Support Vector Machines

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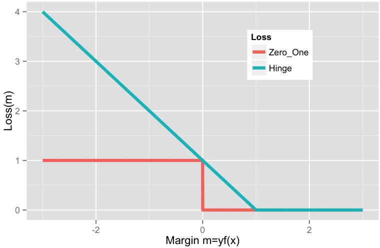
The SVM as a Quadratic Program

Support Vector Machine

- Hypothesis space $\mathcal{F} = \left\{ f(x) = w^T x + b \mid w \in \mathbf{R}^d, b \in \mathbf{R} \right\}$.
- ℓ_2 regularization (Tikhonov style)
- Loss $\ell(m) = (1-m)_+$
  - Margin $m = yf(x)$; "Positive part" $(x)_+ = x1(x \geqslant 0)$.



SVM Optimization Problem

The SVM prediction function is the solution to

$$\min_{w \in \mathbf{R}^d, b \in \mathbf{R}} \frac{1}{2}\|w\|^2 + \frac{c}{n}\sum_{i=1}^{n}\left(1 - y_i\left[w^T x_i + b\right]\right)_+ .$$

- unconstrained optimization
- not differentiable
- Can we reformulate into a differentiable problem?

SVM Optimization Problem

- The SVM optimization problem is equivalent to

$$\begin{array}{ll} \text{minimize} & \frac{1}{2}\|w\|^2 + \frac{c}{n}\sum_{i=1}^{n}\xi_i \\ \text{subject to} & \xi_i \geqslant \left(1 - y_i\left[w^Tx_i + b\right]\right)_+, \end{array}$$

- Which is equivalent to

$$\begin{array}{ll} \text{minimize} & \frac{1}{2}\|w\|^2 + \frac{c}{n}\sum_{i=1}^{n}\xi_i \\ \text{subject to} & \xi_i \geqslant 0 \text{ for } i = 1, \dots, n \\ & \xi_i \geqslant \left(1 - y_i\left[w^Tx_i + b\right]\right) \text{ for } i = 1, \dots, n \end{array}$$

SVM as a Quadratic Program

- The SVM optimization problem is equivalent to

$$
\begin{array}{ll}
\text{minimize} & \frac{1}{2}\|w\|^2 + \frac{c}{n}\sum_{i=1}^{n}\xi_i \\
\text{subject to} & -\xi_i \leqslant 0 \text{ for } i = 1, \ldots, n \\
& \left(1 - y_i\left[w^T x_i + b\right]\right) - \xi_i \leqslant 0 \text{ for } i = 1, \ldots, n
\end{array}
$$

- Differentiable objective function
- $n + d + 1$ unknowns and $2n$ affine constraints.
- A quadratic program that can be solved by any off-the-shelf QP solver.
- Let's learn more by examining the dual.

The SVM Dual Problem

SVM Lagrange Multipliers

$$
\begin{aligned}
\text{minimize} \quad & \frac{1}{2}\|w\|^2 + \frac{c}{n}\sum_{i=1}^{n}\xi_i \\
\text{subject to} \quad & -\xi_i \leqslant 0 \text{ for } i = 1,\ldots,n \\
& \left(1 - y_i\left[w^T x_i + b\right]\right) - \xi_i \leqslant 0 \text{ for } i = 1,\ldots,n
\end{aligned}
$$

Lagrange Multiplier	Constraint
λ_i	$-\xi_i \leqslant 0$
α_i	$\left(1 - y_i\left[w^T x_i + b\right]\right) - \xi_i \leqslant 0$

$$
\begin{aligned}
L(w,b,\xi,\alpha,\lambda) &= \frac{1}{2}\|w\|^2 + \frac{c}{n}\sum_{i=1}^{n}\xi_i \\
&\quad + \sum_{i=1}^{n}\alpha_i\left(1 - y_i\left[w^T x_i + b\right] - \xi_i\right) + \sum_{i=1}^{n}\lambda_i\left(-\xi_i\right)
\end{aligned}
$$

SVM Lagrangian

- The Lagrangian for this formulation is

$$\begin{aligned}
& L(w,b,\xi,\alpha,\lambda) \\
= \quad & \frac{1}{2}\|w\|^2 + \frac{c}{n}\sum_{i=1}^n \xi_i + \sum_{i=1}^n \alpha_i \left(1 - y_i \left[w^T x_i + b\right] - \xi_i\right) - \sum_i \lambda_i \xi_i \\
= \quad & \frac{1}{2} w^T w + \sum_{i=1}^n \xi_i \left(\frac{c}{n} - \alpha_i - \lambda_i\right) + \sum_{i=1}^n \alpha_i \left(1 - y_i \left[w^T x_i + b\right]\right).
\end{aligned}$$

- Primal and dual:

$$\begin{aligned}
p^* &= \inf_{w,\xi,b} \sup_{\alpha,\lambda \succeq 0} L(w,b,\xi,\alpha,\lambda) \\
&\geqslant \sup_{\alpha,\lambda \succeq 0} \inf_{w,b,\xi} L(w,b,\xi,\alpha,\lambda) = d^*
\end{aligned}$$

- Do we have $p^* = d^*$?

