Sequential Minimal Optimization

SMO (Platt, 1998)

$\in \mathbb{R}^k$

Problem: Given sets $A^{\pm} = \{x_1^{\pm}, \ldots, x_{n_\pm}^{\pm}\}$, minimize

-2α

$\in C(A^+)$ $\in C(A^-)$

$$Q(\lambda^+, \lambda^-) = \| \sum_{i=1}^{n_+} \lambda_i^+ x_i^+ - \sum_{i=1}^{n_-} \lambda_i^- x_i^- \|^2 - \sum_{i=1}^{n_+} \lambda_i^+ - \sum_{i=1}^{n_-} \lambda_i^-$$

subject to the constraints $\lambda_i^{\pm} \geq 0$ for all i and

$$\sum_{i=1}^{n_+} \lambda_i^+ = \sum_{i=1}^{n_-} \lambda_i^- = \alpha. \quad = \alpha(\lambda^+, \lambda^-)$$

Strategy:

0. Start at a random point λ^+, λ^- satisfying the constraints.

1. Pick a pair λ_i^+ and λ_j^-.

2. Holding all other $\lambda^{\pm}$ constant, change λ_i^+ and λ_j^- by *the same amount* δ so that

$$\lambda_i^+ + \delta \geq 0 \text{ and } \lambda_j^- + \delta \geq 0$$

   and $Q(\lambda^+, \lambda^-)$ decreases when you replace λ_i^+ by $\lambda_i^+ + \delta$ and λ_j^- by $\lambda_j^- + \delta$. Note the constraints are still satisfied.

   $\alpha \mapsto \alpha + \delta$

3. Repeat this process until the $\lambda^{\pm}$ change by an amount less than some preset tolerance.

4. $p(\lambda^+) = \sum_{i=1}^{n_+} \lambda_i^+ x_i^+$ and $q(\lambda^-) = \sum_{i=1}^{n_-} \lambda_i^- x_i^-$ are the closest points.

SMO algorithm continued

Following this strategy, consider Q as a function of λ_i^+ and λ_j^-, with all other $\lambda^\pm$ treated as constants. Recall that

$$w(\lambda^+, \lambda^-) = \sum_{i=1}^{n_+} \lambda_i^+ x_i^+ - \sum_{i=1}^{n_-} \lambda^- x_i^-$$

and that

$$Q(\lambda^+, \lambda^-) = \|w(\lambda^+, \lambda^-)\|^2 - \sum_{i=1}^{n_+} \lambda^+ - \sum_{i=1}^{n_-} \lambda^- .$$

Changing $\lambda_i^+ \mapsto \lambda_i^+ + \delta$ and $\lambda_j^- \mapsto \lambda_j^- + \delta$ amounts to replacing $w(\lambda^+, \lambda^-)$ by

$$w_{\delta,i,j}(\lambda^+, \lambda^-) = w(\lambda^+, \lambda^-) + \boxed{\delta(x_i^+ - x_j^-).}$$

$$\sum \underset{\uparrow\ \lambda_i^+ + \delta}{\lambda_i^+} x_i^+ - \sum \underset{\uparrow\ \lambda_j^- + \delta}{\lambda_j^-} x_j^-$$

Also, $\alpha \mapsto \alpha + \delta$.

To make the change that makes Q get as much smaller as possible, we want to choose δ to minimize

$\lambda_i^+ + \delta \geq 0$

$$Q_{new}(\delta) = \|w_{\delta,i,j}(\lambda^+, \lambda^-)\|^2 - 2\alpha - 2\delta$$

$\lambda_j^- + \delta \geq 0$

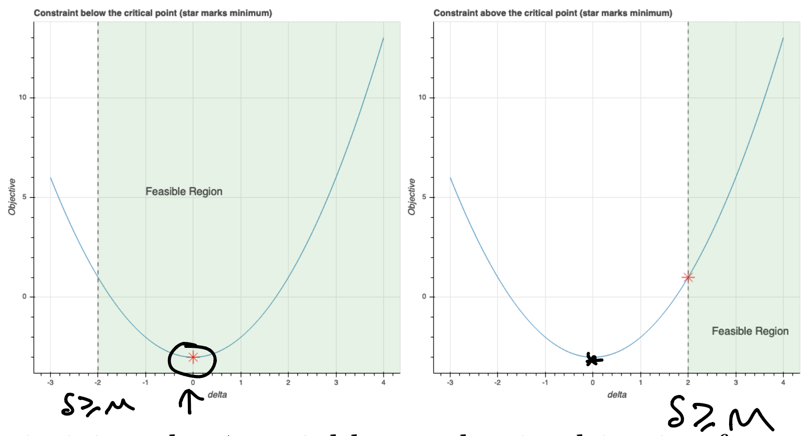
subject to the constraint that $\delta \geq \max\{-\lambda_i^+, -\lambda_j^-\}$.

$\delta \geq -\lambda_i^+$

$\delta \geq -\lambda_j^-$

This is a one variable minimization problem of a quadratic polynomial.

SMO continued



Minimizing the 1-variable quadratic objective function

Remember that $\delta \geq \overset{\max}{\cancel{\min}}\{-\lambda_i^+, -\lambda_j^-\}$.

$w_{\delta,i,j} = w + \delta(x_i^+ - x_j^-)$

$d/d\delta\, w_{\delta,i,j} = x_i^+ - x_j^-$

SMO continued.

