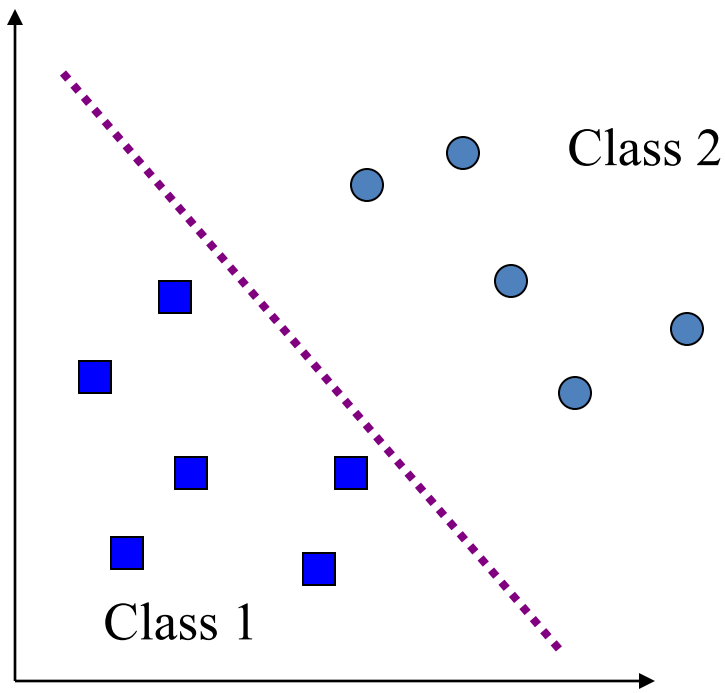
[3] V. Vapnik. The Nature of Statistical Learning Theory. 2nd edition, Springer, 1999.

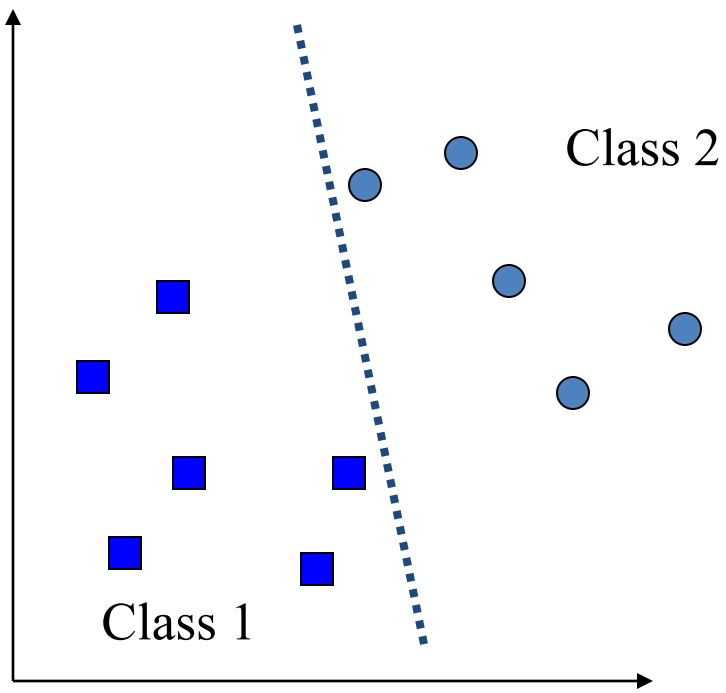
What is a good Decision Boundary?

- 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 (DHS ch. 5)
- Are all decision boundaries equally good?



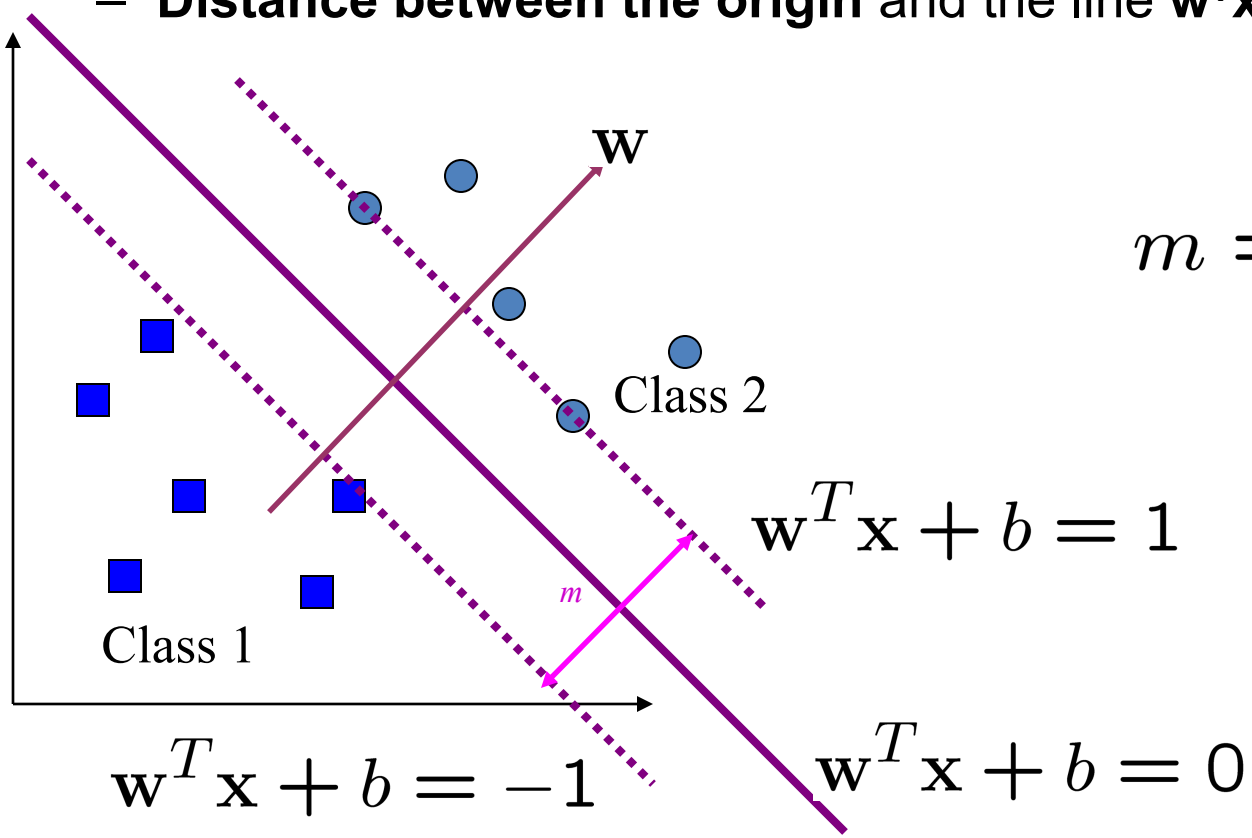
Examples of Bad Decision Boundaries





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/||**w**||



$$m = \frac{2}{||\mathbf{w}||}$$

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

- 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

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

- 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

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

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

- This is a **quadratic programming** (QP) problem
  - A global maximum of α_i can always be found

