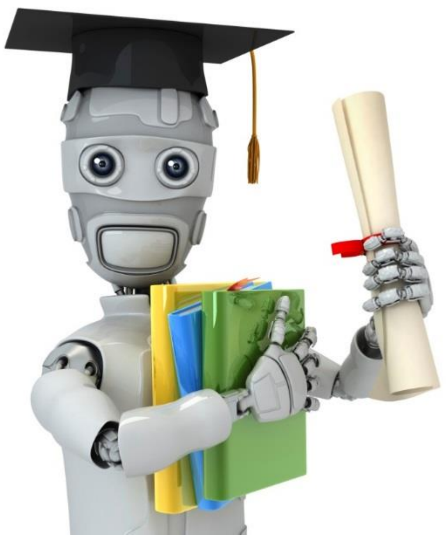

Machine Learning

支持向量机 (Support Vector Machines)

梁毅雄

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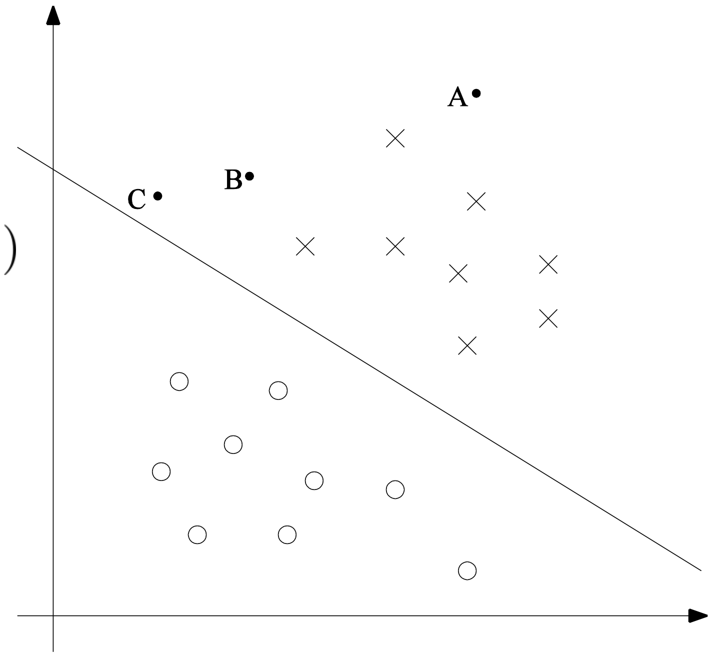
Some materials from Andrew Ng, Barnabás Póczos and others

Margins: Intuition

Logistic regression: $p(y=1|x;\theta) = h_\theta(x) = g(\theta^T x)$



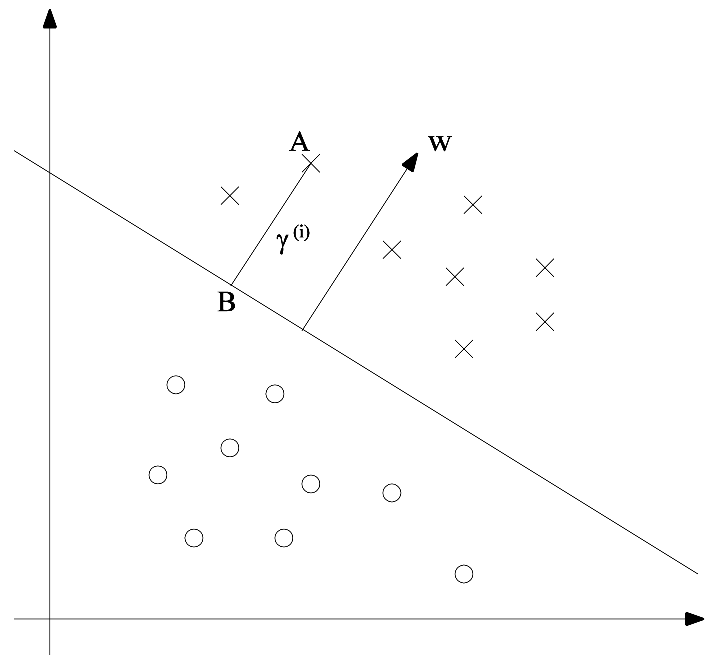
在测试新样本时，当 $\theta^T x \gg 0$ 或者 $\theta^T x \ll 0$ 我们可以“very confident”给出预测结果

While in trainining, we'd have found a good fit to the training data if we can find θ so that $\theta^T x^{(i)} \gg 0$ whenever $y^{(i)} = 1$, and $\theta^T x^{(i)} \ll 0$ whenever $y^{(i)} = 0$

Margins: Intuition

重新定义符号如下：

$$
\begin{aligned}
y = \{0,1\} \quad & \Rightarrow y = \{-1,+1\} \\
\theta_0 \quad & \Rightarrow b \\
\begin{bmatrix} \theta_1 \\ \theta_2 \\ \vdots \\ \theta_n \end{bmatrix} \quad & \Rightarrow w = \begin{bmatrix} w_1 \\ w_2 \\ \vdots \\ w_n \end{bmatrix}
\end{aligned}
$$



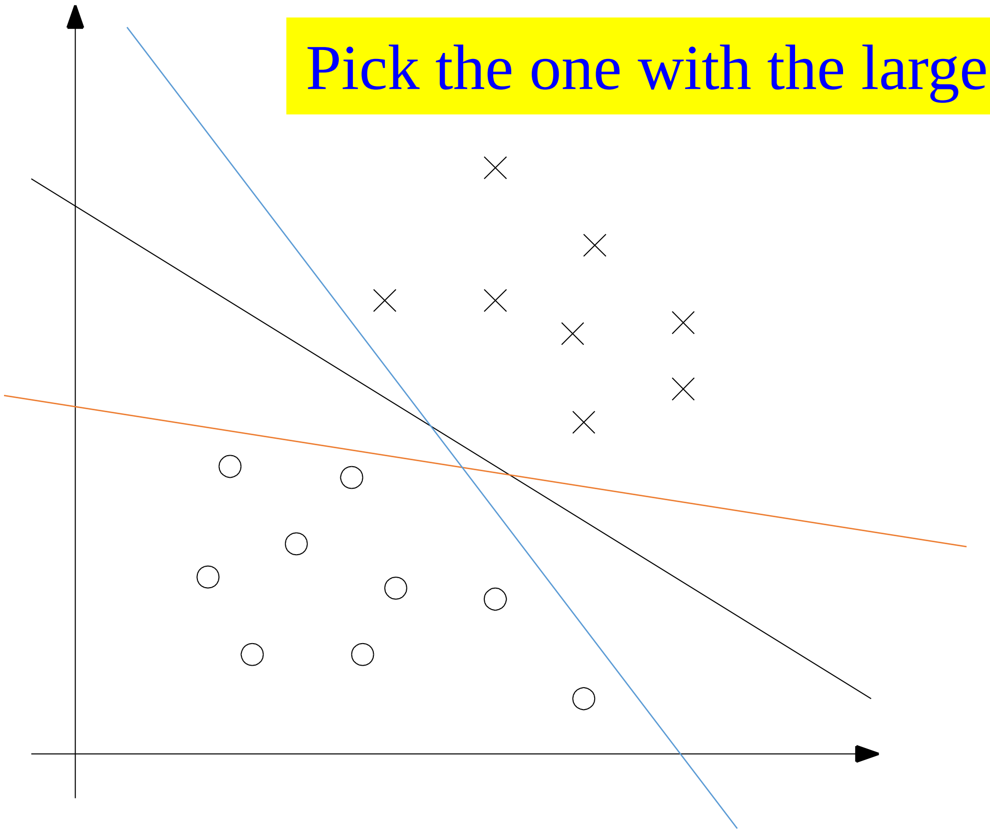
"Confidence": $\hat{\gamma}^{(i)} = y^{(i)}(w^T x^{(i)} + b)$

$$y = \mathrm{sign}(w^T x + b) = \begin{cases} +1, & w^T x + b > 0 \\ -1, & w^T x + b < 0 \end{cases}$$

正确分类的条件： $y^{(i)}(w^T x^{(i)} + b) > 0$

Margins: Intuition

Which line is better?



Pick the one with the largest margin!

最大间隔分类器(Max Margin Classifier)

Pick the one with the largest margin!

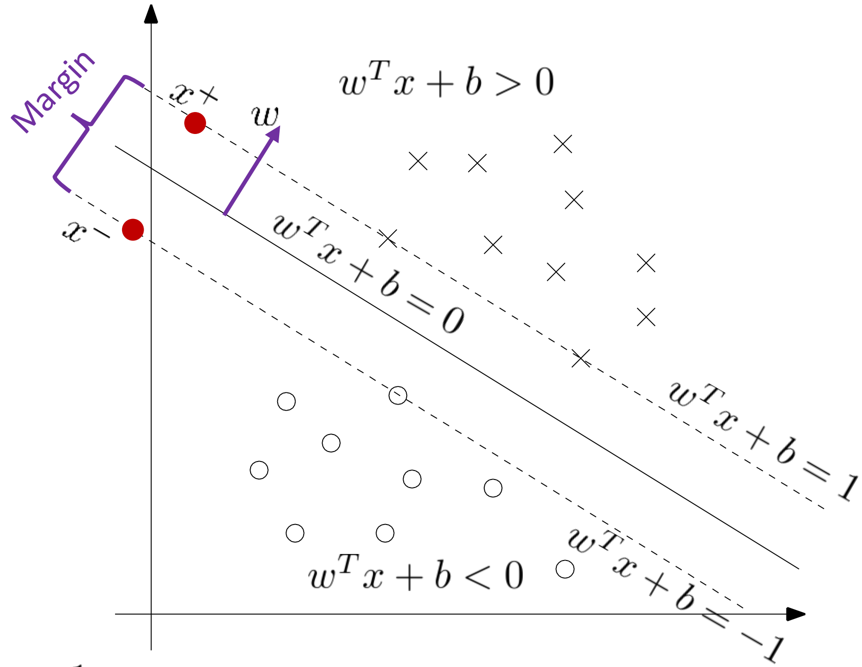
如何计算margin？

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

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

$$\text{margin} = \|x^+ - x^-\| = ?$$

$$w^T(x^+ - x^-) = 2$$
$$\lambda = \frac{2}{w^T w}$$
$$\text{margin} = \|x^+ - x^-\| = \|\lambda w\| = \frac{2}{\|w\|}$$