Strong Duality by Slater's constraint qualification

- The SVM optimization problem:

$$
\begin{aligned}
\text{minimize} \quad & \frac{1}{2}\|w\|^2 + \frac{c}{n}\sum_{i=1}^{n}\xi_i \\
\text{subject to} \quad & -\xi_i \leqslant 0 \text{ for } i = 1,\ldots,n \\
& \left(1 - y_i\left[w^T x_i + b\right]\right) - \xi_i \leqslant 0 \text{ for } i = 1,\ldots,n
\end{aligned}
$$

- Convex problem + affine constraints $\implies$ strong duality iff problem is feasible
- Constraints are satisfied by $w = b = 0$ and $\xi_i = 1$ for $i = 1,\ldots,n$,
  - so **we have strong duality** $\implies$

$$
\begin{aligned}
p^* &= \inf_{w,\xi,b}\ \sup_{\alpha,\lambda\succeq 0} L(w,b,\xi,\alpha,\lambda) \\
&= \sup_{\alpha,\lambda\succeq 0}\ \inf_{w,b,\xi} L(w,b,\xi,\alpha,\lambda) = d^*
\end{aligned}
$$

SVM Dual Function

- Lagrange dual is the inf over primal variables of the Lagrangian:

$$
\begin{aligned}
g(\alpha,\lambda) &= \inf_{w,b,\xi} L(w,b,\xi,\alpha,\lambda) \\
&= \inf_{w,b,\xi} \left[\frac{1}{2} w^T w + \sum_{i=1}^n \xi_i \left(\frac{c}{n} - \alpha_i - \lambda_i \right) + \sum_{i=1}^n \alpha_i \left(1 - y_i \left[w^T x_i + b \right] \right) \right]
\end{aligned}
$$

- Taking inf of convex and differentiable function of w, b, ξ.
    - Quadratic in w and linear in ξ and b.
- Thus optimal point iff $\partial_w L = 0$ $\partial_b L = 0$ $\partial_\xi L = 0$
- Note: $g(\alpha,\lambda) = -\infty$ when $\frac{c}{n} - \alpha_i - \lambda_i \neq 0$. (send $\xi_i \to \pm\infty$)

SVM Dual Function: First Order Conditions

- Lagrange dual function is the inf over primal variables of L:

$$
\begin{aligned}
g(\alpha,\lambda) &= \inf_{w,b,\xi} L(w,b,\xi,\alpha,\lambda) \\
&= \inf_{w,b,\xi}\left[\frac{1}{2}w^Tw+\sum_{i=1}^n \xi_i\left(\frac{c}{n}-\alpha_i-\lambda_i\right)+\sum_{i=1}^n \alpha_i\left(1-y_i\left[w^Tx_i+b\right]\right)\right]
\end{aligned}
$$

$$\partial_w L = 0 \iff w-\sum_{i=1}^n \alpha_i y_i x_i = 0 \iff \boxed{w=\sum_{i=1}^n \alpha_i y_i x_i}$$

$$\partial_b L = 0 \iff -\sum_{i=1}^n \alpha_i y_i = 0 \iff \boxed{\sum_{i=1}^n \alpha_i y_i = 0}$$

$$\partial_{\xi_i} L = 0 \iff \frac{c}{n}-\alpha_i-\lambda_i = 0 \iff \boxed{\alpha_i+\lambda_i=\frac{c}{n}}$$

SVM Dual Function

- Substituting these conditions back into L, the second term disappears.
- First and third terms become

$$
\begin{aligned}
\frac{1}{2}w^T w &= \frac{1}{2}\sum_{i,j=1}^{n}\alpha_i\alpha_j y_i y_j x_i^T x_j \\
\sum_{i=1}^{n}\alpha_i(1-y_i\left[w^T x_i+b\right]) &= \sum_{i=1}^{n}\alpha_i-\sum_{i,j=1}^{n}\alpha_i\alpha_j y_i y_j x_j^T x_i-b\underbrace{\sum_{i=1}^{n}\alpha_i y_i}_{=0}.
\end{aligned}
$$