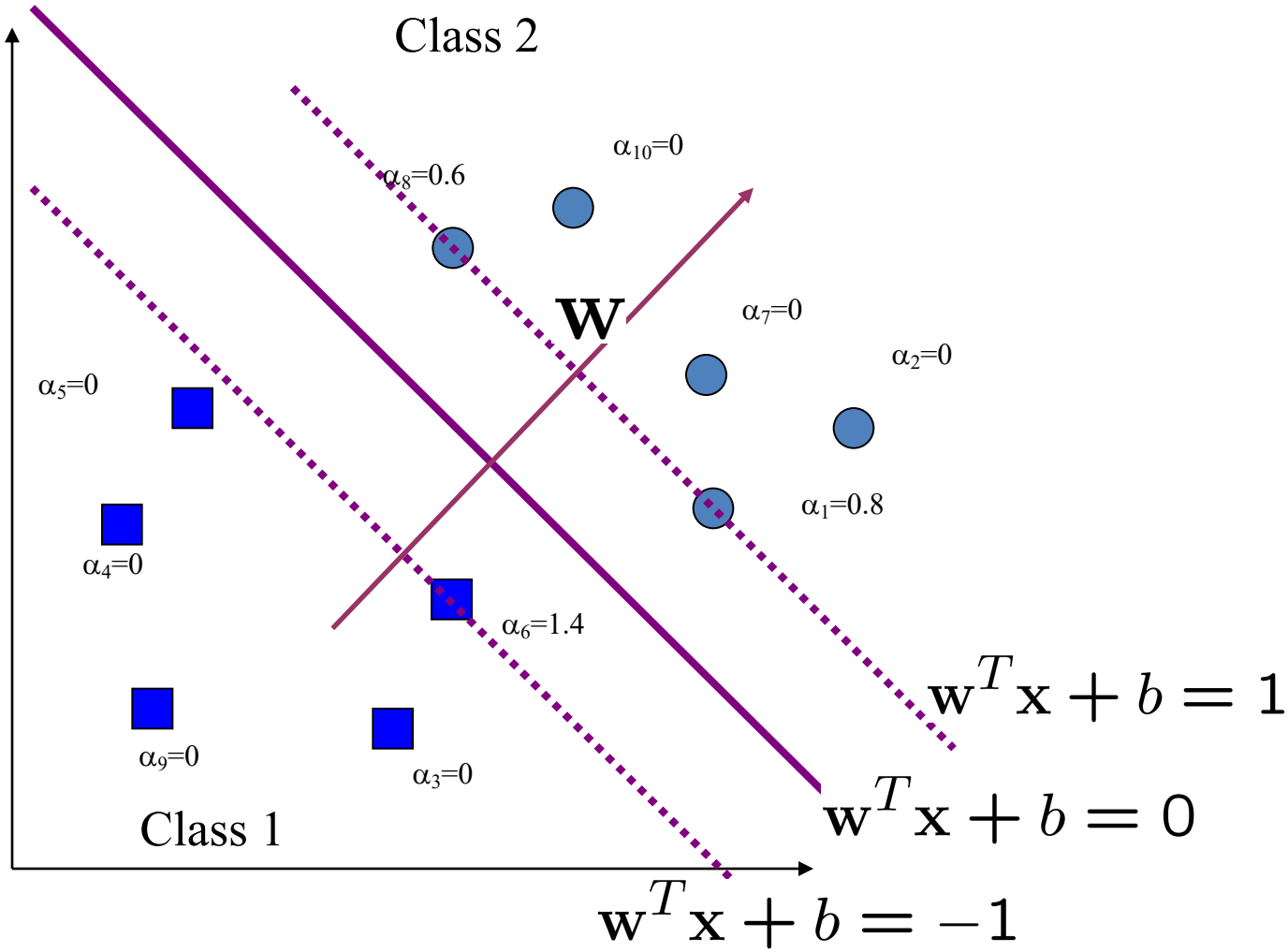
- **w** can be recovered by

$$\mathbf{w} = \sum_{i=1}^{n} \alpha_i y_i \mathbf{x}_i$$

The Quadratic Programming Problem

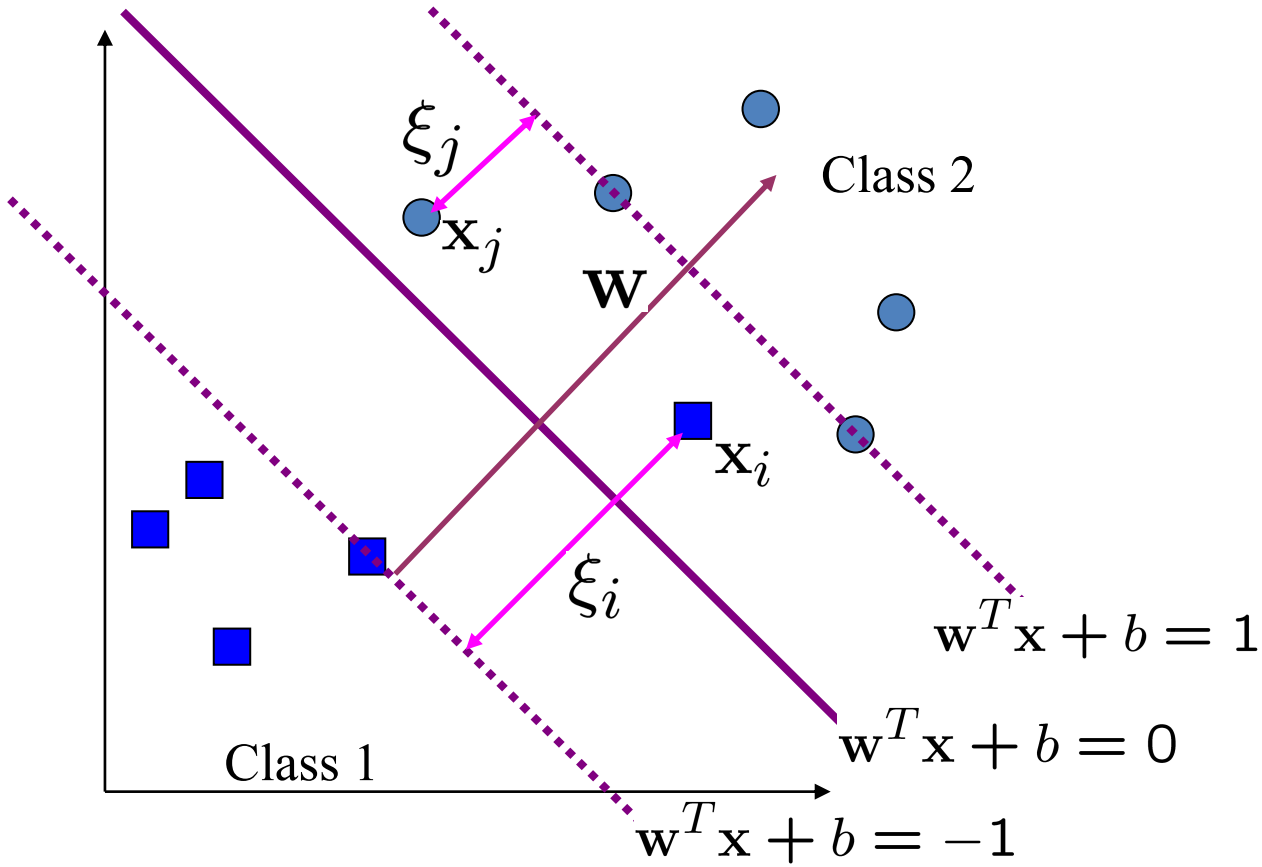
- Many approaches have been proposed
  - Loqo, cplex, etc. (see http://www.numerical.rl.ac.uk/qp/qp.html)
- Most are "interior-point" methods
  - Start with an **initial solution that can violate the constraints**
  - Improve this solution by optimizing the objective function and/or **reducing the amount 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