最大化margin: $\max_w \frac{2}{\|w\|}$ 等价于 $\min_w \frac{1}{2}\|w\|^2$

The Primal Hard SVM

假设数据线性可分，即 $y^{(i)}(w^T x^{(i)} + b) \geq 1$

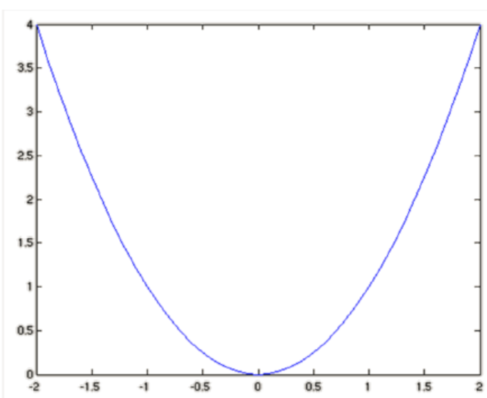
$$
\begin{aligned}
\min_{w,b} \quad & \frac{1}{2}||w||^2 \\
\text{s.t.} \quad & y^{(i)}(w^T x^{(i)} + b) \geq 1, \;\; i = 1, \ldots, m
\end{aligned}
$$

- 属于带约束的优化问题(线性约束条件 + 二次目标函数)
- 典型的二次规划（ Quadratic Programming, QP ）问题
- Efficient algorithms and commercial code exist for QP

Constrained Optimization

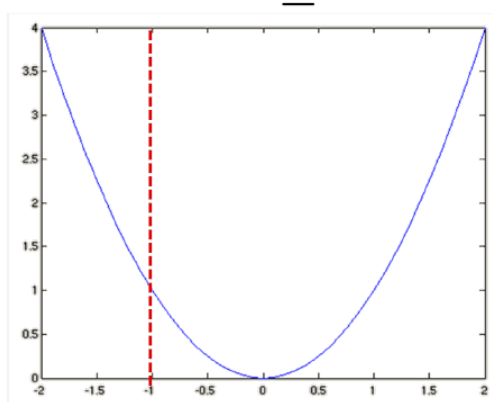
$$\min_x \ x^2$$
$$\text{s.t.} \quad x \geq b$$

$\min_x \ x^2$



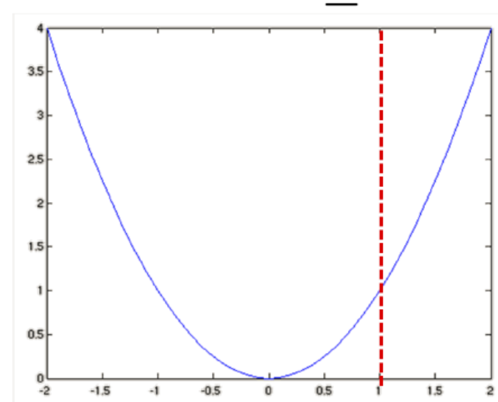
$x^* = 0$

$\min_x \ x^2$
$\text{s.t.} \quad x \geq -1$



$x^* = 0$

$\min_x \ x^2$
$\text{s.t.} \quad x \geq 1$



$x^* = 1$

Lagrange Multiplier

$$\begin{aligned} \min_w \quad & f(w) \\ \text{s.t.} \quad & h_i(w) = 0, \quad i = 1, \ldots, l. \end{aligned}$$

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

β_i: **Lagrange multipliers**.

$$\frac{\partial \mathcal{L}}{\partial w_i} = 0; \quad \frac{\partial \mathcal{L}}{\partial \beta_i} = 0,$$

Lagrange Multiplier

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

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

$$\theta_{\mathcal{P}}(w) = \max_{\alpha, \beta \,:\, \alpha_i \geq 0} \mathcal{L}(w, \alpha, \beta).$$

α_i, β_i: **Lagrange multipliers**.

Let some w be given. If w violates any of the primal constraints (i.e., if either $g_i(w) > 0$ or $h_i(w) \neq 0$ for some i), then you should be able to verify that

$$
\begin{aligned}
\theta_{\mathcal{P}}(w) &= \max_{\alpha, \beta \,:\, \alpha_i \geq 0} f(w) + \sum_{i=1}^{k} \alpha_i g_i(w) + \sum_{i=1}^{l} \beta_i h_i(w) \\
&= \infty.
\end{aligned}
$$

Lagrange Multiplier

$$\theta_{\mathcal{P}}(w) = \max_{\alpha,\beta\,:\,\alpha_i \geq 0} \mathcal{L}(w,\alpha,\beta) \qquad \mathcal{L}(w,\alpha,\beta) = f(w) + \sum_{i=1}^{k} \alpha_i g_i(w) + \sum_{i=1}^{l} \beta_i h_i(w)$$

$$\theta_{\mathcal{P}}(w) = \begin{cases} f(w) & \text{if } w \text{ satisfies primal constraints} \\ \infty & \text{otherwise.} \end{cases}$$

$$\min_{w} \theta_{\mathcal{P}}(w) = \min_{w} \max_{\alpha,\beta\,:\,\alpha_i \geq 0} \mathcal{L}(w,\alpha,\beta)$$

等价于原来的优化问题 (Primal problem)

$$\theta_{\mathcal{D}}(\alpha,\beta) = \min_{w} \mathcal{L}(w,\alpha,\beta) \qquad \max_{\alpha,\beta\,:\,\alpha_i \geq 0} \theta_{\mathcal{D}}(\alpha,\beta) = \max_{\alpha,\beta\,:\,\alpha_i \geq 0} \min_{w} \mathcal{L}(w,\alpha,\beta)$$

对偶优化问题(Dual problem)

$$d^* = \max_{\alpha,\beta\,:\,\alpha_i \geq 0} \min_{w} \mathcal{L}(w,\alpha,\beta) \leq \min_{w} \max_{\alpha,\beta\,:\,\alpha_i \geq 0} \mathcal{L}(w,\alpha,\beta) = p^*$$

弱对偶性

Lagrange Multiplier

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

Under certain conditions, we will have $d^* = p^*$ 强对偶性

- f and the g_i's are convex (its Hessian is positive semi-definite)
- h_i's are affine, i.e., there exists a_i, b_i, so that $h_i(w) = a_i^T w + b_i$

Under our above assumptions, there must exist w^*, α^*, β^* so that w^* is the solution to the primal problem, α^*, β^* are the solution to the dual problem, and moreover $p^* = d^* = \mathcal{L}(w^*, \alpha^*, \beta^*)$.

Lagrange Multiplier

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

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

Moreover, w^*, α^* and β^* satisfy the **Karush-Kuhn-Tucker (KKT) conditions**, which are as follows:

$$\begin{aligned} \frac{\partial}{\partial w_i} \mathcal{L}(w^*, \alpha^*, \beta^*) &= 0, \quad i = 1, \ldots, n \\ \frac{\partial}{\partial \beta_i} \mathcal{L}(w^*, \alpha^*, \beta^*) &= 0, \quad i = 1, \ldots, l \\ \boxed{\alpha_i^* g_i(w^*) = 0, \quad i = 1, \ldots, k} & \\ g_i(w^*) &\le 0, \quad i = 1, \ldots, k \\ \alpha^* &\ge 0, \quad i = 1, \ldots, \end{aligned}$$

The KKT **dual complementarity** condition:
If $\alpha_i^* > 0$, then $g_i(w^*) = 0$

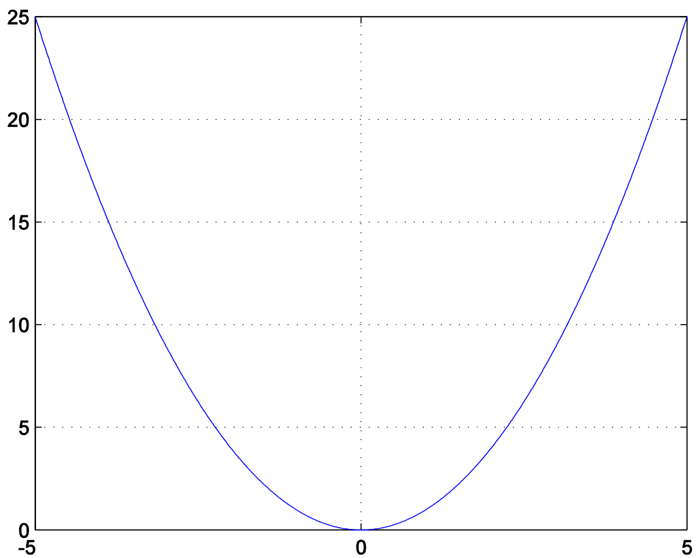
Moreover, if some w^*, α^*, β^* satisfy the KKT conditions, then it is also a solution to the primal and dual problems.