To minimize Q_{new} we compute the derivative with respect to δ:

$Q_{new}(\delta)$

$$\frac{d}{d\delta}(\|w_{\delta,i,j}(\lambda^+,\lambda^-)\|^2 - \cancel{2\alpha} - 2\delta) = 2w_{\delta,i,j}(\lambda^+,\lambda^-)\cdot(x_i^+ - x_j^-) - 2.$$

Setting this equal to zero yields the formula

$$\delta_{i,j} = \frac{1 - w(\lambda^+,\lambda^-)\cdot(x_i^+ - x_j^-)}{\|x_i^+ - x_j^-\|^2}.$$

$$(w + \delta(x_i^+ - x_j^-))\cdot(x_i^+ - x_j^-) = 1$$

$$\delta_{i,j} = \frac{1 - w\cdot(x_i^+ - x_j^-)}{\|x_i^+ - x_j^-\|^2}$$

To reduce the size of Q_{new} as much as possible, while preserving the constraints:

- If $\delta_{i,j} \geq \max\{-\lambda_i^+, -\lambda_j^-\}$, then replace λ_i^+ and λ_j^- by $\lambda_i^+ + \delta_{i,j}$ and $\lambda_j^- + \delta_{i,j}$ respectively.
- Otherwise let $M = \max\{-\lambda_i^+, -\lambda_j^-\}$ and replace λ_i^+ and λ_j^- by $\lambda_i^+ + M$ and $\lambda_j^- + M$ respectively – so one of the λ's will become zero.

The SMO algorithm summarized.

Algorithm (SMO)

Given: Two linearly separable sets of points $A^+ = \{x_1^+, \ldots, x_{n_+}^+\}$ and $A^- = \{x_1^-, \ldots, x_{n_-}^-\}$ in $\mathbf{R}^k$.

Find: Points p and q belonging to $C(A^+)$ and $C(A^-)$ respectively such that

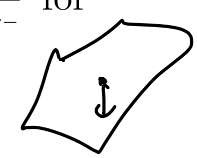
$$\|p - q\|^2 = \min_{p' \in C(A^+), q' \in C(A^-)} \|p' - q'\|^2$$

Initialization: Set $\lambda_i^+ = \frac{1}{n_+}$ for $i = 1, \ldots, n_+$ and $\lambda_i^- = \frac{1}{n_-}$ for $i = 1, \ldots, n_-$. Set

$\sum \lambda_i^+ = 1$

$$p(\lambda^+) = \sum_{i=1}^{n_+} \lambda_i^+ x_i^+$$

$\lambda_i^+ = \frac{1}{n_+}$

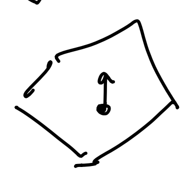


and

$\sum \lambda_i^- = 1$

$$q(\lambda^-) = \sum_{i=1}^{n_-} \lambda_i^- x_i^-$$

$\lambda_i^- = 1/n_-$



Notice that $w(\lambda^+, \lambda^-) = p(\lambda^+) - q(\lambda^-)$. Let $\alpha = \sum_{i=1}^{n_+} \lambda^+ = \sum_{i=1}^{n_-} \lambda^-$. These sums will remain equal to each other throughout the operation of the algorithm.

SMO continued

Iteration: Repeat the following steps until maximum value of δ^* computed in each iteration is smaller than some tolerance (so that the change in all of the λ's is very small):

- For each pair i, j with $1 \leq i \leq n_+$ and $1 \leq j \leq n_-$, compute

$$M_{i,j} = \max\{-\lambda_i^+, -\lambda_j^-\}$$

and

$$\delta_{i,j} = \frac{1 - (p(\lambda^+) - q(\lambda^-)) \cdot (x_i^+ - x_j^-)}{\|x_i^+ - x_j^-\|^2}.$$

If $\delta_{i,j} \geq M$ then set $\delta^* = \delta_{i,j}$; otherwise set $\delta^* = M$. Then update the $\lambda^\pm$ by the equations:

$$\begin{aligned} \lambda_i^+ &= \lambda_i^+ + \delta^* \\ \lambda_j^+ &= \lambda_j^- + \delta^* \end{aligned}$$

When this algorithm finishes, $p \approx p(\lambda^+)$ and $q \approx q(\lambda^-)$ will be very good approximations to the desired closest points.

SMO conclusion

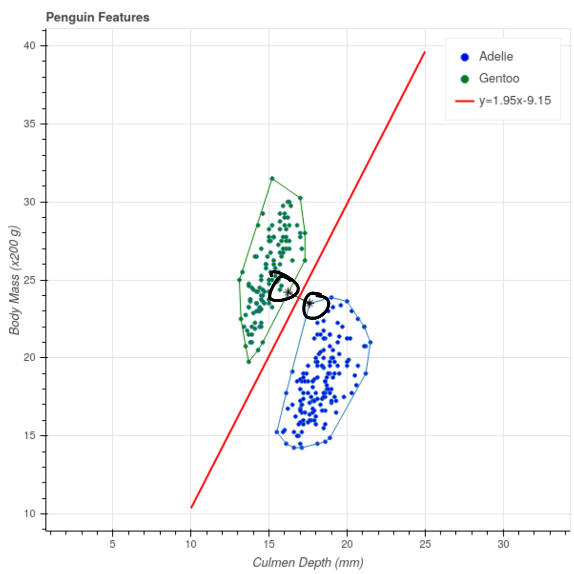
Recall that if we set $w = p - q$, then the optimal margin classifier is

$$f(x) = w \cdot x - \frac{B^+ + B^-}{2} = 0$$

$w = p - q$

where $B^+ = w \cdot p$ and $B^- = w \cdot q$. Since $w = p - q$ we can simplify this to obtain

$$f(x) = (p - q) \cdot x - \frac{\|p\|^2 - \|q\|^2}{2} = 0.$$



$y = 1.95x - 9.15$

Figure 1: Closest points in convex hulls of penguin data