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

$$\text{Minimize } \frac{1}{2}||\mathbf{w}||^2 + C\sum_{i=1}^n \xi_i$$

$$\text{subject to } y_i(\mathbf{w}^T\mathbf{x}_i + b) \geq 1 - \xi_i, \quad \xi_i \geq 0$$

Feature Mapping and Kernel Trick

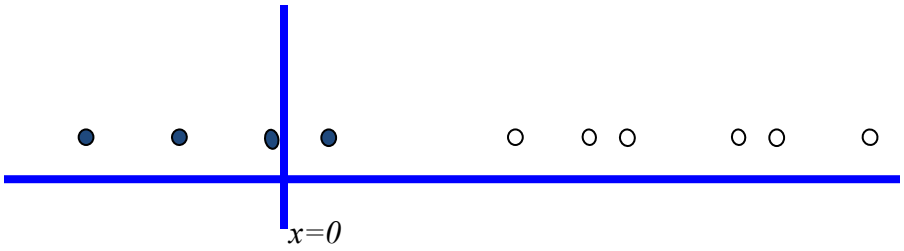
- Non-linear separable problem can be **mapped to linearly mapped high-dimension space**
- Feature **mapping can be done implicitly by Kernel Trick**

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

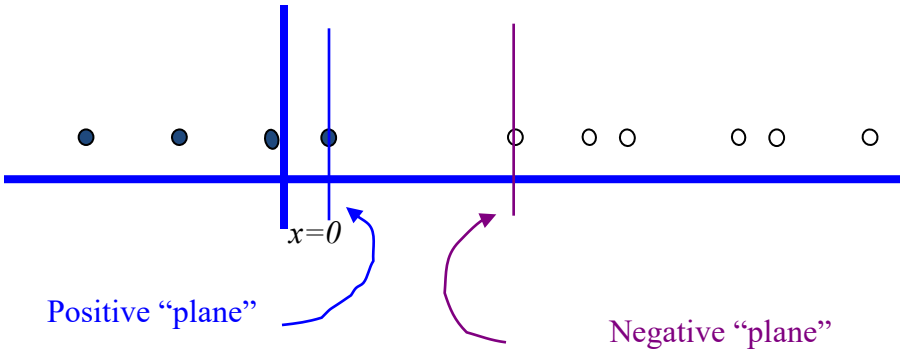
Suppose we're in 1-dimension

What would SVMs do with this data?

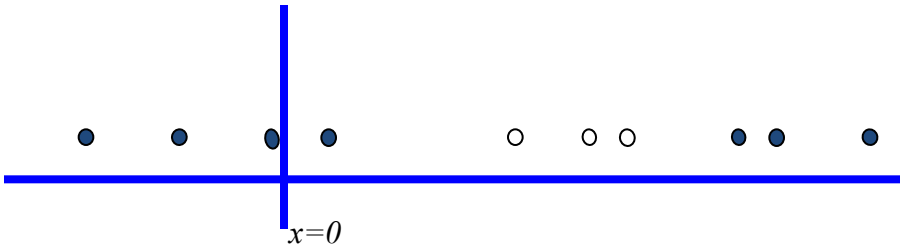


Suppose we're in 1-dimension

Not a big surprise



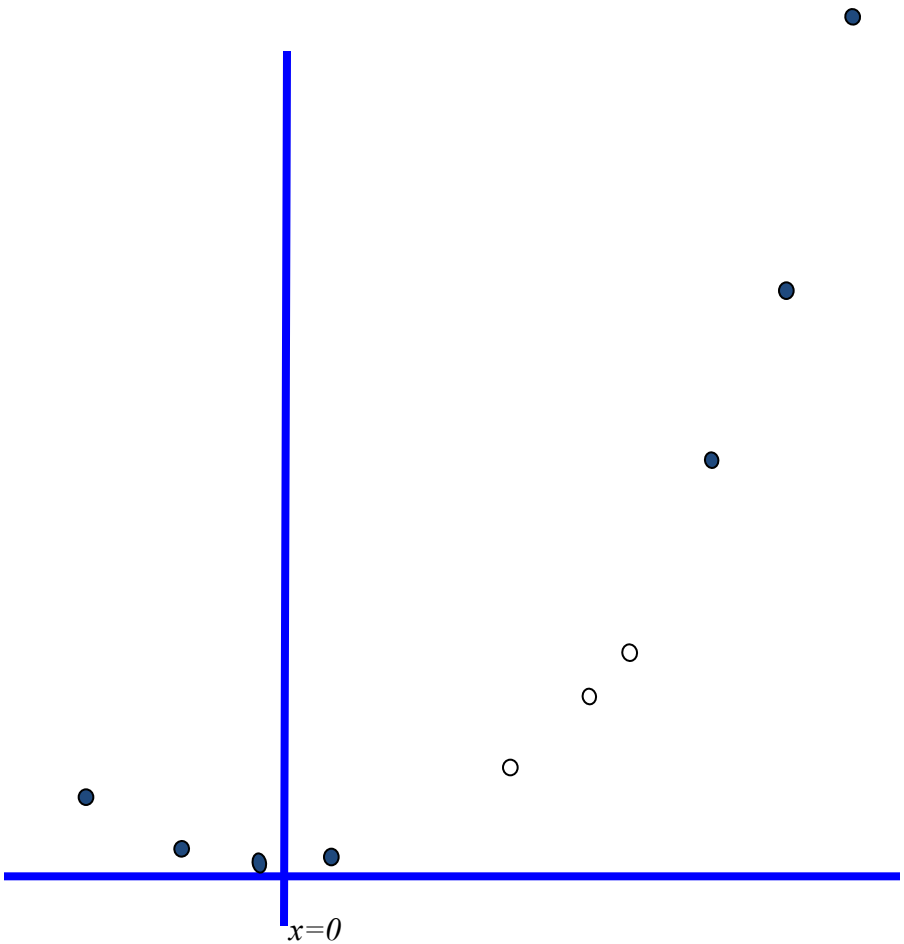
Harder 1-dimensional dataset



That's wiped the smirk off SVM's face.