Lagrange Multiplier

$$\begin{aligned} \min_w \quad & f(w) \\ \text{s.t.} \quad & g_i(w) \boxed{\leq} 0, \quad i = 1, \dots, k \\ & h_i(w) = 0, \quad i = 1, \dots, l. \end{aligned}$$

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

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



$$\begin{aligned} \min_x \quad & f(x) = x^2 \\ \text{s.t.} \quad & x \boxed{\geq} b \end{aligned}$$

满足强对偶条件

$$\mathcal{L}(x,\alpha) = x^2 - \alpha(x - b)$$

$$\begin{aligned} \min_x \max_\alpha \quad & \mathcal{L}(x,\alpha) \\ \text{s.t.} \quad & \alpha \geq 0 \end{aligned}$$

Lagrange Multiplier

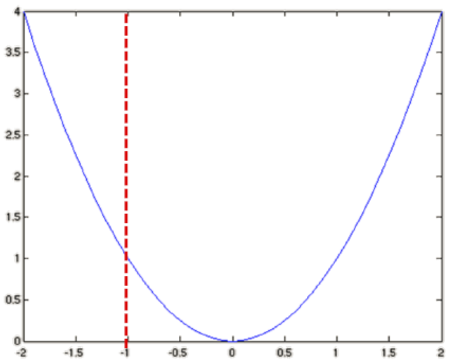
$$\begin{aligned} \min_x \quad & f(x) = x^2 \\ \text{s.t.} \quad & x \geq b \end{aligned}$$

$$\begin{aligned} \min_x \max_\alpha \quad & \mathcal{L}(x, \alpha) = x^2 - \alpha(x - b) \\ \text{s.t.} \quad & \alpha \geq 0 \end{aligned}$$

$$\frac{\partial \mathcal{L}}{\partial x} = 0 \Rightarrow x^* = \frac{\alpha}{2}$$

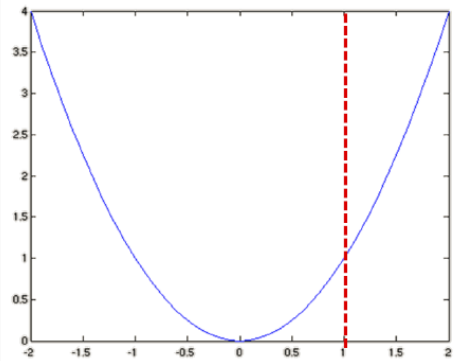
$$\frac{\partial \mathcal{L}}{\partial \alpha} = 0 \Rightarrow \alpha^* = \max(2b, 0)$$

$$\begin{aligned} \min_x \quad & x^2 \\ \text{s.t.} \quad & x \geq -1 \end{aligned}$$



$x^* = 0$

$$\begin{aligned} \min_x \quad & x^2 \\ \text{s.t.} \quad & x \geq 1 \end{aligned}$$



$x^* = 1$

SVM: From Primal to Dual

Primal problem:

$$\begin{aligned} \min_{w,b} \quad & \frac{1}{2}||w||^2 \\ \text{s.t.} \quad & y^{(i)}(w^T x^{(i)} + b) \geq 1, \quad i = 1, \ldots, m \end{aligned}$$

Lagrange function:

满足强对偶条件

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

$$\nabla_w \mathcal{L}(w, b, \alpha) = w - \sum_{i=1}^{m} \alpha_i y^{(i)} x^{(i)} = 0 \Rightarrow \boxed{w^* = \sum_{i=1}^{m} \alpha_i y^{(i)} x^{(i)}}$$

$$\frac{\partial}{\partial b} \mathcal{L}(w, b, \alpha) = \boxed{\sum_{i=1}^{m} \alpha_i^* y^{(i)} = 0}$$

SVM: From Primal to Dual

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

$$\Big\downarrow \quad w^* = \sum_{i=1}^{m} \alpha_i y^{(i)} x^{(i)}$$

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

$$\Big\downarrow \quad \sum_{i=1}^{m} \alpha_i y^{(i)} = 0$$

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

Solving the Dual: The SMO Algorithm

$$
\begin{aligned}
\max_\alpha \quad & W(\alpha) = \sum_{i=1}^m \alpha_i - \frac{1}{2} \sum_{i,j=1}^m y^{(i)} y^{(j)} \alpha_i \alpha_j \langle x^{(i)}, x^{(j)} \rangle \\
\text{s.t.} \quad & \alpha_i \geq 0, \quad i = 1, \ldots, m \\
& \sum_{i=1}^m \alpha_i y^{(i)} = 0
\end{aligned}
$$

- 这仍然是一个二次规划问题，可采用通用的QP算法求解，但其规模正比于训练样本数
- Sequential Minimal Optimization (SMO) algorithm是一种高效算法，基本思想是采用坐标下降法，在更新α_i时固定其他α_j, 由于$\sum_{i=1}^m \alpha_i y^{(i)} = 0$, α_i的值可由其他的 α_j $(j \neq i)$表示

The Dual Hard SVM

$$\begin{aligned}
\max_\alpha \quad & W(\alpha) = \sum_{i=1}^{m} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{m} y^{(i)} y^{(j)} \alpha_i \alpha_j \langle x^{(i)}, x^{(j)} \rangle \\
\text{s.t.} \quad & \alpha_i \geq 0, \quad i = 1, \ldots, m \\
& \sum_{i=1}^{m} \alpha_i y^{(i)} = 0
\end{aligned}$$

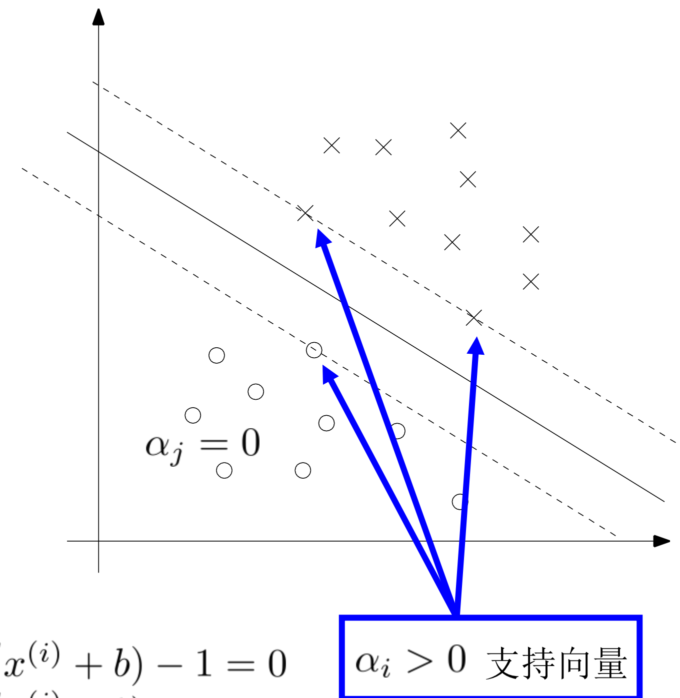
得到上式的最优解α^*后，可代入$w = \sum_{i=1}^{m} \alpha_i y^{(i)} x^{(i)}$得到最优解$w^*$

如何求b？

$$b^* = -\frac{\max_{i:y^{(i)}=-1} w^{*T} x^{(i)} + \min_{i:y^{(i)}=1} w^{*T} x^{(i)}}{2}$$

分类：$y = \operatorname{sign}(w^T x + b) = \begin{cases} +1, & w^T x + b > 0 \\ -1, & w^T x + b < 0 \end{cases}$

The Dual Hard SVM



$$
\begin{aligned}
w^T x + b &= \left(\sum_{i=1}^{m} \alpha_i y^{(i)} x^{(i)}\right)^T x + b \\
&= \sum_{i=1}^{m} \alpha_i y^{(i)} \langle x^{(i)}, x \rangle + b
\end{aligned}
$$

- The KKT **dual complementarity** condition:
  $\alpha_i \left[y^{(i)}(w^T x^{(i)} + b) - 1 \right] = 0, \ \forall i \quad \Rightarrow \begin{cases} \alpha_i > 0, & y^{(i)}(w^T x^{(i)} + b) - 1 = 0 \\ \alpha_i = 0, & y^{(i)}(w^T x^{(i)} + b) - 1 > 0 \end{cases}$
- $y = \mathrm{sign}\left(\sum_{i=1}^{m} \alpha_i y^{(i)} \langle x^{(i)}, x \rangle + b\right)$

  - 一般情况下只有少数训练样本对应的Lagrange Multiplier大于零(支持向量)，分类面则是由这些支持向量决定
  - 决策时只需计算新样本与所有支持向量的内积

From Hard SVM to Soft SVM

$$(w^*_{\text{hard}}, b^*_{\text{hard}}) = \quad \arg\min_{w,b} \quad \frac{1}{2}||w||^2$$

$$\text{s.t.} \qquad y^{(i)}(w^T x^{(i)} + b) \geq 1, \quad i = 1, \ldots, m$$

$$(w^*_{\text{hard}}, b^*_{\text{hard}}) = \arg\min_{w,b} \sum_{i=1}^{m} \boxed{\ell_{0-\infty}\left(y^{(i)}(w^T x^{(i)} + b) \geq 1\right)} + \boxed{\frac{1}{2}||w||^2}$$