- Putting it together, the dual function is

$$
g(\alpha,\lambda)=\begin{cases}\sum_{i=1}^{n}\alpha_i-\frac{1}{2}\sum_{i,j=1}^{n}\alpha_i\alpha_j y_i y_j x_j^T x_i & \begin{array}{c}\sum_{i=1}^{n}\alpha_i y_i=0\\ \alpha_i+\lambda_i=\frac{c}{n},\text{ all } i\end{array}\\ -\infty & \text{otherwise.}\end{cases}
$$

SVM Dual Problem

- The **dual function** is

$$g(\alpha,\lambda) = \begin{cases} \sum_{i=1}^n \alpha_i - \frac{1}{2}\sum_{i,j=1}^n \alpha_i\alpha_j y_i y_j x_j^T x_i & \sum_{i=1}^n \alpha_i y_i = 0 \\ & \alpha_i + \lambda_i = \frac{c}{n}, \text{ all } i \\ -\infty & \text{otherwise.} \end{cases}$$

- The **dual problem** is $\sup_{\alpha,\lambda \succeq 0} g(\alpha,\lambda)$:

$$\begin{aligned} \sup_{\alpha,\lambda} \quad & \sum_{i=1}^n \alpha_i - \frac{1}{2}\sum_{i,j=1}^n \alpha_i\alpha_j y_i y_j x_j^T x_i \\ \text{s.t.} \quad & \sum_{i=1}^n \alpha_i y_i = 0 \\ & \alpha_i + \lambda_i = \frac{c}{n} \quad \alpha_i, \lambda_i \geqslant 0, \; i = 1, \ldots, n \end{aligned}$$

SVM Dual Problem: Eliminating a Variable

- Can eliminate the λ variables:

$$\begin{aligned} \sup_{\alpha} \quad & \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{n} \alpha_i \alpha_j y_i y_j x_j^T x_i \\ \text{s.t.} \quad & \sum_{i=1}^{n} \alpha_i y_i = 0 \\ & \alpha_i \in \left[0, \frac{c}{n}\right] \; i = 1, \ldots, n. \end{aligned}$$

- Quadratic objective in n unknowns and $2n$ constraints
- Efficient minimization algorithm: SMO (sequential minimal optimization)
- Now let's see what we can learn from dual formulation...

The Form of the Primal Solution (w^*)

The Form of w^*

- Recall

$$\partial_w L = 0 \iff w = \sum_{i=1}^{n} \alpha_i y_i x_i$$

- If α^* is a solution to the dual problem, then primal solution is

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

- We now now the form of w^*: **a linear combination of x_i's.**
- Recall $\alpha_i^* \in [0, \frac{c}{n}]$. So c controls max weight on each example. (**Robustness**!)
- What's b^*? We'll come back to that.

Support Vectors

- If α^* is a solution to the dual problem, then primal solution is

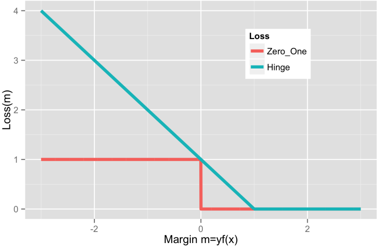
$$w^* = \sum_{i=1}^{n} \alpha_i^* y_i x_i$$

  with $\alpha_i^* \in [0, \frac{c}{n}]$.
- We'll soon show that we often have $\alpha_i^* = 0$.
- The x_i's corresponding to $\alpha_i^* > 0$ are called **support vectors.**
- This can give a **sparsity in input examples**.
    - This becomes more relevant after "kernelization", next week.

The Margin and Support Vectors

The Margin and Some Terminology

- For notational convenience, define $f^*(x) = x_i^T w^* + b^*$.
- Margin $yf^*(x)$



- Incorrect classification: $yf^*(x) \leqslant 0$.
- Margin error: $yf^*(x) < 1$.
- "On the margin": $yf^*(x) = 1$.
- "Good side of the margin": $yf^*(x) > 1$.

