Support Vector Machines

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February 13, 2018

Contents

- The SVM as a Quadratic Program
- The SVM Dual Problem
- Insights From Complementary Slackness: Margin and Support Vectors
- Complementary Slackness To Get b*
- Teaser for Kernelization

The SVM as a Quadratic Program

The Margin

Definition

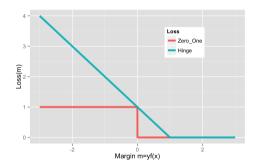
The margin (or functional margin) for predicted score \hat{y} and true class $y \in \{-1, 1\}$ is $y\hat{y}$.

- The margin often looks like yf(x), where f(x) is our score function.
- The margin is a measure of how correct we are.
- We want to maximize the margin.
- Most classification losses depend only on the margin.

(This is distinct from but related to geometric margin.)

Hinge Loss

- SVM/Hinge loss: $\ell_{\text{Hinge}} = \max\{1-m, 0\} = (1-m)_{+}$
- Margin m = yf(x); "Positive part" $(x)_+ = x1(x \ge 0)$.



Hinge is a **convex**, **upper bound** on 0-1 loss. Not differentiable at m=1. We have a "margin error" when m<1.

Support Vector Machine

- Hypothesis space $\mathcal{F} = \{ f(x) = w^T x + b \mid w \in \mathbb{R}^d, b \in \mathbb{R} \}.$
- ℓ_2 regularization (Tikhonov style)
- Loss $\ell(m) = \max\{1-m, 0\} = (1-m)_+$
- The SVM prediction function is the solution to

$$\min_{w \in \mathbf{R}^{d}, b \in \mathbf{R}} \frac{1}{2} ||w||^{2} + \frac{c}{n} \sum_{i=1}^{n} \max (0, 1 - y_{i} [w^{T} x_{i} + b]).$$

SVM Optimization Problem (Tikhonov Version)

The SVM prediction function is the solution to

$$\min_{w \in \mathbf{R}^d, b \in \mathbf{R}} \frac{1}{2} ||w||^2 + \frac{c}{n} \sum_{i=1}^n \max (0, 1 - y_i [w^T x_i + b]).$$

- unconstrained optimization
- not differentiable because of the max (right at the border of a margin error)
- Can we reformulate into a differentiable problem?

SVM Optimization Problem

The SVM optimization problem is equivalent to

minimize
$$\frac{1}{2}||w||^2 + \frac{c}{n}\sum_{i=1}^n \xi_i$$

subject to
$$\xi_i \geqslant \max(0, 1 - y_i [w^T x_i + b]).$$

Which is equivalent to

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

SVM as a Quadratic Program

The SVM optimization problem is equivalent to

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

- 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

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

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

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

SVM Lagrangian

• The Lagrangian for this formulation is

$$L(w, b, \xi, \alpha, \lambda) = \frac{1}{2} ||w||^{2} + \frac{c}{n} \sum_{i=1}^{n} \xi_{i} + \sum_{i=1}^{n} \alpha_{i} \left(1 - y_{i} \left[w^{T} x_{i} + b\right] - \xi_{i}\right) - \sum_{i} \lambda_{i} \xi_{i}$$

$$= \frac{1}{2} w^{T} w + \sum_{i=1}^{n} \xi_{i} \left(\frac{c}{n} - \alpha_{i} - \lambda_{i}\right) + \sum_{i=1}^{n} \alpha_{i} \left(1 - y_{i} \left[w^{T} x_{i} + b\right]\right).$$

Primal and dual:

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

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

• Do we have $p^* = d^*$?

Strong Duality by Slater's constraint qualification

• The SVM optimization problem:

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

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

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

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

SVM Dual Function

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

$$g(\alpha, \lambda) = \inf_{w, b, \xi} L(w, b, \xi, \alpha, \lambda)$$

$$= \inf_{w, b, \xi} \left[\frac{1}{2} w^{T} w + \sum_{i=1}^{n} \xi_{i} \left(\frac{c}{n} - \alpha_{i} - \lambda_{i} \right) + \sum_{i=1}^{n} \alpha_{i} \left(1 - y_{i} \left[w^{T} x_{i} + b \right] \right) \right]$$

- 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 $\xi_i \to \pm \infty$). This inf is NOT an optimum because it is never attained.

SVM Dual Function: First Order Conditions

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

$$g(\alpha, \lambda) = \inf_{w,b,\xi} L(w, b, \xi, \alpha, \lambda)$$

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

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

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

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

SVM Dual Function

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

$$\frac{1}{2} w^T w = \frac{1}{2} \sum_{i,j=1}^n \alpha_i \alpha_j y_i y_j x_i^T x_j$$

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

Putting it together, the dual function is

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

SVM Dual Problem

The dual function is

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

• The dual problem is $\sup_{\alpha,\lambda \succ 0} g(\alpha,\lambda)$:

$$\sup_{\alpha,\lambda} \qquad \sum_{i=1}^{n} \alpha_{i} - \frac{1}{2} \sum_{i,j=1}^{n} \alpha_{i} \alpha_{j} y_{i} y_{j} x_{j}^{T} x_{i}$$
s.t.
$$\sum_{i=1}^{n} \alpha_{i} y_{i} = 0$$

$$\alpha_{i} + \lambda_{i} = \frac{c}{n} \quad \alpha_{i}, \lambda_{i} \geqslant 0, \ i = 1, \dots, n$$