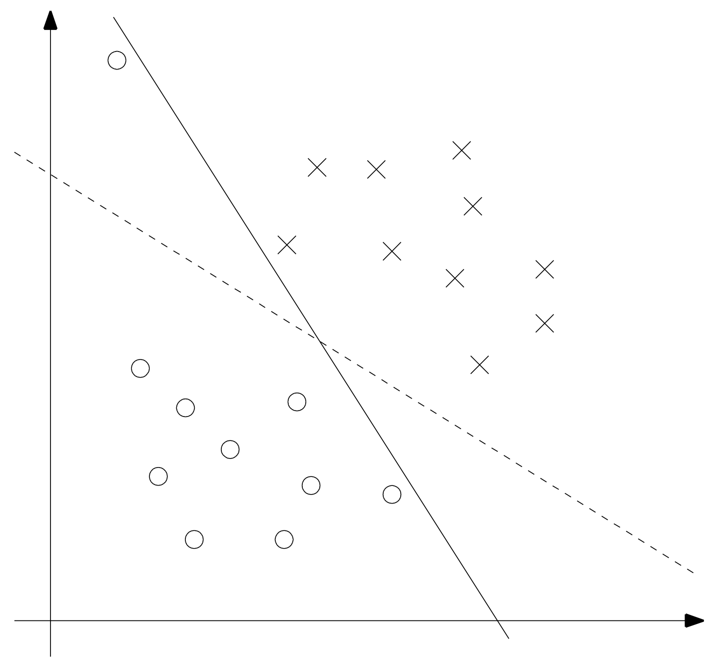
$$\ell_{0-\infty}\left(y^{(i)}(w^T x^{(i)} + b) \geq 1\right) = \begin{cases} 0, & \text{if } y^{(i)}(w^T x^{(i)} + b) \geq 1 \\ \infty, & \text{otherwise} \end{cases}$$

$$J(\theta) = L(\theta) + \lambda R(\theta)$$

From Hard SVM to Soft SVM

$$(w^*_{\text{hard}}, b^*_{\text{hard}}) = \arg\min_{w,b} \sum_{i=1}^{m} \ell_{0-\infty}\left(y^{(i)}(w^T x^{(i)} + b) \geq 1\right) + \frac{1}{2}||w||^2$$

- 仅能处理线性可分问题
- 实际情况下训练数据中可能存在“特异点”(outlier)，把这些点去掉后数据是线性可分的
- 或者是去掉这些数据后，能得到更大的margin

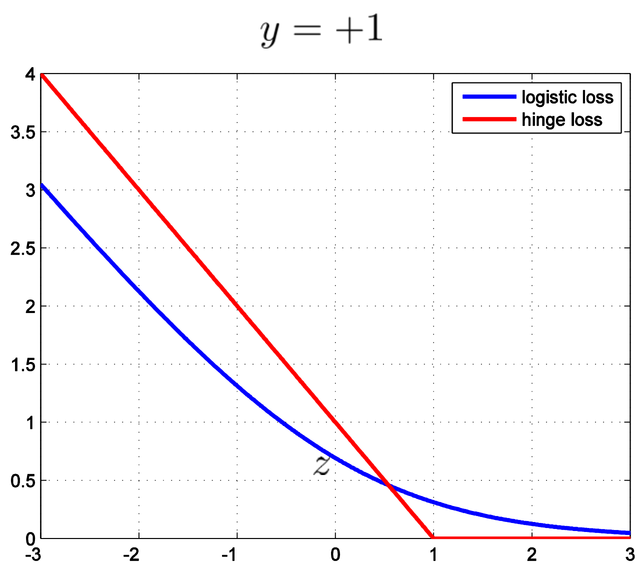


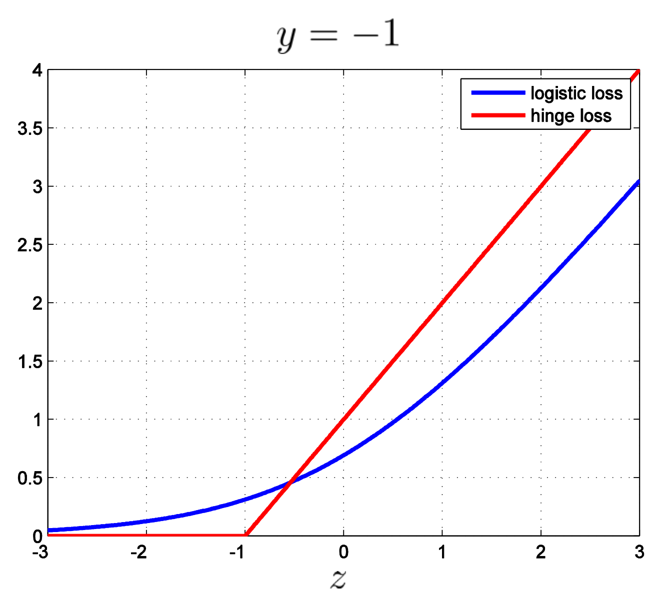
From Logistic Loss to Hinge Loss

$$z = \theta^T x = w^T x + b$$

$$\text{Logistic Loss: } \ell = \begin{cases} -\log(\frac{1}{1+e^{-z}}) = \log(1 + e^{-z}), & y = +1 \\ -\log(1 - \frac{1}{1+e^{-z}}) = \log(1 + e^{z}), & y = -1 \end{cases} \quad \Rightarrow \ell = \log(1 + e^{-yz})$$

$$\text{Hinge Loss: } \ell = \max(1 - yz, 0)$$





From Logistic Loss to Hinge Loss

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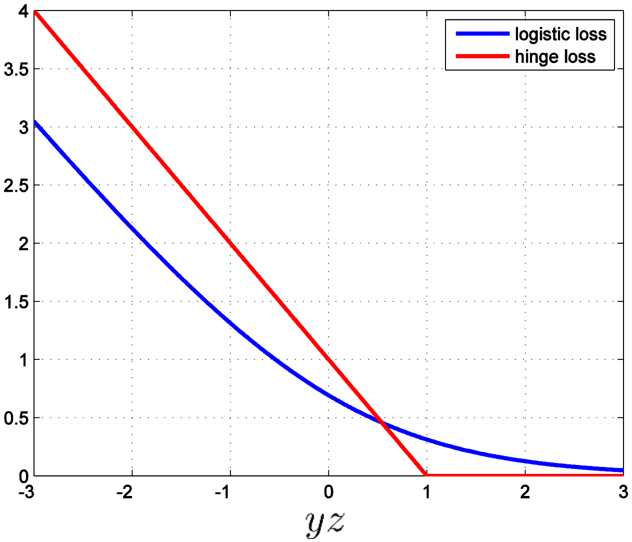
$$\Rightarrow \ell = \log(1+e^{-yz})$$

$$\text{Hinge Loss: } \ell = \max(1 - yz, 0)$$



The Primal Soft SVM problem

$$(w^*_{\text{hard}}, b^*_{\text{hard}}) = \arg\min_{w,b} \sum_{i=1}^{m} \ell_{0-\infty}\left(y^{(i)}(w^T x^{(i)} + b) \geq 1\right) + \frac{1}{2}||w||^2$$

换成hinge loss

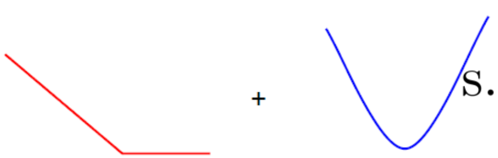
$$(w^*_{\text{soft}}, b^*_{\text{soft}}) = \arg\min_{w,b} C \sum_{i=1}^{m} \max\left(1 - y^{(i)}(w^T x^{(i)} + b), 0\right) + \frac{1}{2}||w||^2$$

$$\xi_i = \max\left(1 - y^{(i)}(w^T x^{(i)} + b), 0\right)$$ 松弛因子

等价于

$$(w^*_{\text{soft}}, b^*_{\text{soft}}) = \arg\min_{w,b,\xi} \quad \frac{1}{2}||w||^2 + C \sum_{i=1}^{m} \xi_i$$

C: 惩罚因子



s.t.

$$y^{(i)}(w^T x^{(i)} + b) \geq 1 - \xi_i, \quad i = 1, \ldots, m$$

$$\xi_i \geq 0, \quad i = 1, \ldots, m.$$

The Dual Soft SVM

$$(w^*_{\text{soft}}, b^*_{\text{soft}}) = \arg\min_{w,b,\xi} \quad \frac{1}{2}||w||^2 + C\sum_{i=1}^{m}\xi_i$$

$$\text{s.t.} \qquad y^{(i)}(w^T x^{(i)} + b) \geq 1 - \xi_i, \quad i = 1, \ldots, m$$

$$\xi_i \geq 0, \quad i = 1, \ldots, m.$$

$$\mathcal{L}(w, b, \xi, \alpha, r) = \frac{1}{2}w^T w + C\sum_{i=1}^{m}\xi_i - \sum_{i=1}^{m}\alpha_i\left[y^{(i)}(x^T w + b) - 1 + \xi_i\right] - \sum_{i=1}^{m} r_i\xi_i.$$

另$\mathcal{L}(w, b, \xi, \alpha, r)$对$w, b, \xi$的偏导数为零，有

$$w^* = \sum_{i=1}^{m}\alpha_i y^{(i)} x^{(i)}$$

$$\sum_{i=1}^{m}\alpha_i^* y^{(i)} = 0$$

$$C = \alpha_i + r_i$$

The Dual Soft SVM

$$(w^*_{\text{soft}}, b^*_{\text{soft}}) = \arg\min_{w,b,\xi} \quad \frac{1}{2}||w||^2 + C\sum_{i=1}^{m}\xi_i$$

思考：是否可以用梯度下降法求解？

Primal problem

$$\text{s.t.} \quad y^{(i)}(w^T x^{(i)} + b) \geq 1 - \xi_i, \quad i = 1, \ldots, m$$

$$\xi_i \geq 0, \quad i = 1, \ldots, m.$$

$$\max_\alpha \quad W(\alpha) = \sum_{i=1}^{m}\alpha_i - \frac{1}{2}\sum_{i,j=1}^{m} y^{(i)}y^{(j)}\alpha_i\alpha_j\langle x^{(i)}, x^{(j)}\rangle$$

Dual problem

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

$$\sum_{i=1}^{m}\alpha_i y^{(i)} = 0,$$

The Dual Soft SVM

$$\max_\alpha \quad W(\alpha) = \sum_{i=1}^{m} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{m} y^{(i)} y^{(j)} \alpha_i \alpha_j \langle x^{(i)}, x^{(j)} \rangle$$

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

$$\sum_{i=1}^{m} \alpha_i y^{(i)} = 0$$

The Dual Hard SVM

$$\max_\alpha \quad W(\alpha) = \sum_{i=1}^{m} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{m} y^{(i)} y^{(j)} \alpha_i \alpha_j \langle x^{(i)}, x^{(j)} \rangle$$

$$\text{s.t.} \quad 0 \leq \alpha_i \boxed{\leq C,} \quad i = 1, \ldots, m$$

$$\sum_{i=1}^{m} \alpha_i y^{(i)} = 0,$$

The Dual Soft SVM

思考:惩罚因子C趋近无穷大会发生什么情况?

