

# Support Vector Machine

A supervised learning model.

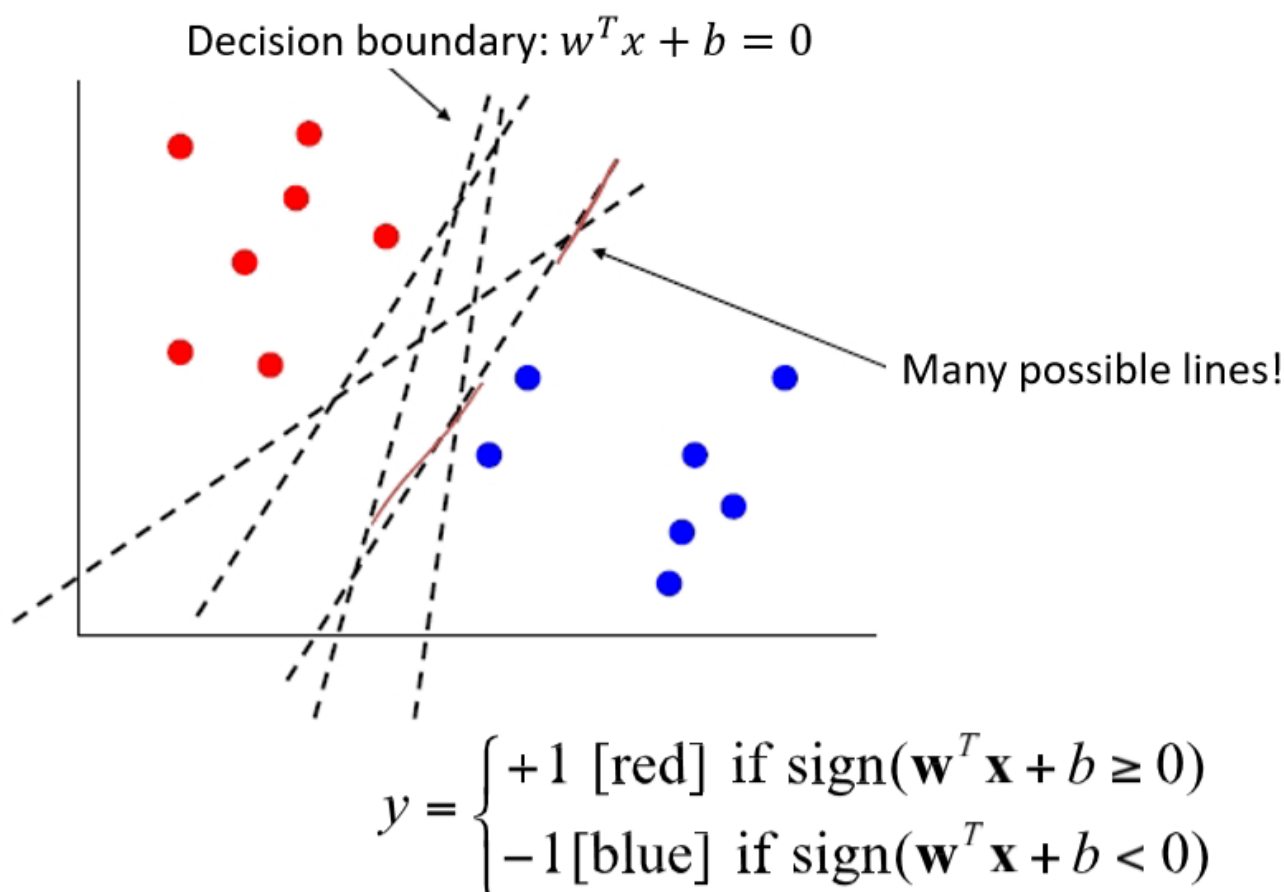
## Motivation and Logistics

- A **maximum margin method**, can be used for classification or regression.
- SVMs can efficiently perform a non-linear classification using what is called the **kernel trick**, implicitly mapping their inputs into high-dimensional feature spaces.
- First, we will derive **linear, hard-margin SVM** for linearly separable data, later for non-separable (soft margin SVM), and for nonlinear boundaries (kernel SVM).