What can be done about this?

Harder 1-dimensional dataset

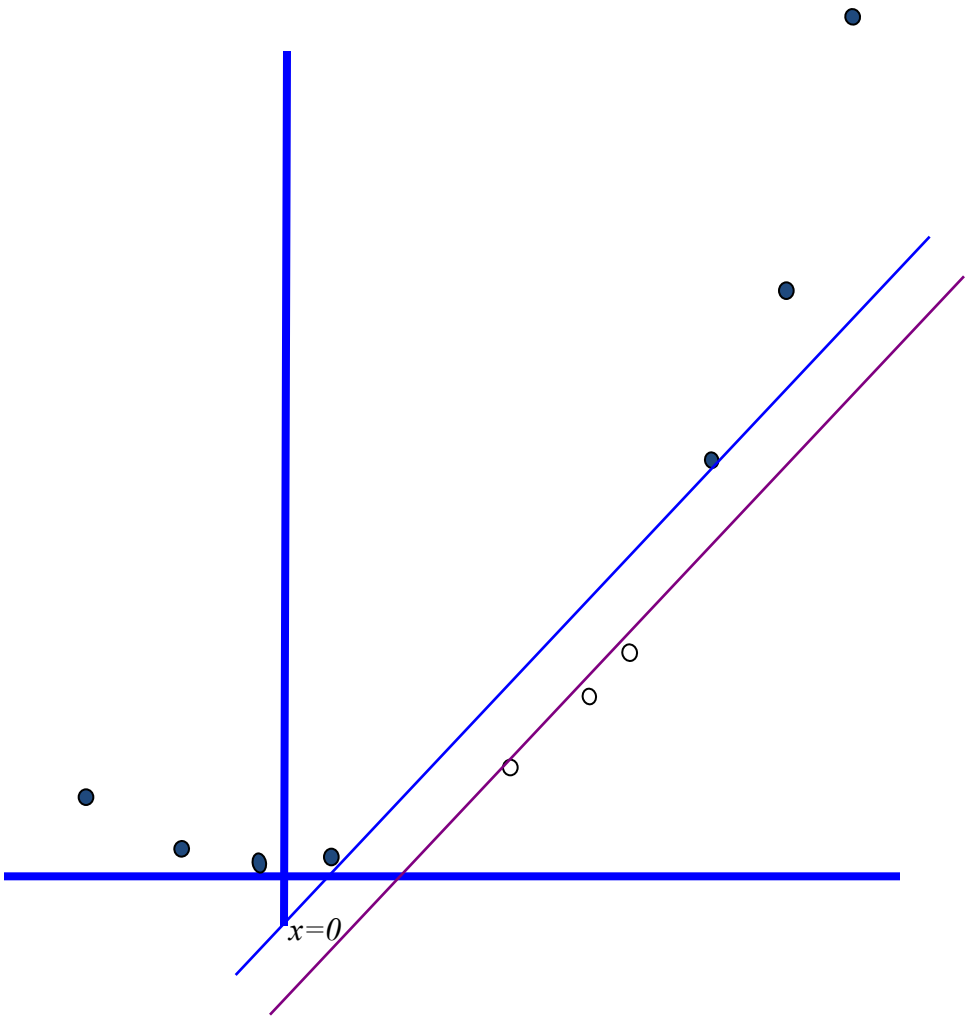


Remember how permitting non-linear basis functions made linear regression so much nicer?

Let's permit them here too

$$\mathbf{z}_k = (x_k, x_k^2)$$

Harder 1-dimensional dataset

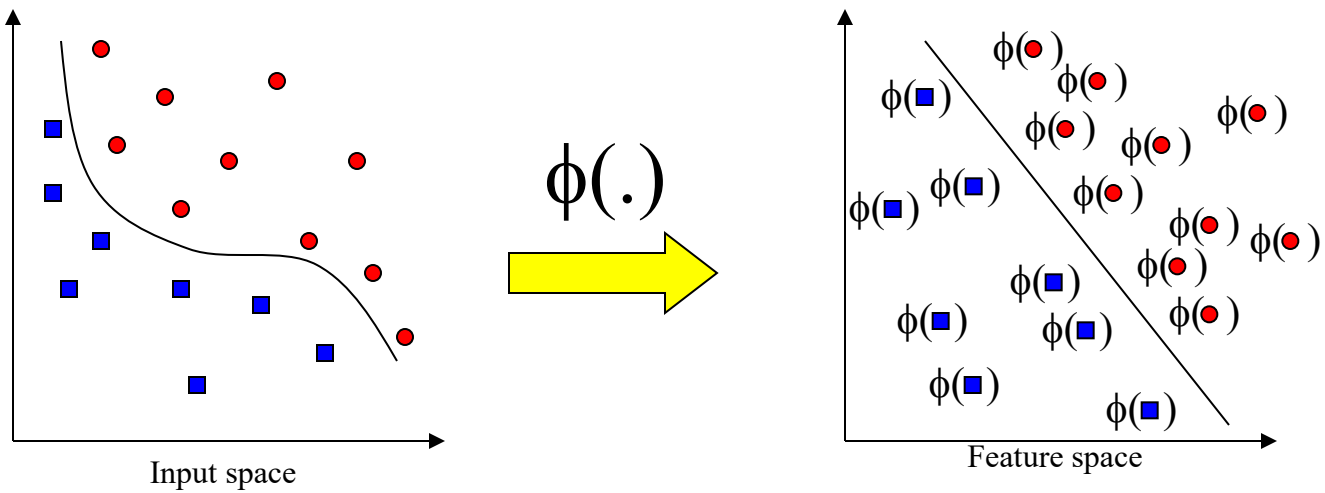


Remember how permitting non-linear basis functions made linear regression so much nicer?