The Dual Soft SVM

$$\max_\alpha \quad W(\alpha) = \sum_{i=1}^{m} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{m} y^{(i)} y^{(j)} \alpha_i \alpha_j \langle x^{(i)}, x^{(j)} \rangle$$

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

$$\sum_{i=1}^{m} \alpha_i y^{(i)} = 0,$$

KKT conditions:

$$\begin{cases} \alpha_i \geq 0, \ r_i \geq 0 \\ y^{(i)}(w^T x^{(i)} + b) - 1 + \xi_i \geq 0 \\ \alpha_i [y^{(i)}(w^T x^{(i)} + b) - 1 + \xi_i] = 0 \\ \xi_i \geq 0, \ r_i \xi_i = 0 \end{cases}$$

$$w^* = \sum_{i=1}^{m} \alpha_i y^{(i)} x^{(i)}$$

$$\sum_{i=1}^{m} \alpha_i^* y^{(i)} = 0$$

$$C = \alpha_i + r_i$$

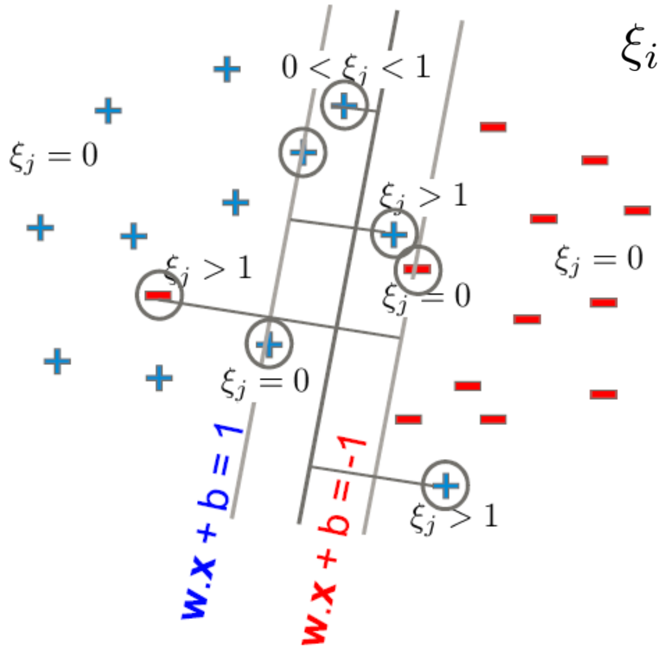
$$\begin{aligned} \alpha_i = 0 \quad &\Rightarrow \quad y^{(i)}(w^T x^{(i)} + b) - 1 + \xi_i \geq 0 \\ \alpha_i > 0 \quad &\Rightarrow \quad y^{(i)}(w^T x^{(i)} + b) - 1 + \xi_i = 0 \\ 0 < \alpha_i < C \quad &\Rightarrow \quad r_i > 0, \xi_i = 0 \\ \alpha_i = C \quad &\Rightarrow \quad r_i = 0 \end{aligned}$$

Support vectors in Soft SVM

$$(w^*_{\text{soft}}, b^*_{\text{soft}}) = \arg\min_{w,b,\xi} \quad \frac{1}{2}||w||^2 + C\sum_{i=1}^{m}\xi_i$$

$$\text{s.t.} \quad y^{(i)}(w^T x^{(i)} + b) \geq 1 - \xi_i, \quad i = 1, \ldots, m$$

$$\xi_i \geq 0, \quad i = 1, \ldots, m.$$



- Margin support vectors: $y^{(i)}(w^T x^{(i)} + b) \geq 1 - \xi_i$
- Nonmargin support vectors: $\xi_i > 0$

The Dual Soft SVM

$$
\begin{aligned}
\max_\alpha \quad & W(\alpha) = \sum_{i=1}^{m} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{m} y^{(i)} y^{(j)} \alpha_i \alpha_j \langle x^{(i)}, x^{(j)} \rangle \\
\text{s.t.} \quad & 0 \leq \alpha_i \leq C, \quad i = 1, \ldots, m \\
& \sum_{i=1}^{m} \alpha_i y^{(i)} = 0,
\end{aligned}
$$

- 这仍然是一个二次规划问题，可采用通用的QP算法求解，但其规模正比于训练样本数

- Sequential Minimal Optimization (SMO) algorithm是一种高效算法，基本思想是采用坐标下降法，在更新α_i时固定其他α_j, 由于$\sum_{i=1}^{m} \alpha_i y^{(i)} = 0$, α_i的值可由其他的 α_j $(j \neq i)$表示

Solving the Dual: The SMO Algorithm

$$\max_\alpha \quad W(\alpha) = \sum_{i=1}^{m} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{m} y^{(i)} y^{(j)} \alpha_i \alpha_j \langle x^{(i)}, x^{(j)} \rangle$$
$$\text{s.t.} \quad 0 \le \alpha_i \le C, \ \ i = 1, \dots, m$$
$$\sum_{i=1}^{m} \alpha_i y^{(i)} = 0,$$

具体而言，SMO算法不断执行下面两个基本步骤直到收敛：

- 选取一对需要更新的变量(假设为α_1和α_2),满足$\alpha_1 y^{(1)} + \alpha_2 y^{(2)} = -\sum_{i=3}^{m} \alpha_i y^{(i)}$;
- 固定$\alpha_3, \dots \alpha_m$, 则$-\sum_{i=3}^{m} \alpha_i y^{(i)} = \zeta$为一常量，求$W(\alpha)$的最优解等价于求一个带约束的二次函数优化问题

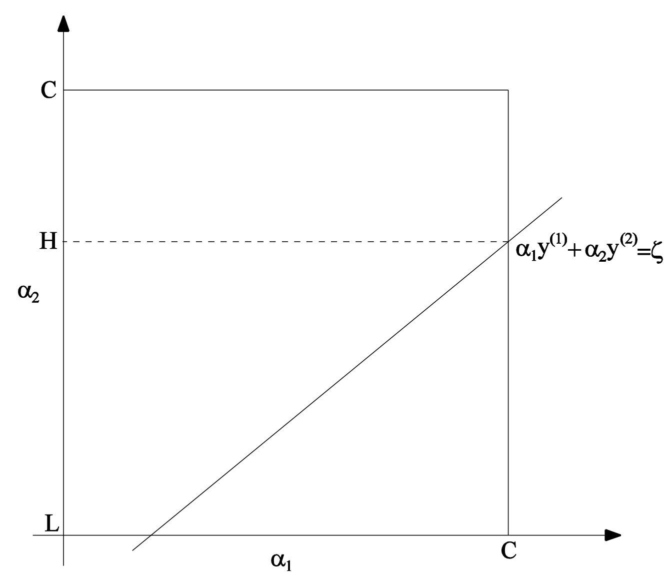
$$\alpha_1 y^{(1)} + \alpha_2 y^{(2)} = \zeta \Rightarrow \alpha_1 = (\zeta - \alpha_2 y^{(2)}) y^{(1)}$$

代入到目标函数中:

$W(\alpha_1, \alpha_2, \dots, \alpha_m) = W((\zeta - \alpha_2 y^{(2)}) y^{(1)}, \alpha_2, \dots, \alpha_m).$

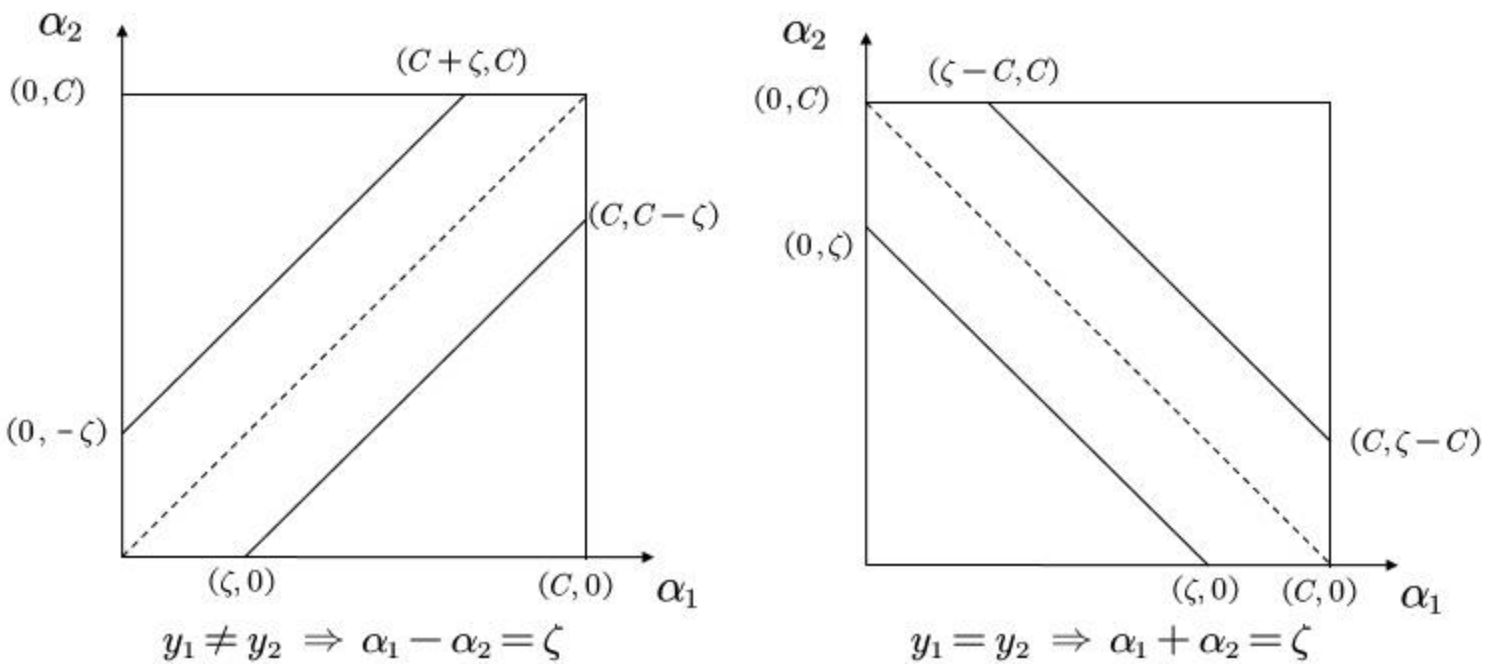
这是个关于α_2的二次函数: $a\alpha_2^2 + b\alpha_2 + c$

约束条件为 $L \le \alpha_2 \le H$, 这里$L = 0$.