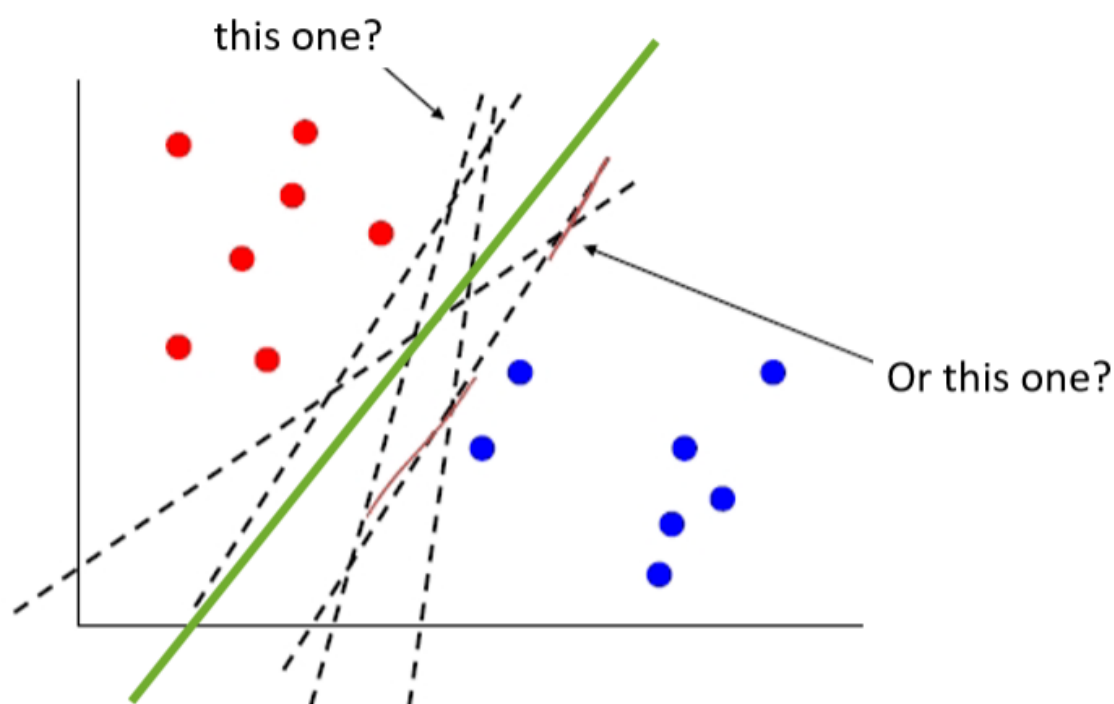
## Maximum Margin

### Motivation

看一个二分类问题，现在可以有很多个Decision boundary，到底哪个才是最好的。



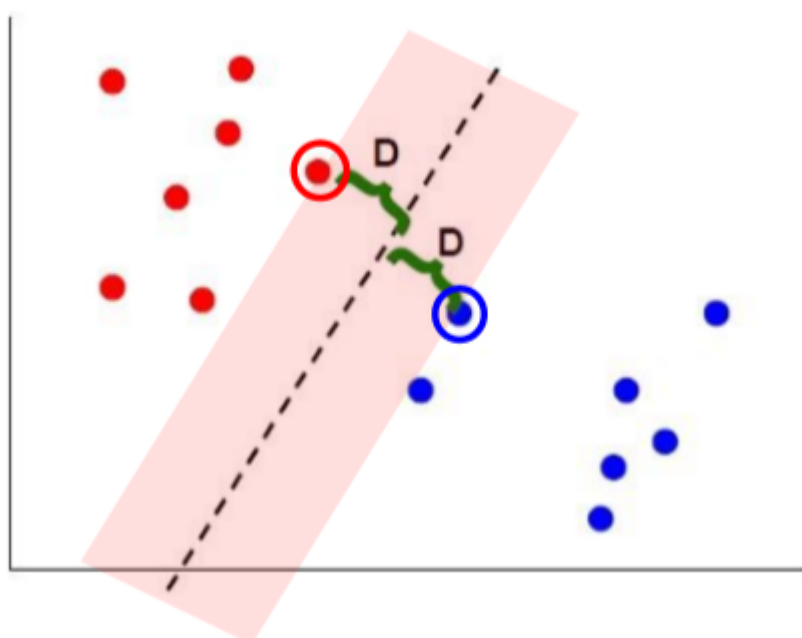
那当然是能远离所有点的那条线是最好的，如下图的绿线。



*It maximizes the margin between the two classes.*

我们只需要关注boundary points.

我们的目标就是：learn a boundary that leads to the largest margin.