Let's permit them here too

$$\mathbf{z}_k = (x_k, x_k^2)$$

Transforming the Data (c.f. DHS Ch. 5)

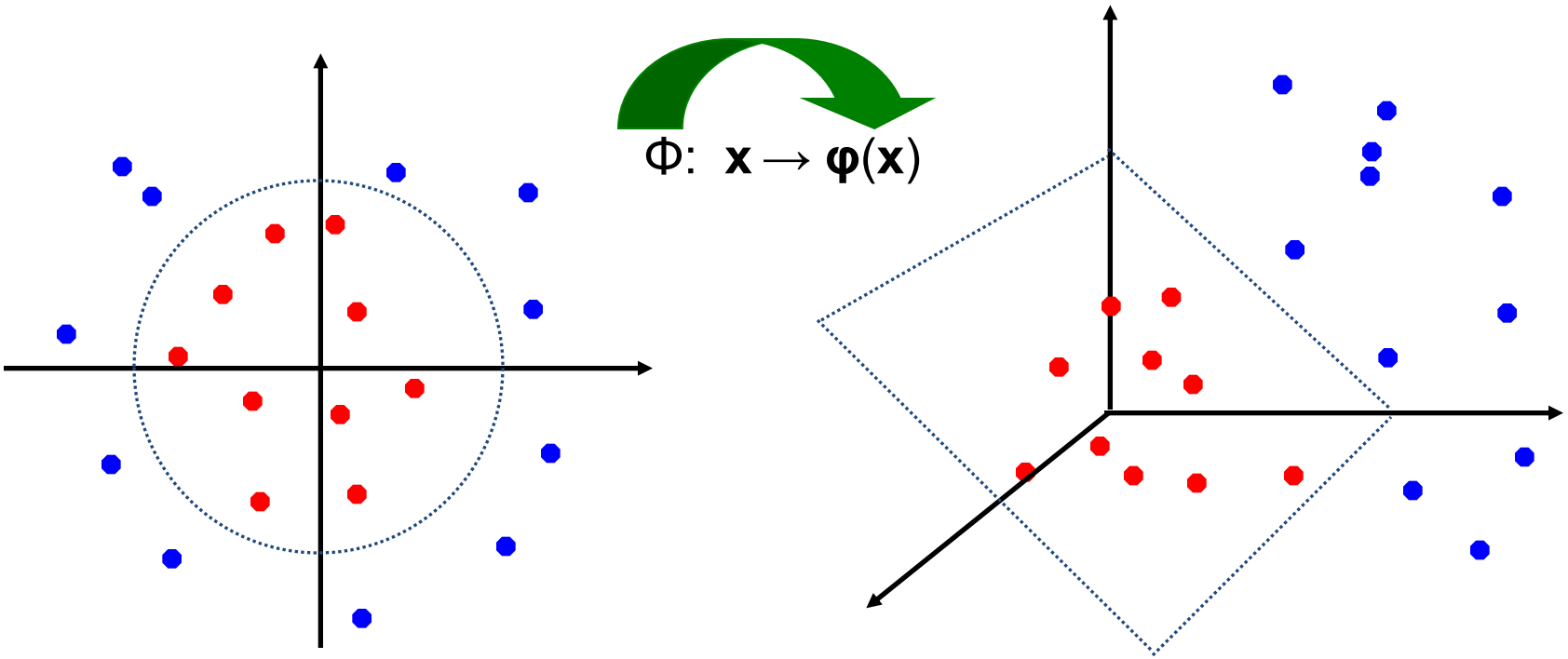


Note: feature space is of higher dimension than the input space in practice

- 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

Non-linear SVMs: Feature spaces

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



What Functions are Kernels?

- For some functions $K(\mathbf{x}_i,\mathbf{x}_j)$ checking that $K(\mathbf{x}_i,\mathbf{x}_j)= \varphi(\mathbf{x}_i)^{\mathsf{T}}\varphi(\mathbf{x}_j)$ can be cumbersome.
- **Mercer's theorem:**

  Every semi-positive definite symmetric function is a kernel
- Semi-positive definite symmetric functions correspond to a semi-positive definite **symmetric Gram matrix**:

K=

$K(\mathbf{x}_1,\mathbf{x}_1)$	$K(\mathbf{x}_1,\mathbf{x}_2)$	$K(\mathbf{x}_1,\mathbf{x}_3)$	…	$K(\mathbf{x}_1,\mathbf{x}_n)$
$K(\mathbf{x}_2,\mathbf{x}_1)$	$K(\mathbf{x}_2,\mathbf{x}_2)$	$K(\mathbf{x}_2,\mathbf{x}_3)$		$K(\mathbf{x}_2,\mathbf{x}_n)$
…	…	…	…	…
$K(\mathbf{x}_n,\mathbf{x}_1)$	$K(\mathbf{x}_n,\mathbf{x}_2)$	$K(\mathbf{x}_n,\mathbf{x}_3)$	…	$K(\mathbf{x}_n,\mathbf{x}_n)$

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

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

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 or Tanh 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

An Example for $\phi(.)$ and $K(.,.)$

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

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

- An inner product in the feature space is

$$\langle \phi(\begin{bmatrix} x_1 \\ x_2 \end{bmatrix}), \phi(\begin{bmatrix} y_1 \\ y_2 \end{bmatrix}) \rangle = (1 + x_1y_1 + x_2y_2)^2$$

- 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

The “Kernel Trick” examples

- The linear classifier relies on inner product between vectors $K(\mathbf{x}_i,\mathbf{x}_j)=\mathbf{x}_i^{\mathbf{T}}\mathbf{x}_j$
- If every datapoint is mapped into high-dimensional space via some transformation Φ: $\mathbf{x} \rightarrow \varphi(\mathbf{x})$, the inner product becomes:

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

- A *kernel function* is a function that is eqiuvalent to an inner product in some feature space.
- Example:

  2-dimensional vectors $\mathbf{x}=[x_1 \;\; x_2]$; let $K(\mathbf{x}_i,\mathbf{x}_j)=(1 + \mathbf{x}_i^{\mathbf{T}}\mathbf{x}_j)^2$,

  Need to show that $K(\mathbf{x}_i,\mathbf{x}_j)= \boldsymbol{\varphi}(\mathbf{x}_i)^{\mathbf{T}}\boldsymbol{\varphi}(\mathbf{x}_j)$:

  $K(\mathbf{x}_i,\mathbf{x}_j)=(1 + \mathbf{x}_i^{\mathbf{T}}\mathbf{x}_j)^2 = 1+ x_{i1}^2x_{j1}^2 + 2\, x_{i1}x_{j1}\, x_{i2}x_{j2}+ x_{i2}^2x_{j2}^2 + 2x_{i1}x_{j1} + 2x_{i2}x_{j2}=$