Solving the Dual: The SMO Algorithm

$$\alpha_1 y_1 + \alpha_2 y_2 = \zeta \Rightarrow \alpha_1 = (\zeta - \alpha_2 y_2) y_1$$



https://zhuanlan.zhihu.com/p/32152421

The SMO Algorithm Implementation (optional)

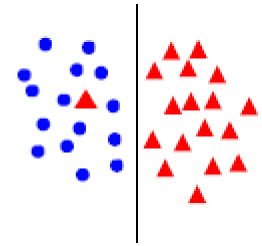
$$
\begin{aligned}
\max_\alpha \quad & W(\alpha)=\sum_{i=1}^{m}\alpha_i-\frac{1}{2}\sum_{i,j=1}^{m}y^{(i)}y^{(j)}\alpha_i\alpha_j\langle x^{(i)},x^{(j)}\rangle \\
\text{s.t.} \quad & \alpha_i\geq 0,\quad i=1,\ldots,m \\
& \sum_{i=1}^{m}\alpha_i y^{(i)}=0
\end{aligned}
$$

每次如何选择需要更新的α_i和α_j?

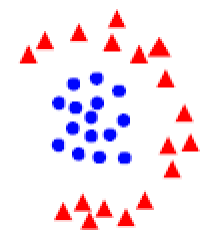
选取最不符合要求的两个参数:

- 选出违反 KKT 条件最严重的样本点、以其对应的参数作为第一个参数
- 选出与第一个参数对应的样本点间隔最大的样本对应的参数

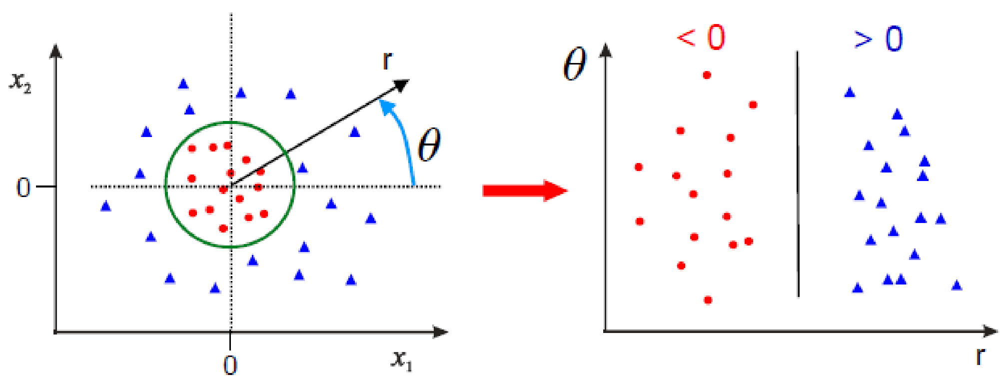
核 (Kernel)



- 通过引入松弛因子，Soft SVM能处理部分“特异点”outlier导致的线性不可分问题



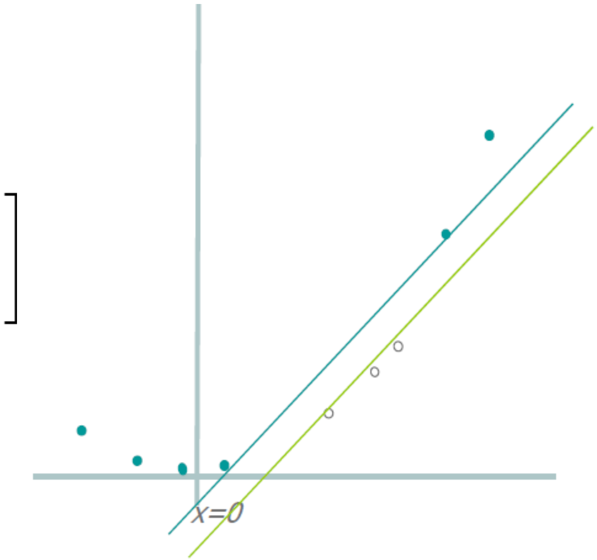
- 但如果数据本身是线性不可分的，如何处理？
  - 显式将数据变换到新的空间(如采用极坐标、多项式升维)，使其线性可分，如

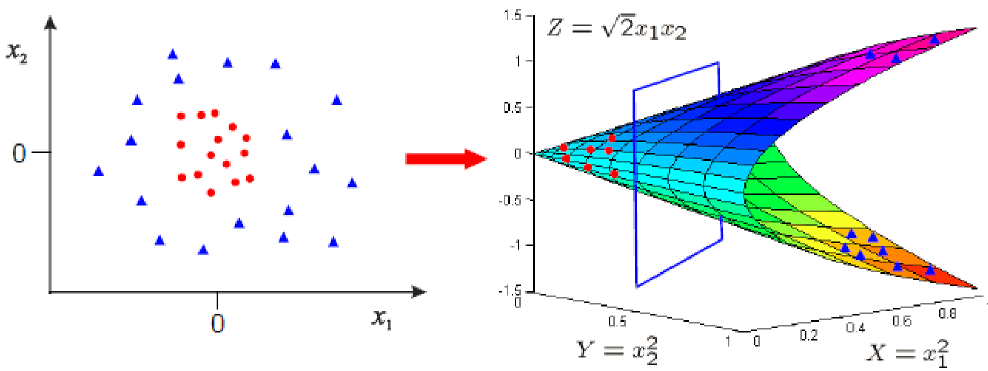


$$\phi : \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \rightarrow \begin{bmatrix} r \\ \theta \end{bmatrix}$$

核 (Kernel)

$$\phi(x) = \begin{bmatrix} x \\ x^2 \end{bmatrix}$$





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

核 (Kernel)

$$\text{映射为: } x \to \phi(x)$$

$$\text{对应的SVM分类准则为: } y = \text{sign}\left(\sum_{i=1}^{m} \alpha_i y^{(i)} \boxed{\langle \phi(x^{(i)}), \phi(x) \rangle} + b\right)$$

- 只有少数的$\alpha > 0$
- 只需要知道测试样本x与支持所有支持向量的内积，无需明确知道对应的映射

$$\text{可以直接定义核函数来计算内积: } k(x,z) = \langle \phi(x), \phi(z) \rangle = \phi(x)^T \phi(z)$$

$$\text{SVM分类准则: } y = \text{sign}\left(\sum_{i=1}^{m} \alpha_i y^{(i)} k(x^{(i)}, x) + b\right)$$

核 (Kernel)

如: $k(x,z) = (x^T z)^2$, 其中$x, z \in \mathbb{R}^n$

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

若$n = 3$, $\phi(x) = \begin{bmatrix} x_1x_1 \\ x_1x_2 \\ x_1x_3 \\ x_2x_1 \\ x_2x_2 \\ x_2x_3 \\ x_3x_1 \\ x_3x_2 \\ x_3x_3 \end{bmatrix}$

$O(n^2)$

核 (Kernel)

$$\begin{aligned} k(x,z) &= (x^T z + c)^2 \\ &= \sum_{i,j=1}^{n}(x_i x_j)(z_i z_j) + \sum_{i=1}^{n}(\sqrt{2c}x_i)(\sqrt{2c}z_i) + c^2 \end{aligned}$$

如$n = 3$,对应的映射为$\phi(x) = \begin{bmatrix} x_1x_1 \\ x_1x_2 \\ x_1x_3 \\ x_2x_1 \\ x_2x_2 \\ x_2x_3 \\ x_3x_1 \\ x_3x_2 \\ x_3x_3 \\ \sqrt{2c}x_1 \\ \sqrt{2c}x_2 \\ \sqrt{2c}x_3 \\ c \end{bmatrix}$

多项式核: $k(x,z) = (x^T z + c)^d$, 对应$\phi(x)$的维度$\approx n^d$

高斯核(RBF Kernel): $k(x,z) = \exp\left(-\frac{||x-z||^2}{2\sigma^2}\right)$,
对应$\phi(x)$的维度∞

RBF Kernel

高斯核(RBF Kernel)： $k(x,z) = \exp\left(-\frac{||x-z||^2}{2\sigma^2}\right)$，对应$\phi(x)$的维度 ∞，因为(这里省略σ)

$$
\begin{aligned}
k(x,z) &= \exp\left(-\frac{1}{2}||x-z||^2\right) = \phi(x)^T\phi(z)? \\
&= \exp\left(-\frac{1}{2}\left(||x||^2 + ||z||^2 - 2x^T z\right)\right) \\
&= \exp\left(-\frac{1}{2}||x||^2\right)\exp\left(-\frac{1}{2}||z||^2\right)\exp\left(x^T z\right) \\
&= C_x C_z \exp\left(x^T z\right) = C_x C_z \sum_{i=0}^{\infty} \frac{(x^T z)^i}{i!} \\
&= C_x C_z + C_x C_z (x^T z) + C_x C_z \frac{1}{2}(x^T z)^2 + \cdots
\end{aligned}
$$