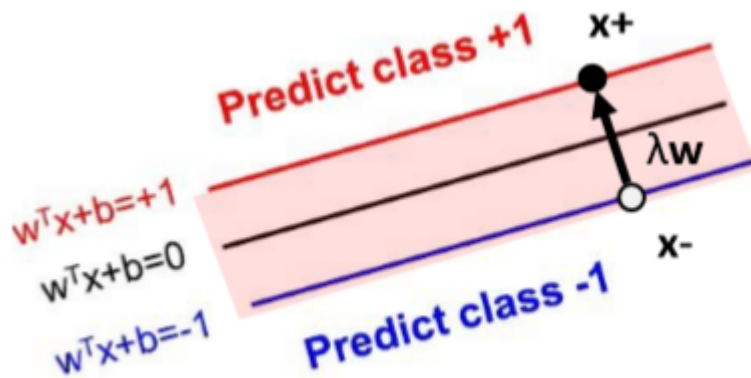


为什么叫支持向量？

Subset of vectors that support determine boundary are called the **support vectors (circled)**.

Max Margin Classifier

我们对刚刚得到的decision boundary进行平移，得到一个margin.



我们看二分类问题，标签为1和-1，当然也可以标记为两个常数。

$$Class : +1 \quad if \quad w^T x + b \geq 1$$

$$Class : -1 \quad if \quad w^T x + b \leq -1$$

$$Class : Undefined \quad if \quad -1 < w^T x + b < 1$$

我们怎么确定支持向量？

假设现在如图这两个点  $x^+$  和  $x^-$ ，是两个支持向量。

易知，

$$w^T x^+ + b = 1$$

$$w^T x^- + b = -1$$

则，

$$w^T (x^+ - x^-) = 2$$

我们需要maximize

$$\|x^+ - x^-\|$$

那我们如何用  $w$  来表示上式呢？

我们，需要引入一个中间变量  $\lambda$ 。令

$$x^+ - x^- = \lambda w$$

代入下式，

$$w^T x^+ + b = 1$$

得到：

$$w^T (\lambda w + x^-) + b = 1$$

$$w^T x^- + b + \lambda w^T w = 1$$

$$-1 + \lambda w^T w = 1$$

$$\lambda = \frac{2}{w^T w}$$

现在我们可以求

$$\|x^+ - x^-\| = \|\lambda w\| = \lambda \sqrt{w^T w} = \frac{2}{\sqrt{w^T w}}$$

Maximizing the margin is equivalent to regularization.

最大化这个margin相当于防止overfitting.

## Linear SVM

对于可以线性分类的问题。我们这个模型要学习的是\$w\$和\$b\$这两个参数。

### Formulation

Objective function:

$$\min \frac{1}{2} \|w\|^2$$

$$s.t. (w^T x_i + b)y_i \geq 1, \forall i$$

如果样本标签为1，分类结果为-1或者0.5或者-0.5，都会破坏这个约束。

This is the primal formulation.

Apply Lagrange multipliers: formulate equivalent problem.

使用拉格朗日乘子，转化为没有约束的等价问题。

### Lagrange multipliers

Convert the primal constrained minimization to an unconstrained optimization problem: represent constraints as penalty terms:

$$\min_{w,b} \frac{1}{2} \|w\|^2 + \text{penalty}$$

对每个样本\$\{(x\_i, y\_i)\}\$的惩罚求和，

$$\text{penalty} = \sum_{i=1}^n \max_{\alpha_i \geq 0} \alpha_i [1 - (w^T x_i + b)y_i]$$

其中，n是样本数量，\$\alpha\_i\$是拉格朗日乘子。

**max**在这里到底是约束还是变量？

如果约束满足：

$$1 - (w^T x_i + b)y_i \leq 0$$

如果约束不满足：

$$1 - (w^T x_i + b)y_i > 0$$

大的拉格朗日乘子 $\alpha_i$ ，确保惩罚足够大。

提问，阿尔法怎么设？

得到，

$$\min_{w,b} \frac{1}{2} \|w\|^2 + \sum_{i=1}^n \max_{\alpha_i \geq 0} \alpha_i [1 - (w^T x_i + b)y_i]$$

代价函数：

$$\max_{\alpha_i \geq 0} \min_{w,b} J(w, b; \alpha) = \max_{\alpha_i \geq 0} \min_{w,b} \frac{1}{2} \|w\|^2 + \sum_{i=1}^n \alpha_i [1 - (w^T x_i + b)y_i]$$