  $= [1 \;\; x_{i1}^2 \;\; \sqrt{2}\, x_{i1}x_{i2} \;\; x_{i2}^2 \;\; \sqrt{2}x_{i1} \;\; \sqrt{2}x_{i2}]^{\mathbf{T}}\, [1 \;\; x_{j1}^2 \;\; \sqrt{2}\, x_{j1}x_{j2} \;\; x_{j2}^2 \;\; \sqrt{2}x_{j1} \;\; \sqrt{2}x_{j2}] =$

  $= \boldsymbol{\varphi}(\mathbf{x}_i)^{\mathbf{T}}\boldsymbol{\varphi}(\mathbf{x}_j)$, where $\boldsymbol{\varphi}(\mathbf{x}) = [1 \;\; x_1^2 \;\; \sqrt{2}\, x_1x_2 \;\; x_2^2 \;\; \sqrt{2}x_1 \;\; \sqrt{2}x_2]$
- Thus, a kernel function *implicitly* maps data to a high-dimensional space (without the need to compute each $\boldsymbol{\varphi}(\mathbf{x})$ explicitly).

Examples of Kernel Functions

- Linear: $K(\mathbf{x}_i,\mathbf{x}_j)= \mathbf{x}_i^T\mathbf{x}_j$
  - Mapping Φ: $\mathbf{x} \rightarrow \boldsymbol{\varphi}(\mathbf{x})$, where $\boldsymbol{\varphi}(\mathbf{x})$ is $\mathbf{x}$ itself

- Polynomial of power p: $K(\mathbf{x}_i,\mathbf{x}_j)= (1+ \mathbf{x}_i^T\mathbf{x}_j)^p$
  - Mapping Φ: $\mathbf{x} \rightarrow \boldsymbol{\varphi}(\mathbf{x})$, where $\boldsymbol{\varphi}(\mathbf{x})$ has $\binom{d+p}{p}$ dimensions

- **Gaussian (radial-basis function):** $K(\mathbf{x}_i,\mathbf{x}_j) = e^{-\frac{\|\mathbf{x}_i-\mathbf{x}_j\|^2}{2\sigma^2}}$
  - Mapping Φ: $\mathbf{x} \rightarrow \boldsymbol{\varphi}(\mathbf{x})$, where $\boldsymbol{\varphi}(\mathbf{x})$ is *infinite-dimensional*: every point is mapped to *a function* (a Gaussian); combination of functions for support vectors is the separator.

- Higher-dimensional space still has *intrinsic* dimensionality d (the mapping is not *onto*), but linear separators in it correspond to *non-linear* separators in original space.

Modification Due to Kernel Function

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

Original

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

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

With kernel function

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

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

Modification Due to Kernel Function

- For testing, the new data **z** is classified as class 1 if *f* ≥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

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

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

Examples

Example 23.3: Let us continue with the example dataset shown in Figure 23.2. The dataset has 14 points as shown in Table 23.1.

Solving the L_{dual} quadratic program yields the following values for the Lagrangian multipliers for the support vectors

$\mathbf{x}_i$	x_{i1}	x_{i2}	y_i	α_i
$\mathbf{x}_1$	3.5	4.25	+1	0.0437
$\mathbf{x}_2$	4	3	+1	0.2162
$\mathbf{x}_4$	4.5	1.75	+1	0.1427
$\mathbf{x}_{13}$	2	2	−1	0.3589
$\mathbf{x}_{14}$	2.5	0.75	−1	0.0437

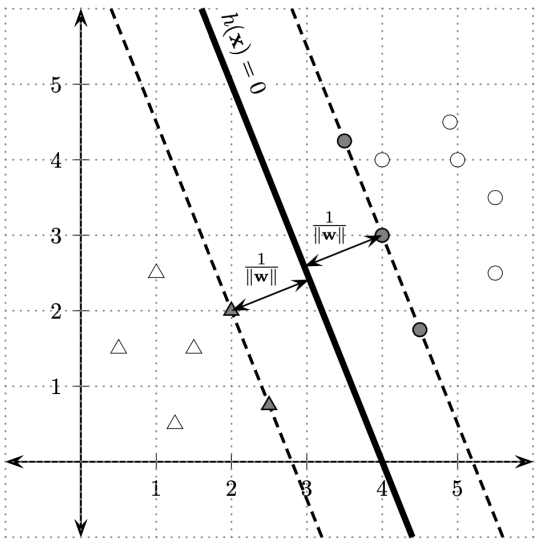


Figure 23.2: Margin of a Separating Hyperplane: $\frac{1}{\|\mathbf{w}\|}$ is the margin, and the shaded points are the support vectors.

Examples

$\mathbf{x}_i$	x_{i1}	x_{i2}	y_i
$\mathbf{x}_1$	3.5	4.25	+1
$\mathbf{x}_2$	4	3	+1
$\mathbf{x}_3$	4	4	+1
$\mathbf{x}_4$	4.5	1.75	+1
$\mathbf{x}_5$	4.9	4.5	+1
$\mathbf{x}_6$	5	4	+1
$\mathbf{x}_7$	5.5	2.5	+1
$\mathbf{x}_8$	5.5	3.5	+1
$\mathbf{x}_9$	0.5	1.5	−1
$\mathbf{x}_{10}$	1	2.5	−1
$\mathbf{x}_{11}$	1.25	0.5	−1
$\mathbf{x}_{12}$	1.5	1.5	−1
$\mathbf{x}_{13}$	2	2	−1
$\mathbf{x}_{14}$	2.5	0.75	−1

Table 23.1: Dataset corresponding to Figure 23.2

All other points are not support vectors, so they have $\alpha_i = 0$. Using (23.27) we can compute the weight vector for the hyperplane

$$\begin{aligned}\mathbf{w} &= \sum_{i,\alpha_i>0} \alpha_i y_i \mathbf{x}_i \\ &= 0.0437\begin{pmatrix}3.5\\4.25\end{pmatrix} + 0.2162\begin{pmatrix}4\\3\end{pmatrix} + 0.1427\begin{pmatrix}4.5\\1.75\end{pmatrix} - 0.3589\begin{pmatrix}2\\2\end{pmatrix} - 0.0437\begin{pmatrix}2.5\\0.75\end{pmatrix} \\ &= \begin{pmatrix}0.833\\0.334\end{pmatrix}\end{aligned}$$

We can compute the final bias as the average of the bias obtained from each support vector using (23.28)

$\mathbf{x}_i$	$\mathbf{w}^T\mathbf{x}_i$	$b_i = y_i - \mathbf{w}^T\mathbf{x}_i$
$\mathbf{x}_1$	4.332	−3.332
$\mathbf{x}_2$	4.331	−3.331
$\mathbf{x}_4$	4.331	−3.331
$\mathbf{x}_{13}$	2.333	−3.333
$\mathbf{x}_{14}$	2.332	−3.332
$b = \text{avg}\{b_i\}$		−3.332