Kernel Matrix and Mercer Kernel

假定存在某个核函数$K(\cdot,\cdot)$对应某个隐式映射$\phi(\cdot)$, 给定训练集$\{x^{(1)},\ldots,x^{(m)}\}$, 对应的核矩阵$K\in\mathbb{R}^{m\times m}$为对称矩阵, 其元素$K_{ij}=K(x^{(i)},x^{(j)})$

容易证明该矩阵是半正定的:

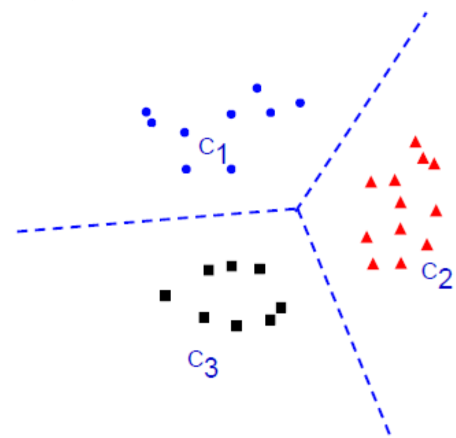
$$
\begin{aligned}
z^TKz &= \sum_i\sum_j z_iK_{ij}z_j \\
&= \sum_i\sum_j z_i\phi(x^{(i)})^T\phi(x^{(j)})z_j \\
&= \sum_i\sum_j z_i\sum_k \phi_k(x^{(i)})\phi_k(x^{(j)})z_j \\
&= \sum_k\sum_i\sum_j z_i\phi_k(x^{(i)})\phi_k(x^{(j)})z_j \\
&= \sum_k\left(\sum_i z_i\phi_k(x^{(i)})\right)^2 \\
&\geq 0.
\end{aligned}
$$

Mercer定理. 函数$K(\cdot,\cdot):\mathbb{R}^n\times\mathbb{R}^n\mapsto\mathbb{R}$为核函数的充要条件为：给定训练集$\{x^{(1)},\ldots,x^{(m)}\}$，对应的核矩阵$K\in\mathbb{R}^{m\times m}$为对称半正定矩阵.

Multi-Class SVM

- 将二分类器拓展处理多分类问题的基本思路：
  - 训练：采用one vs. rest策略训练K个分类器$h_{\theta^{(k)}}(x)$
  - 测试：选择分类器输出最大的值

$\max_k h_{\theta^{(k)}}(x)$



- 是否可以采用该策略拓展SVM?

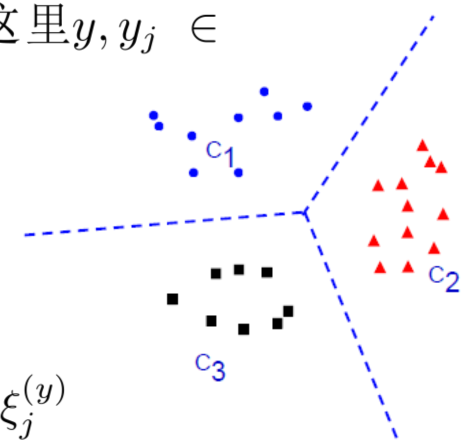
$$y = \arg\max_k \left({w^{(k)}}^T x + b^{(k)} \right)$$

But $(w^{(k)}, b^{(k)})$ may not be based on the same scale

Multi-Class SVM

- 采用类似Softmax的思想，同时学习K个参数$(w^{(k)}, b^{(k)})$，满足： $\max_k h_{\theta^{(k)}}(x)$
  ${w^{(y_j)}}^T x_j + b^{(y_j)} \geq {w^{(y)}}^T x_j + b^{(y)} + 1, \ \forall y \neq y_j, \ \forall j.$ 这里$y, y_j \in \{1, 2, \cdots, K\}$

- Margin: gap between correct class and nearest other class



$$
\begin{aligned}
(w^*_{\text{multiclass}}, b^*_{\text{multiclass}}) = \arg\min_{w,b,\xi} \quad & \frac{1}{2}\sum_{k=1}^{K} ||w^{(k)}||^2 + C\sum_{j=1}^{m}\sum_{y\neq y_j} \xi_j^{(y)} \\
\text{s.t.} \quad & {w^{(y_j)}}^T x_j + b^{(y_j)} \geq {w^{(y)}}^T x_j + b^{(y)} + 1, \ \forall y \neq y_j, \ \forall j \\
& \xi_j^{(y)} \geq 0, \ \forall y \neq y_j, \ \forall j.
\end{aligned}
$$

采用了joint optimization，保证各类的参数矢量 $(w^{(k)}, b^{(k)})$ have the same scale

SVM vs. Logistic Regression

	SVM	Logistic Regression
Loss function	Hinge Loss	Logistic Loss (Cross-Entropy Loss)
High dimensional features with kernels	Yes!	No (but there is kernel logistic regression too)
Solution sparse	Often yes!	Almost always no!
Semantics of output	“Margin”	“Real probabilities”

支持向量回归

- Soft SVM Classifier:

$$\min_{w,b} C\sum_{i=1}^{m} \max\left(1-y^{(i)}(w^T x^{(i)}+b),0\right)+\frac{1}{2}||w||^2$$

- 可以写成更一般的形式

$$\min_{w,b} C\sum_{i=1}^{m} \ell\left(y^{(i)},h_{w,b}(x^{(i)})\right)+\frac{1}{2}||w||^2$$

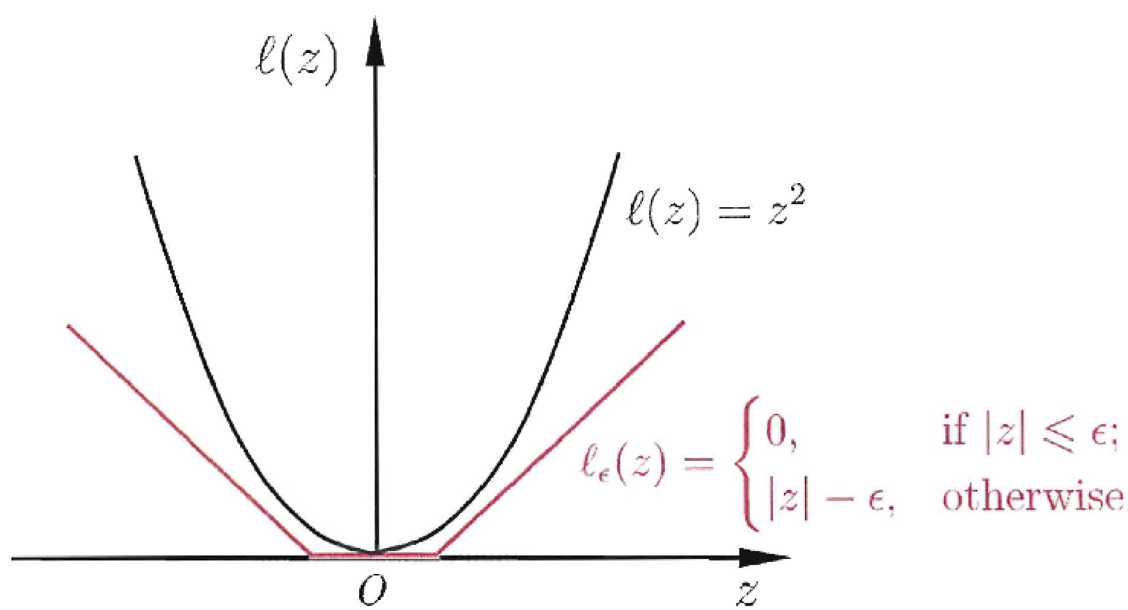
- 若$\ell(\cdot,\cdot)$为平方损失，则演变成Ridge regression，当且仅当$h(x)=y$时，损失才为零. SVR的基本思想是可以容忍一定的错误，即当预测的值$h(x)$和实际的值差别不大于ϵ时，损失仍为零，对应的损失函数为

$$\ell_\epsilon(z)=\begin{cases} 0, & \text{if } |z|\le\epsilon; \\ |z|-\epsilon, & \text{otherwise} \end{cases}$$

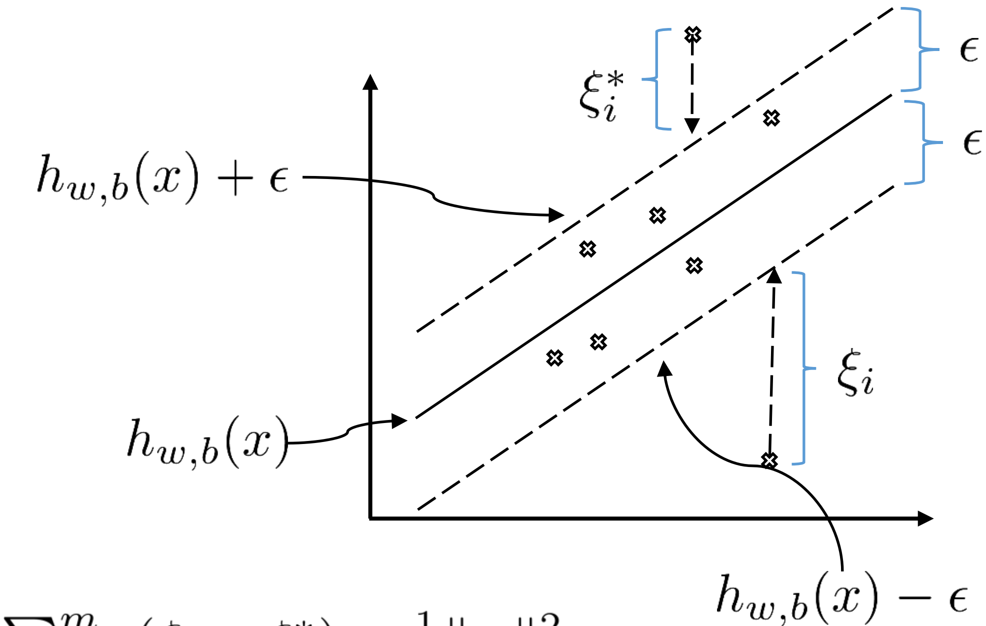
支持向量回归

$\epsilon-$不敏感损失函数$\ell_\epsilon(z)$

$$\ell_\epsilon(z) = \begin{cases} 0, & \text{if } |z| \leq \epsilon; \\ |z| - \epsilon, & \text{otherwise} \end{cases}$$



