

参考文档

了解SVM

Logistic回归

给定一些数据点，它们分别属于两个不同的类，现在要找到一个线性分类器把这些数据分成两类。如果用 x 表示数据点，用 y 表示类别（ y 可以取1或者-1，分别代表两个不同的类，一个线性分类器的学习目标便是要在 n 维的数据空间中找到一个超平面（hyper plane），这个超平面的方程可以表示为

$$[1] w^T x + b = 0$$

Cost Function

<https://yoyoyohamapi.gitbooks.io/mit-ml/content/SVM/articles/代价函数.html>

[2]

$$\min_{\theta} \frac{1}{m} \left[\sum_{i=1}^n y^i (-\log h_{\theta}(x^i)) + (1 - y^i)(1 - \log(1 - h_{\theta}(x^i))) \right] + \frac{1}{2} \sum_{j=1}^n \theta_j^2$$

$$h_{\theta}(x) = \frac{1}{1 + \exp^{-\theta^T x}}$$

Large Margin Classifier

点到直线的距离

(x_0, y_0) 到 $Ax + By + C = 0$ 距离可用如下公式表示: $d = \frac{|Ax_0 + By_0 + C|}{\sqrt{A^2 + B^2}}$

then:

(x_0, y_0) 到 $w^T X + b = 0$ 距离可用如下公式表示: $d = \frac{|wx_0 + b|}{\sqrt{A^2 + B^2}}$

Margin

1. 为了预测精度足够高, $y=1$ 时, 希望 $\theta^T x \geq 1$, $y=0$ 时, 希望 $\theta^T x \leq -1$

2. margin线上的点 (x_0, y_0) 到直线 $w^T X + b = 0$ 的距离为 [3] $d = \frac{1}{||w||}$, 因为margin线为 $w^T x + b = 1$ 或 $w^T x + b = -1$
3. 将margin线加入y, 即 $y(w^T x + b) = -1$

问题求解变为

[4]

$$\max \frac{1}{||w||}$$

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

$$i = 1, \dots, n$$

深入SVM

从线性可分到线性不可分

由于求的最大值相当于求的最小值，所以上述目标函数等价于[5]

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

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

$$i = 1, \dots, n$$

最优解问题分类

1. 无约束问题优化，可通过求导
2. 有等式约束优化，可通过拉格朗日乘子法
3. 有不等式约束优化，可通过拉格朗日对偶性解决，满足KKT条件

拉格朗日对偶性

我们的问题符合第三类最优解问题:

$$\ell(w, b, \alpha) = \frac{1}{2} \|w\|^2 - \sum_{i=1}^n \alpha_i (y_i (w^T x_{(i)} + b) - 1)$$

令:

$$\psi(w) = \max_{\alpha_i \geq 0} \ell(w, b, \alpha)$$

\Rightarrow

$$\psi(w) = \min_{w, b} \max_{\alpha_i \geq 0} \ell(w, b, \alpha)$$

有兰格朗日对偶性:

$$P^* = \min_{w, b} \max_{\alpha_i \geq 0} \ell(w, b, \alpha)$$

$$D^* = \max_{\alpha_i \geq 0} \min_{w, b} \ell(w, b, \alpha)$$

$$D^* \leq P^*$$

在满足KKT条件，这两者相等，这个时候就可以通过求解对偶问题来间接地求解原始问题, KKT条件:

$$\text{optimize } f(x)$$

s.t.

$$g(x) \leq 0$$

$$h(x) \equiv 0$$

\Rightarrow

$$\ell(x, \alpha, \lambda) = f(x) + \alpha g(x) + \lambda h(x)$$

s.t.

$$\alpha_i \geq 0, g(x) \leq 0, \sum_{i=1}^n \alpha_i g(x_i) = 0, \lambda \neq 0$$

此问题可变为:

[6]

$$\ell(w, b, \alpha) = \frac{1}{2} \|w\|^2 + \sum_{i=1}^n \alpha_i (1 - y_i (w^T x_i + b))$$

$$\alpha_i \geq 0, g(x) = 1 - y_i (w^T x_i + b) \leq 0, \sum_{i=1}^n \alpha_i g(x_i) = 0$$

$\ell(w, b, \alpha)$ 有最大值, 因为 $\alpha_i \geq 0, g(x) \leq 0$, 分别对 w, b 求导:

$$\frac{\partial \ell}{\partial w} = 0 \Rightarrow w = \sum_{i=1}^n \alpha_i y_i x_i$$

$$\frac{\partial \ell}{\partial b} = 0 \Rightarrow \sum_{i=1}^n \alpha_i y_i = 0$$