对w, b求偏导，

$$\frac{\partial J(w, b; \alpha)}{\partial w} = w - \sum_{i=1}^n \alpha_i x_i y_i = 0$$

$$\frac{\partial J(w, b; \alpha)}{\partial b} = - \sum_{i=1}^n \alpha_i y_i = 0$$

## Dual problem

重新代进原式，得到Dual problem，现在我们需要优化 $\alpha$ ，训练的时候，我们

$$L = \max_{\alpha_i \geq 0} \sum_{i=1}^n \alpha_i - \frac{1}{2} \sum_{i,j=1}^n y_i y_j \alpha_i \alpha_j (x_i^T x_j)$$

$$s.t. \alpha_i \geq 0; \sum_{i=1}^n \alpha_i y_i = 0$$

Then use the obtained  $\alpha_i$ 's to solve for the weights and bias:

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

$$b = y_i - w^T x_i$$

In practice, predict

$$y = \text{sign}[w^T x + b]$$

## Primal v.s. Dual Problem

## Soft margin and slack variables

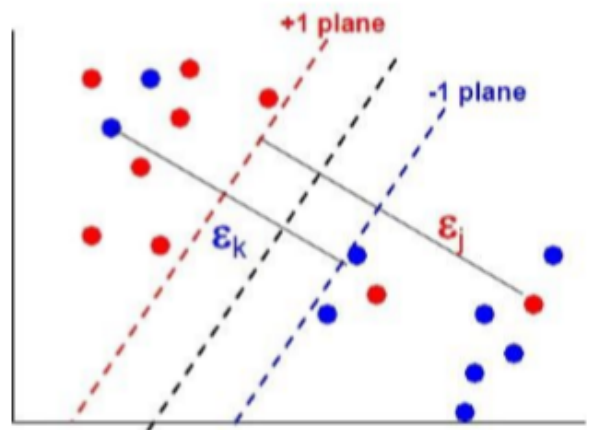
Introduce **slack variables**  $\xi_i$

$$\min \left[ \frac{1}{2} \|\mathbf{w}\|^2 + \lambda \sum_{i=1}^n \xi_i \right]$$

subject to constraints (for all  $i$ ):

$$y_i (\mathbf{w} \cdot \mathbf{x}_i + b) \geq 1 - \xi_i$$

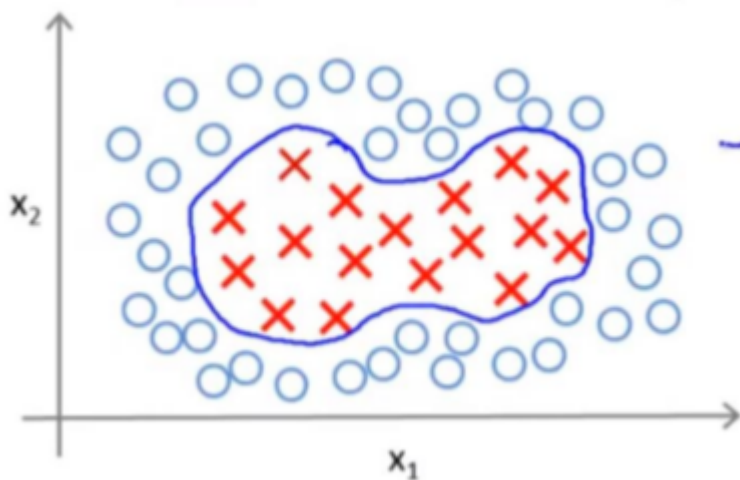
$$\xi_i \geq 0$$



Example lies on wrong side of hyperplane:  $\xi_i > 1 \Rightarrow \sum_i \xi_i$   
is upper bound on number of training errors

$\xi_i$  的取值，如图所示，如果红点在 +1 平面的左方， $\xi_i$  为 0，如果在决策平面的左方，+1 平面的右方，取值则为 (0,1)，如果在决策平面另一侧，取值则大于 1。

Kernel trick for non-linear decision boundary



虽然可以用 high order polynomial features，我们就希望用一个变换，把这些数据变得 linear separable, 然后用 linear SVM.