Support Vectors and The Margin

- Recall $\xi_i^* = (1 - y_i f^*(x_i))_+$ the hinge loss on (x_i, y_i).
- Suppose $\xi_i^* = 0$.
- Then $y_i f^*(x_i) \geqslant 1$
    - "on the margin" $(=1)$, or
    - "on the good side" (>1)

Complementary Slackness Consequences

- For our SVM primal, the complementary slackness conditions are:

$$\alpha_i^*\left(1 - y_i f^*(x_i) - \xi_i^*\right) = 0$$
$$\lambda_i^* \xi_i^* = \left(\frac{c}{n} - \alpha_i^*\right)\xi_i^* = 0$$

- If $y_i f^*(x) > 1$ then the margin loss is $\xi_i^* = 0$, and we get $\alpha_i^* = 0$.
- If $y_i f^*(x_i) < 1$ then the margin loss is $\xi_i^* > 0$, so $\alpha_i^* = \frac{c}{n}$.
- If $\alpha_i^* = 0$, then $\xi_i^* = 0$, which implies no loss, so $y_i f^*(x) \geqslant 1$.
- If $\alpha_i^* \in \left(0, \frac{c}{n}\right)$, then $\xi_i^* = 0$, which implies $1 - y_i f^*(x_i) = 0$.

Complementary Slackness Results: Summary

$$
\begin{aligned}
\alpha_i^* = 0 \quad &\implies \quad y_i f^*(x_i) \geqslant 1 \\
\alpha_i^* \in \left(0, \frac{c}{n}\right) \quad &\implies \quad y_i f^*(x_i) = 1 \\
\alpha_i^* = \frac{c}{n} \quad &\implies \quad y_i f^*(x_i) \leqslant 1
\end{aligned}
$$

$$
\begin{aligned}
y_i f^*(x_i) < 1 \quad &\implies \quad \alpha_i^* = \frac{c}{n} \\
y_i f^*(x_i) = 1 \quad &\implies \quad \alpha_i^* \in \left[0, \frac{c}{n}\right] \\
y_i f^*(x_i) > 1 \quad &\implies \quad \alpha_i^* = 0
\end{aligned}
$$

Complementary Slackness To Get b^*

Complementary Slackness

- By strong duality, we have the following **complementary slackness** condition:
  - Lagrange multiplier is zero unless the [primal] constraint is active at the optimum: "$\lambda_i^* f_i(x^*) = 0$"
- Our primal constraints:

$$
\begin{aligned}
(\alpha_i) &\qquad \left(1 - y_i\left[x_i^T w + b\right]\right) - \xi_i \leqslant 0 \text{ for } i = 1, \ldots, n \\
(\lambda_i) &\qquad -\xi_i \leqslant 0 \text{ for } i = 1, \ldots, n
\end{aligned}
$$

- Complementary slackness is about **optimal** primal and dual variables
  - Let $\left(w^*, b^*, \xi_i^*\right)$ be primal optimal
  - Let(α^*, λ^*) be dual optimal

The Bias Term: b

- For our SVM primal, the complementary slackness conditions are:

$$\alpha_i^* \left(1 - y_i \left[x_i^T w^* + b\right] - \xi_i^*\right) = 0 \quad (1)$$

$$\lambda_i^* \xi_i^* = \left(\frac{c}{n} - \alpha_i^*\right) \xi_i^* = 0 \quad (2)$$

- Suppose there's an i such that $\alpha_i^* \in \left(0, \frac{c}{n}\right)$.
- (2) implies $\xi_i^* = 0$.
- (1) implies

$$\begin{aligned} & y_i \left[x_i^T w^* + b^*\right] = 1 \\ \iff \quad & x_i^T w^* + b^* = y_i \text{ (use } y_i \in \{-1, 1\}) \\ \iff \quad & \boxed{b^* = y_i - x_i^T w^*} \end{aligned}$$

The Bias Term: b

- The optimal b is

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

- We get the same b^* for any choice of i with $\alpha_i^* \in \left(0, \frac{c}{n}\right)$
  - **With exact calculations!**
- With numerical error, more robust to average over all eligible i's:

$$b^* = \text{mean}\left\{ y_i - x_i^T w^* \mid \alpha_i^* \in \left(0, \frac{c}{n}\right) \right\}.$$

- If there are no $\alpha_i^* \in \left(0, \frac{c}{n}\right)$?
  - Then we have a **degenerate SVM training problem**[1] ($w^* = 0$).

[1] See Rifkin et al.'s "A Note on Support Vector Machine Degeneracy", an MIT AI Lab Technical Report.

Kernelization?

Dual Problem: Dependence on x through inner products

- SVM Dual Problem:

$$
\begin{aligned}
\sup_{\alpha} \quad & \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{n} \alpha_i \alpha_j y_i y_j x_j^T x_i \\
\text{s.t.} \quad & \sum_{i=1}^{n} \alpha_i y_i = 0 \\
& \alpha_i \in \left[0, \frac{c}{n}\right] \quad i = 1, \ldots, n.
\end{aligned}
$$