带入方程, \Rightarrow

$$\ell(w, b, \alpha) = \frac{1}{2} \|w\|^2 + \sum_{i=1}^n \alpha_i (1 - y_i (w^T x_i + b))$$

$$\ell(w, b, \alpha) = \frac{1}{2} w^T w + \sum_{i=1}^n \alpha_i - \sum_{i=1}^n \alpha_i y_i w^T x_i - b \sum_{i=1}^n \alpha_i y_i$$

$$\ell(w, b, \alpha) = \frac{1}{2} w^T w + \sum_{i=1}^n \alpha_i - \sum_{i=1}^n \alpha_i y_i w^T x_i$$

$$\ell(w, b, \alpha) = \frac{1}{2} (\sum_{i=1}^n \alpha_i y_i x_i)^T (\sum_{i=1}^n \alpha_i y_i x_i) + \sum_{i=1}^n \alpha_i - \sum_{i=1}^n \alpha_i y_i (\sum_{j=1}^n \alpha_j y_j x_j)^T x_i$$

$$\ell(w, b, \alpha) = \frac{1}{2} \sum_{i=1, j=1}^n \alpha_i \alpha_j y_i y_j x_i^T x_j + \sum_{i=1}^n \alpha_i - \sum_{i=1, j=1}^n \alpha_i \alpha_j y_i y_j x_i^T x_j$$

$$\ell(w, b, \alpha) = \sum_{i=1}^n \alpha_i - \frac{1}{2} \sum_{i=1, j=1}^n \alpha_i \alpha_j y_i y_j x_i^T x_j$$

当 $\ell(w, b, \alpha)$ 取到极值时[7]:

$$\ell(w, b, \alpha) = \sum_{i=1}^n \alpha_i - \frac{1}{2} \sum_{i=1, j=1}^n \alpha_i \alpha_j y_i y_j x_i^T x_j = f(x)$$

核函数(mercer定理, 半正定)

分类:

1. 线性核函数 $K(x_i, x_j) = x_i^T x_j$
2. 多项式核函数 $K(x_i, x_j) = (\gamma_i^T x_j + b)$
3. 高斯核函数 $K(x_i, x_j) = \exp(-\gamma \|x_i - x_j\|^2)$

4. 拉格拉斯核函数

5. sigmod核函数

假设:

$$x = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$$

映射到

$$\phi = \begin{bmatrix} x_1 x_1 \\ x_1 x_2 \\ x_2 x_1 \\ x_2 x_2 \end{bmatrix}$$

\Rightarrow

$$K(\phi(m), \phi(n)) = \phi(m)^T \phi(n)$$

$$K(m, n) = m_1 m_1 n_1 n_1 + m_1 m_2 n_1 n_2 + m_2 m_1 n_2 n_1 + m_2 m_2 n_2 n_2$$

$$K(m, n) = m_1 m_1 n_1 n_1 + 2m_1 m_2 n_1 n_2 + m_2 m_2 n_2 n_2$$

$$K(m, n) = (m_1 n_1 + m_2 n_2)^2$$

$$K(m, n) = (m^T n)^2$$

SMO

取 α_1, α_2 作为参数

$$D^* = \max_{\alpha_i \geq 0} \min_{w, b} \ell(w, b, \alpha)$$

$$\ell(w, b, \alpha) = \sum_{i=1}^n \alpha_i - \frac{1}{2} \sum_{i=1, j=1}^n \alpha_i \alpha_j y_i y_j x_i^T x_j = f(x)$$

$$\ell(w, b, \alpha) = \alpha_1 + \alpha_2 + \sum_{i=3}^n \alpha_i - \frac{1}{2} [\alpha_1 y_1 \sum_{j=1}^n \alpha_j y_j (x_1^T x_j) + \alpha_2 y_2 \sum_{j=1}^n \alpha_j y_j (x_2^T x_j) + \sum_{i=3, j=1}^n \alpha_i \alpha_j y_i y_j (x_i^T x_j)] + \sum_{i=3}^n \alpha_i$$

$$\ell(w, b, \alpha) = \alpha_1 + \alpha_2 + \sum_{i=3}^n \alpha_i - \frac{1}{2} [\alpha_1 y_1 \alpha_1 y_1 (x_1^T x_1) + \alpha_1 y_1 \alpha_2 y_2 (x_1^T x_2) + \alpha_1 y_1 \sum_{j=3}^n \alpha_j y_j (x_1^T x_j) + \alpha_2 y_2 \alpha_1 y_1 (x_2^T x_1) + \alpha_2 y_2 \alpha_2 y_2 (x_2^T x_2) + \alpha_2 y_2 \sum_{j=3}^n \alpha_j y_j (x_2^T x_j) + \sum_{i=3, j=3}^n \alpha_i \alpha_j y_i y_j (x_i^T x_j)]$$