Thus the optimal hyperplane is given as follows

$$h(\mathbf{x}) = \begin{pmatrix}0.833\\0.334\end{pmatrix}^T \mathbf{x} - 3.332 = 0 \tag{23.31}$$

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

Algorithm 23.1: Dual SVM Algorithm: Stochastic Gradient Ascent

SVM-DUAL $(\mathbf{D}, K, C, \epsilon)$:

foreach $\mathbf{x}_i \in \mathbf{D}$ **do** $\mathbf{x}_i \leftarrow \begin{pmatrix} \mathbf{x}_i \\ 1 \end{pmatrix}$ `// map to` $\mathbb{R}^{d+1}$

if $loss =$ `hinge` **then**

  $\mathbf{K} \leftarrow \{K(\mathbf{x}_i, \mathbf{x}_j)\}_{i,j=1,\ldots,n}$ `// kernel matrix, hinge loss`

else if $loss =$ `quadratic` **then**

  $\mathbf{K} \leftarrow \{K(\mathbf{x}_i, \mathbf{x}_j) + \frac{1}{2C}\delta_{ij}\}_{i,j=1,\ldots,n}$ `// kernel matrix, quadratic loss`

for $k = 1, \cdots, n$ **do** $\eta_k \leftarrow \frac{1}{K(\mathbf{x}_k, \mathbf{x}_k)}$ `// set step size`

$t \leftarrow 0$

$\boldsymbol{\alpha}_0 \leftarrow (0, \ldots, 0)^T$

repeat

  $\boldsymbol{\alpha} \leftarrow \boldsymbol{\alpha}_t$

  for $k = 1$ *to* n **do**

    `// update` k`-th component of` $\boldsymbol{\alpha}$

    $$\alpha_k \leftarrow \alpha_k + \eta_k \Big(1 - y_k \sum_{i=1}^{n} \alpha_i y_i K(\mathbf{x}_i, \mathbf{x}_k)\Big)$$

    if $\alpha_k < 0$ **then** $\alpha_k \leftarrow 0$

    if $\alpha_k > C$ **then** $\alpha_k \leftarrow C$

  $\boldsymbol{\alpha}_{t+1} = \boldsymbol{\alpha}$

  $t \leftarrow t + 1$

until $\|\boldsymbol{\alpha}_t - \boldsymbol{\alpha}_{t-1}\| \leq \epsilon$

Suppose: 3 training examples, 3 classes.
With some W the scores $f(x, W) = Wx$ are:



cat	**3.2**	1.3	2.2
car	5.1	**4.9**	2.5
frog	-1.7	2.0	**-3.1**

Multiclass SVM loss:

Given an example (x_i, y_i)
where x_i is the image and
where y_i is the (integer) label,

and using the shorthand for the scores vector: $s = f(x_i, W)$

the SVM loss has the form:

$$L_i = \sum_{j \neq y_i} \begin{cases} 0 & \text{if } s_{y_i} \geq s_j + 1 \\ s_j - s_{y_i} + 1 & \text{otherwise} \end{cases}$$

$$= \sum_{j \neq y_i} \max(0, s_j - s_{y_i} + 1)$$

Slide Credit: Fei-Fei Li, Justin Johnson, Serena Yeung, CS 231n

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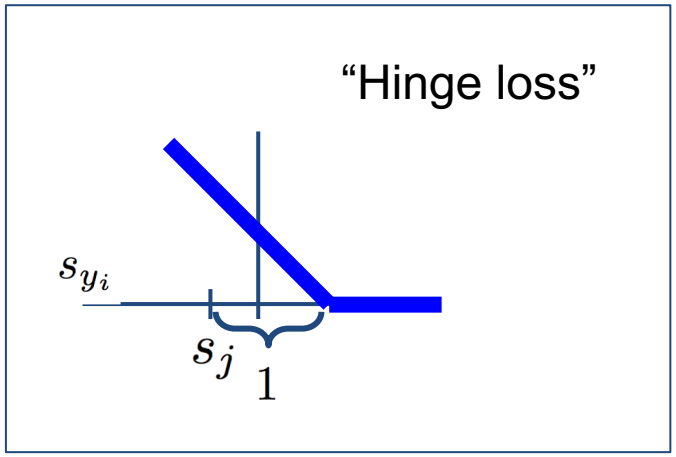
Multiclass SVM loss:



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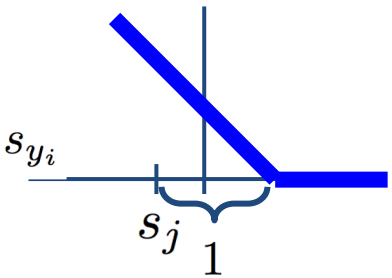
Multiclass SVM loss:

"Hinge loss"



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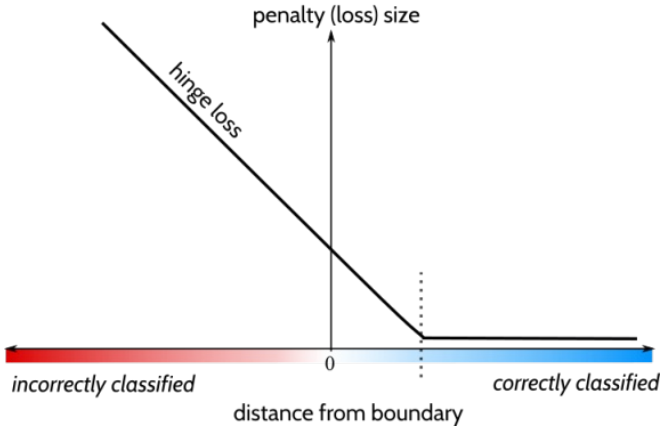

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Losses:	2.9		

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the SVM loss has the form:

$$L_i = \sum_{j \neq y_i} \max(0, s_j - s_{y_i} + 1)$$

= max(0, 5.1 - 3.2 + 1)
+max(0, -1.7 - 3.2 + 1)
= max(0, 2.9) + max(0, -3.9)
= 2.9 + 0
= 2.9

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the SVM loss has the form:

$$L_i = \sum_{j \neq y_i} \max(0, s_j - s_{y_i} + 1)$$

= max(0, 1.3 - 4.9 + 1)
+max(0, 2.0 - 4.9 + 1)
= max(0, -2.6) + max(0, -1.9)
= 0 + 0
= 0

Slide Credit: Fei-Fei Li, Justin Johnson, Serena Yeung, CS 231n

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Losses:	2.9	0	12.9

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the SVM loss has the form:

$$\boxed{L_i = \sum_{j \neq y_i} \max(0, s_j - s_{y_i} + 1)}$$

= max(0, 2.2 - (-3.1) + 1)
+max(0, 2.5 - (-3.1) + 1)
= max(0, 6.3) + max(0, 6.6)
= 6.3 + 6.6
= 12.9

Slide Credit: Fei-Fei Li, Justin Johnson, Serena Yeung, CS 231n

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Loss over full dataset is average:

$$L = \frac{1}{N} \sum_{i=1}^{N} L_i$$

L = (2.9 + 0 + 12.9)/3
= **5.27**

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Q: What happens to loss if car image scores change a bit?