支持向量回归：线性回归



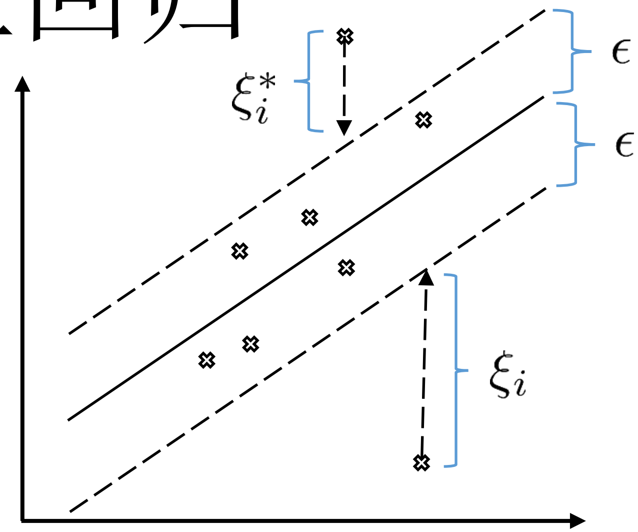
- 引入松弛因子ξ_i, ξ_i^*

$$
\begin{aligned}
\min_{w,b,\xi_i,\xi_i^*} \quad & C\sum_{i=1}^m(\xi_i+\xi_i^*)+\frac{1}{2}\|w\|^2 \\
\text{s.t.} \quad & h_{w,b}(x^{(i)})-y^{(i)} \le \epsilon+\xi_i, \\
& y^{(i)}-h_{w,b}(x^{(i)}) \le \epsilon+\xi_i^*, \\
& \xi_i \ge 0,\ \xi_i^* \ge 0,\ i=1,2,\cdots,m
\end{aligned}
$$

这里$h_{w,b}(x)=w^Tx+b=\langle w,x\rangle+b$

支持向量回归：线性回归

$$
\begin{aligned}
\min_{w,b,\xi_i,\xi_i^*} \quad & C\sum_{i=1}^{m}(\xi_i+\xi_i^*)+\frac{1}{2}\|w\|^2 \\
\text{s.t.} \quad & h_{w,b}(x^{(i)})-y^{(i)} \le \epsilon+\xi_i, \\
& y^{(i)}-h_{w,b}(x^{(i)}) \le \epsilon+\xi_i^*, \\
& \xi_i \ge 0,\ \xi_i^* \ge 0,\ i=1,2,\cdots,m
\end{aligned}
$$



- 再次引入拉格朗日乘子$r_i \ge 0, r_i^* \ge 0, \alpha_i \ge 0, \alpha_i^* \ge 0$, 对应的拉个朗日函数为

$$
L(w,b,\alpha,\alpha^*,\xi,\xi^*,r,r^*) = C\sum_{i=0}^{m}(\xi_i+\xi_i^*)+\frac{1}{2}\|w\|^2-\sum_{i=1}^{m} r_i\xi_i-\sum_{i=1}^{m} r_i^*\xi_i^*
$$
$$
+\sum_{i=1}^{m}\alpha_i(h_{w,b}(x^{(i)})-y^{(i)}-\epsilon-\xi_i)+\sum_{i=1}^{m}\alpha_i^*(y^{(i)}-h_{w,b}(x^{(i)})-\epsilon-\xi_i^*)
$$

- 令拉格朗日函数$L(w,b,\alpha,\alpha^*,\xi,\xi^*,r,r^*)$对$w,b,\xi,\xi^*$的偏导数为零有

$$
w=\sum_{i=1}^{m}(\alpha_i^*-\alpha_i)x^{(i)},\ 0=\sum_{i=1}^{m}(\alpha_i^*-\alpha_i),\ C=\alpha_i+r_i,\ C=\alpha_i^*+r_i^*
$$

支持向量回归：线性回归

- 将

$$w=\sum_{i=1}^{m}(\alpha_i^*-\alpha_i)x^{(i)},\ 0=\sum_{i=1}^{m}(\alpha_i^*-\alpha_i),\ C=\alpha_i+r_i,\ C=\alpha_i^*+r_i^*$$

代入到拉格朗日函数中化简得到只关于α_i,α_i^*的函数，最大化该函数可得SVR的对偶问题

$$\begin{aligned}\max_{\alpha,\alpha^*}\quad & \sum_{i=1}^{m}y^{(i)}(\alpha_i^*-\alpha_i)-\epsilon(\alpha_i^*+\alpha_i)-\frac{1}{2}\sum_{i,j=1}^{m}(\alpha_i^*-\alpha_i)(\alpha_j^*-\alpha_j)\langle x^{(i)},x^{(j)}\rangle\\ \text{s.t.}\quad & 0\le\alpha_i,\alpha_i^*\le C,\ \ i=1,\ldots,m\\ & \sum_{i=1}^{m}(\alpha_i^*-\alpha_i)=0.\end{aligned}$$

仍然属于典型的二次规划问题.

支持向量回归：线性回归

- KKT条件为

$$\begin{cases} \alpha_i(h_{w,b}(x^{(i)}) - y^{(i)} - \epsilon - \xi_i) = 0, \\ \alpha_i^*(y^{(i)} - h_{w,b}(x^{(i)}) - \epsilon - \xi_i^*) = 0, \\ (C - \alpha_i)\xi_i = 0,\ (C - \alpha_i^*)\xi_i^* = 0 \end{cases}$$

- 将$w = \sum_{i=1}^m (\alpha_i^* - \alpha_i) x^{(i)}$代入$h_{w,b}(x) = w^T x + b$ 有

$$h_{w,b}(x) = \sum_{i=1}^m (\alpha_i^* - \alpha_i)\langle x^{(i)}, x\rangle + b$$

- 如果$\left(x^{(i)}, y^{(i)}\right)$满足$|y^{(i)} - h_{w,b}(x^{(i)})| < \epsilon$，无需惩罚，即$\xi_i = 0, \xi_i^* = 0$，则$h_{w,b}(x^{(i)}) - y^{(i)} - \epsilon - \xi_i \neq 0$, $y^{(i)} - h_{w,b}(x^{(i)}) - \epsilon - \xi_i^* \neq 0$，根据KKT条件，必有$\alpha_i^* = 0, \alpha_i = 0$

- 当果$\left(x^{(i)}, y^{(i)}\right)$落在间隔带边界或者外时，方有$(\alpha_i^* - \alpha_i) \neq 0$，对应的样本为SVR的支持向量。

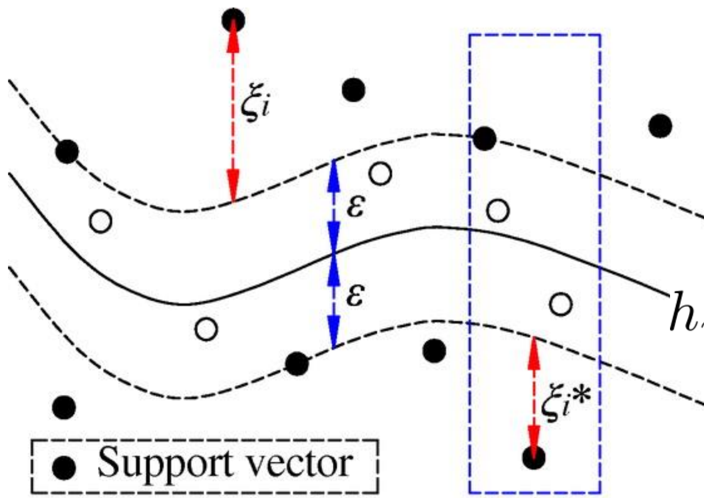
支持向量回归：线性回归

- 如何求b? 根据KKT条件, 对任意训练样本$(x^{(i)}, y^{(i)})$, 有$\alpha_i(h_{w,b}(x^{(i)}) - y^{(i)} - \epsilon - \xi_i) = 0$和$(C-\alpha_i)\xi_i = 0$，若满足$0 < \alpha_i < C$，则必有$\xi_i = 0$, 从而有

$$b = y^{(i)} + \epsilon - \sum_{i=1}^{m}(\alpha_i^* - \alpha_i)\langle x^{(i)}, x\rangle$$

- 理论上可以去任意满足$0 < \alpha_i < C$的样本进行计算，实际应用中取多个(或所有)满足条件的样本计算后取平均值。

支持向量回归：非线性回归



$$h_{w,b}(x) = \langle w, \phi(x) \rangle + b$$

$$h_{w,b}(x) = \sum_{i=1}^{m} (\alpha_i^* - \alpha_i) \langle x^{(i)}, x \rangle + b$$

变为

$$h_{w,b}(x) = \sum_{i=1}^{m} (\alpha_i^* - \alpha_i) \langle \phi(x^{(i)}), \phi(x) \rangle + b = \sum_{i=1}^{m} (\alpha_i^* - \alpha_i) k(x^{(i)}, x) + b$$

Thanks!

Any questions?