$$\ell(w, b, \alpha) = \alpha_1 + \alpha_2 - \frac{1}{2} [\alpha_1 y_1 \alpha_1 y_1 (x_1^T x_1) + \alpha_1 y_1 \alpha_2 y_2 (x_1^T x_2) + \alpha_1 y_1 \sum_{j=3}^n \alpha_j y_j (x_1^T x_j) + \alpha_2 y_2 \alpha_1 y_1 (x_2^T x_1) + \alpha_2 y_2 \alpha_2 y_2 (x_2^T x_2) + \alpha_2 y_2 \sum_{j=3}^n \alpha_j y_j (x_2^T x_j)] + C$$

$$\ell(w, b, \alpha) = \alpha_1 + \alpha_2 - \frac{1}{2}[\alpha_1^2 y_1^2 (x_1^T x_1) + \alpha_1 y_1 \alpha_2 y_2 (x_1^T x_2) + \alpha_1 y_1 \sum_{j=3}^n \alpha_j y_j (x_1^T x_j) + \alpha_2 y_2 \alpha_1 y_1 (x_2^T x_1) + \alpha_2^2 y_2^2 (x_2^T x_2) + \alpha_2 y_2 \sum_{j=3}^n \alpha_j y_j (x_2^T x_j)] + C$$

由于 $y \in \{-1, 1\}$, 所以 $y^2 = 1$, 由于线性核函数 $x_1^T x_2 = x_2^T x_1$

\Rightarrow

$$\ell(w, b, \alpha) = \alpha_1 + \alpha_2 - \frac{1}{2}[\alpha_1^2 (x_1^T x_1) + 2\alpha_1 y_1 \alpha_2 y_2 (x_1^T x_2) + \alpha_1 y_1 \sum_{j=3}^n \alpha_j y_j (x_1^T x_j) + \alpha_2^2 (x_2^T x_2) + \alpha_2 y_2 \sum_{j=3}^n \alpha_j y_j (x_2^T x_j)] + C$$

由 $\Rightarrow \sum_{i=1}^n \alpha_i y_i = 0$, 所以

$$\alpha_1 y_1 + \alpha_2 y_2 + \sum_{i=3}^n \alpha_i y_i = 0$$

\Rightarrow

$$\begin{aligned} \alpha_1 y_1 + \alpha_2 y_2 &= \zeta \\ \alpha_1^{old} y_1 + \alpha_2^{old} y_2 &= \alpha_1^{new} y_1 + \alpha_2^{new} y_2 = \zeta \end{aligned}$$

\Rightarrow

$$\alpha_1^{old} y_1 y_1 + \alpha_2^{old} y_2 y_1 = \zeta y_1$$

\Rightarrow

$$\alpha_1^{old} = \zeta y_1 - \alpha_2^{old} y_2 y_1$$

\Rightarrow

$$\alpha_1^{old} = \zeta' - s \alpha_2^{old}$$

\Rightarrow

$$\ell(w, b, \alpha) = \alpha_1 + \alpha_2 - \frac{1}{2}[\alpha_1^2 (x_1^T x_1) + 2\alpha_1 y_1 \alpha_2 y_2 (x_1^T x_2) + \alpha_1 y_1 \sum_{j=3}^n \alpha_j y_j (x_1^T x_j) + \alpha_2^2 (x_2^T x_2) + \alpha_2 y_2 \sum_{j=3}^n \alpha_j y_j (x_2^T x_j)] + C$$

\Rightarrow

$$\ell(w, b, \alpha) = (\zeta' - s \alpha_2) + \alpha_2 - \frac{1}{2}[(\zeta' - s \alpha_2)^2 (x_1^T x_1) + 2(\zeta' - s \alpha_2) y_1 \alpha_2 y_2 (x_1^T x_2) + (\zeta' - s \alpha_2) y_1 \sum_{j=3}^n \alpha_j y_j (x_1^T x_j) + \alpha_2^2 (x_2^T x_2) + \alpha_2 y_2 \sum_{j=3}^n \alpha_j y_j (x_2^T x_j)] + C$$

函数中变量只有 α_2 , 求取最大值, 需要对 α_2 求偏导数:

$$\frac{\partial \ell}{\partial \alpha_2} = 0$$

\Rightarrow

$$\alpha_2 = C'$$

\Rightarrow

$$\alpha_1 = \zeta' - s\alpha_2$$

\Rightarrow

$$\alpha_2^{new} = C''$$

\Rightarrow

$$\alpha_1^{new} = C'''$$