SVM Dual Problem: Eliminating a Variable

Can eliminate the λ variables:

$$\sup_{\alpha} \sum_{i=1}^{n} \alpha_{i} - \frac{1}{2} \sum_{i,j=1}^{n} \alpha_{i} \alpha_{j} y_{i} y_{j} x_{j}^{T} x_{i}$$
s.t.
$$\sum_{i=1}^{n} \alpha_{i} y_{i} = 0$$

$$\alpha_{i} \in \left[0, \frac{c}{n}\right] \ i = 1, \dots, n.$$

- Given solution α^* to dual, primal solution is $w^* = \sum_{i=1}^n \alpha_i^* y_i x_i$.
- w^* is "in the span of the data" i.e. a linear combination of x_1, \ldots, x_n .
- Note $\alpha_i^* \in [0, \frac{c}{n}]$. So c controls max weight on each example.

SVM Dual Problem

$$\sup_{\alpha} \sum_{i=1}^{n} \alpha_{i} - \frac{1}{2} \sum_{i,j=1}^{n} \alpha_{i} \alpha_{j} y_{i} y_{j} x_{j}^{T} x_{i}$$
s.t.
$$\sum_{i=1}^{n} \alpha_{i} y_{i} = 0$$

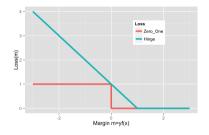
$$\alpha_{i} \in \left[0, \frac{c}{n}\right] \quad i = 1, \dots, n.$$

- Quadratic objective in n unknowns and n+1 constraints
- Efficient minimization algorithm: SMO (sequential minimal optimization)
- What other insights can we get from the dual formulation?

Insights From Complementary Slackness: Margin and Support Vectors

The Margin and Some Terminology

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



- Incorrect classification: $yf^*(x) \leq 0$.
- 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 "slack variable" $\xi_i^* = \max(0, 1 y_i f^*(x_i))$ is 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
 - \bullet "on the good side" (> 1)

Complementary Slackness Conditions

• Recall our primal constraints and Lagrange multipliers:

Lagrange Multiplier	Constraint
λ_i	$-\xi_i \leqslant 0$
α_i	$(1-y_if(x_i))-\xi_i\leqslant 0$

- Recall first order condition $\nabla_{\xi_i} L = 0$ gave us $\lambda_i^* = \frac{c}{n} \alpha_i^*$.
- By strong duality, we must have complementary slackness:

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

Consequences of Complementary Slackness

• By strong duality, we must have **complementary slackness**:

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

- If $y_i f^*(x_i) > 1$ 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 $y_i f^*(x) \ge 1$.
- If $\alpha_i^* \in (0, \frac{c}{n})$, then $\xi_i^* = 0$, which implies $1 y_i f^*(x_i) = 0$.

Complementary Slackness Results: Summary

$$\alpha_{i}^{*} = 0 \implies y_{i}f^{*}(x_{i}) \geqslant 1$$

$$\alpha_{i}^{*} \in \left(0, \frac{c}{n}\right) \implies y_{i}f^{*}(x_{i}) = 1$$

$$\alpha_{i}^{*} = \frac{c}{n} \implies y_{i}f^{*}(x_{i}) \leqslant 1$$

$$y_{i}f^{*}(x_{i}) < 1 \implies \alpha_{i}^{*} = \frac{c}{n}$$

$$y_{i}f^{*}(x_{i}) = 1 \implies \alpha_{i}^{*} \in \left[0, \frac{c}{n}\right]$$

$$y_{i}f^{*}(x_{i}) > 1 \implies \alpha_{i}^{*} = 0$$

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 $\alpha_i^* \in [0, \frac{c}{n}]$.

- The x_i 's corresponding to $\alpha_i^* > 0$ are called **support vectors**.
- Few margin errors or "on the margin" examples \implies sparsity in input examples.

Complementary Slackness To Get b*

The Bias Term: b

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

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

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

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

$$y_{i} \left[x_{i}^{T} w^{*} + b^{*} \right] = 1$$

$$\iff x_{i}^{T} w^{*} + b^{*} = y_{i} \text{ (use } y_{i} \in \{-1, 1\})$$

$$\iff b^{*} = y_{i} - x_{i}^{T} w^{*}$$

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 $\alpha_i^* \in (0, \frac{c}{n})$
 - With exact calculations!
- With numerical error, more robust to average over all eligible i's:

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

- If there are no $\alpha_i^* \in (0, \frac{c}{n})$?
 - Then we have a degenerate SVM training problem¹ ($w^* = 0$).

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

Teaser for Kernelization

Dual Problem: Dependence on x through inner products

SVM Dual Problem:

$$\sup_{\alpha} \sum_{i=1}^{n} \alpha_{i} - \frac{1}{2} \sum_{i,j=1}^{n} \alpha_{i} \alpha_{j} y_{i} y_{j} x_{j}^{T} x_{i}$$
s.t.
$$\sum_{i=1}^{n} \alpha_{i} y_{i} = 0$$

$$\alpha_{i} \in \left[0, \frac{c}{n}\right] \ i = 1, \dots, n.$$

- Note that all dependence on inputs x_i and x_j is through their inner product: $\langle x_j, x_i \rangle = x_j^T x_i$.
- We can replace $x_i^T x_i$ by any other inner product...
- This is a "kernelized" objective function.