Input transformation

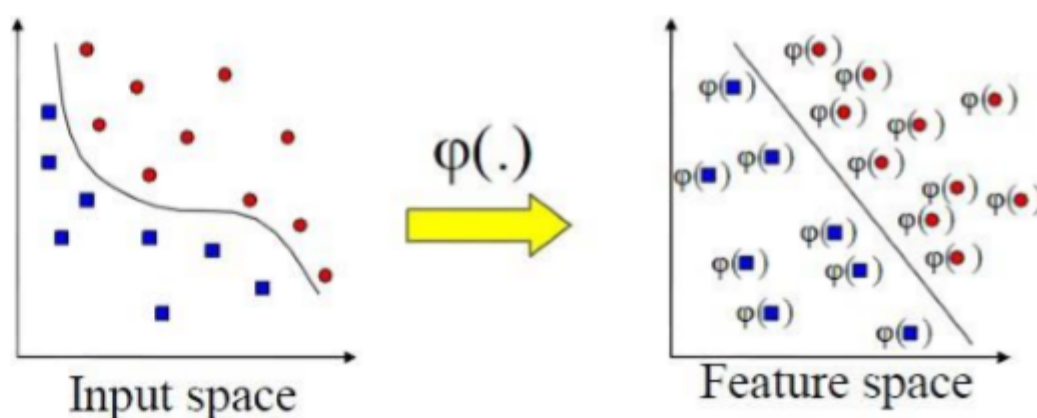
# Input transformation

Mapping to a feature space can produce problems:

- High computational burden due to high dimensionality
- Many more parameters

SVM solves these two issues simultaneously

- Kernel trick produces efficient classification
- Dual formulation only assigns parameters to samples, not features



Lankmark (Kernel Function)

Given data set

$$(x^{(1)}, y^{(1)}), (x^{(2)}, y^{(2)}), \dots, (x^{(m)}, y^{(m)})$$

Choose lankmarks

$$l^{(1)} = x^{(1)}, l^{(2)} = x^{(2)}, \dots, l^{(m)} = x^{(m)}$$

原来的预测函数是这样： Predict "1" when:

$$\theta_0 + \theta_1 x_1 + \theta_2 x_2 + \dots + \theta_n x_n \geq 0$$

经过变换以后： Predict "1" when:

$$\theta_0 + \theta_1 f_1 + \theta_2 f_2 + \dots + \theta_n f_n \geq 0$$

其中， $f_i$ 就是Kernel Function.

Kernel Function需要自行选择，比如选的是高斯分布。

$$f_i = \text{similarity}(x, l^{(i)}) = \exp\left(-\frac{\|x - l^{(i)}\|^2}{2\sigma^2}\right)$$

分布的参数需要自己设定，例如，我们这里设置均值为样本数据点本身，方差另外设定。

## Kernels

Examples of kernels (kernels measure similarity):

1. Polynomial  $K(\mathbf{x}_1, \mathbf{x}_2) = (\mathbf{x}_1 \cdot \mathbf{x}_2 + 1)^2$
2. Gaussian  $K(\mathbf{x}_1, \mathbf{x}_2) = \exp(-\|\mathbf{x}_1 - \mathbf{x}_2\|^2 / 2\sigma^2)$
3. Sigmoid  $K(\mathbf{x}_1, \mathbf{x}_2) = \tanh(\kappa(\mathbf{x}_1 \cdot \mathbf{x}_2) + a)$

Each kernel computation corresponds to dot product calculation for particular mapping  $\varphi(x)$ : implicitly maps to high-dimensional space

Why is this useful?

1. Rewrite training examples using more complex features
2. Dataset not linearly separable in original space may be linearly separable in higher dimensional space



# Classification with non-linear SVMs

Non-linear SVM using kernel function  $K()$ :

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

Maximize  $L_K$  w.r.t.  $\{\alpha\}$ , under constraints  $\alpha \geq 0$

Unlike linear SVM, cannot express  $w$  as linear combination of support vectors – now must retain the support vectors to classify new examples

Final decision function:

$$y = \text{sign}[b - \sum_{i=1}^n y_i \alpha_i K(\mathbf{x}, \mathbf{x}_i)]$$

## Kernel SVM Summary

Advantages:

- Kernels allow very flexible hypotheses
- Poly-time exact optimization methods rather than approximate methods
- Soft-margin extension permits mis-classified examples
- Excellent results (1.1% error rate on handwritten digits vs. LeNet's 0.9%)

Disadvantages:

- Must choose kernel parameters
- Very large problems computationally intractable