Slide Credit: Fei-Fei Li, Justin Johnson, Serena Yeung, CS 231n

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Multiclass SVM loss:

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the SVM loss has the form:

$$\boxed{L_i = \sum_{j \neq y_i} \max(0, s_j - s_{y_i} + 1)}$$

Q2: what is the min/max possible loss?

Slide Credit: Fei-Fei Li, Justin Johnson, Serena Yeung, CS 231n

Multiclass SVM loss:

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the SVM loss has the form:

$$\boxed{L_i = \sum_{j \neq y_i} \max(0, s_j - s_{y_i} + 1)}$$

Q6: What if we used

$$L_i = \sum_{j \neq y_i} \max(0, s_j - s_{y_i} + 1)^2$$

Slide Credit: Fei-Fei Li, Justin Johnson, Serena Yeung, CS 231n

Multiclass SVM Loss

$$L_i = \sum_{j \neq y_i} \max(0, s_j - s_{y_i} + 1)$$

```
def L_i_vectorized(x, y, W):
  scores = W.dot(x)
  margins = np.maximum(0, scores - scores[y] + 1)
  margins[y] = 0
  loss_i = np.sum(margins)
  return loss_i
```

$$f(x, W) = Wx$$

$$L = \frac{1}{N} \sum_{i=1}^{N} \sum_{j \neq y_i} \max(0, f(x_i; W)_j - f(x_i; W)_{y_i} + 1)$$

E.g. Suppose that we found a W such that L = 0. Is this W unique?

No! 2W is also has L = 0!

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frog	-1.7	2.0	**-3.1**
Losses:	2.9	0	

$$L_i = \sum_{j \neq y_i} \max(0, s_j - s_{y_i} + 1)$$

Before:

= max(0, 1.3 - 4.9 + 1)
+max(0, 2.0 - 4.9 + 1)
= max(0, -2.6) + max(0, -1.9)
= 0 + 0
= 0

With W twice as large:

= max(0, 2.6 - 9.8 + 1)
+max(0, 4.0 - 9.8 + 1)
= max(0, -6.2) + max(0, -4.8)
= 0 + 0
= 0

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
  - Inherent feature selection capability
- Weaknesses
  - Need to choose a “good” kernel function.

Overtraining/overfitting

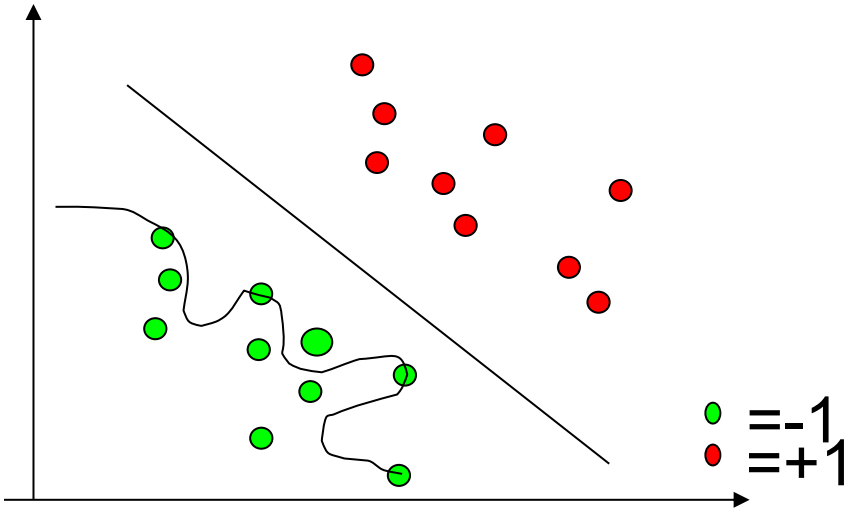
- A well-known problem with machine learning methods is overtraining.
- This means that we have learned the training data very well, but

we can not classify unseen examples correctly.

An example: A botanist really knowing trees.

Every time he sees a new tree,

he claims it is not a tree.



Overtraining/overfitting 2

- A measure of the **risk of overtraining with SVM** (there are also other measures).

- It can be shown that: The portion, **n, of unseen data that will be miss-classified** is bounded by:

  $n \leq$ Number of support vectors / number of training examples

- **Ockham´s razor principle**: Simpler system are better than more complex ones.
  - In SVM case: fewer support vectors mean a simpler representation of the hyperplane.

  Example: Understanding a certain cancer if it can be described by one gene is easier than if we have to describe it with 5000.

SVM applications

- SVMs were originally proposed by Boser, Guyon and Vapnik in 1992 and gained increasing popularity in late 1990s.
- SVMs are currently among the best performers for a number of classification tasks ranging from text to genomic data.
- SVMs can be applied to complex data types beyond feature vectors (e.g. graphs, sequences, relational data) by designing kernel functions for such data.
- SVM techniques have been extended to a number of tasks such as regression [Vapnik *et al.* '97], principal component analysis [Schölkopf *et al.* '99], etc.
- Most popular optimization algorithms for SVMs use *decomposition* to hill-climb over a subset of α_i's at a time, e.g. SMO [Platt '99] and [Joachims '99]
- Tuning SVMs remains a black art: selecting a specific kernel and parameters is usually done in a try-and-see manner.

A Cautionary Example

Image classification of tanks. Autofire when an enemy tank is spotted.

Input data: Photos of own and enemy tanks.

Worked really good with the training set used.

In reality it failed completely.

Reason: All enemy tank photos taken in the morning. All own tanks in dawn.

The classifier could recognize dusk from dawn!!!!

http://www.kernel-machines.org/software.html

Summary

- Support Vector Machine (SVM)
- Kernelization methods
- Strength and weakness of SVM
- Applications of SVM

- What's next?
  - Principle Component Analysis (PCA) and it's variants

Resources

- http://www.kernel-machines.org/
- http://www.support-vector.net/
- http://www.support-vector.net/icml-tutorial.pdf
- http://www.kernel-machines.org/papers/tutorial-nips.ps.gz
- http://www.clopinet.com/isabelle/Projects/SVM/applist.html