SVM Dual Problem

He He

Slides based on Lecture 4c from David Rosenberg's course material.

CDS, NYU

Feb 23, 2021

SVM as a Quadratic Program

- The SVM optimization problem is equivalent to

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

- 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.

Why Do We Care About the Dual?

The Lagrangian

The general [inequality-constrained] optimization problem is:

$$\begin{array}{ll} \text{minimize} & f_0(x) \\ \text{subject to} & f_i(x) \leqslant 0, \quad i = 1, \ldots, m \end{array}$$

Definition

The **Lagrangian** for this optimization problem is

$$L(x, \lambda) = f_0(x) + \sum_{i=1}^{m} \lambda_i f_i(x).$$

- λ_i's are called **Lagrange multipliers** (also called the **dual variables**).
- Weighted sum of the objective and constraint functions
- Hard constraints $\rightarrow$ soft constraints

Lagrange Dual Function

Definition

The **Lagrange dual function** is

$$g(\lambda) = \inf_x L(x,\lambda) = \inf_x \left(f_0(x) + \sum_{i=1}^{m} \underbrace{\overbrace{\lambda_i}^{\geq 0} \overbrace{f_i(x)}^{\leq 0}}_{\leq 0} \right)$$

- $g(\lambda)$ is concave (why?)
- **Lower bound property**: if $\lambda \succeq 0$, $g(\lambda) \leqslant p^*$ where p^* is the optimal value of the optimization problem.
- $g(\lambda)$ can be $-\infty$ (uninformative lower bound)

The Primal and the Dual

- For any **primal form** optimization problem,

$$\begin{array}{ll} \text{minimize} & f_0(x) \\ \text{subject to} & f_i(x) \leqslant 0, \;\; i = 1, \dots, m, \end{array}$$

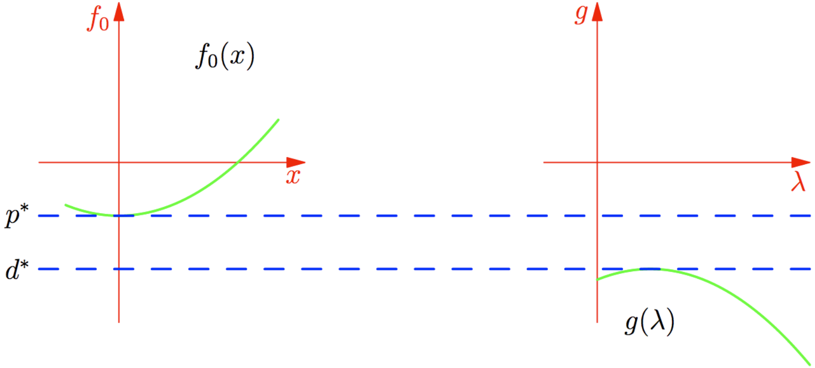
  there is a recipe for constructing a corresponding **Lagrangian dual problem:**

$$\begin{array}{ll} \text{maximize} & g(\lambda) \\ \text{subject to} & \lambda_i \geqslant 0, \;\; i = 1, \dots, m, \end{array}$$

- The dual problem is always a convex optimization problem.
- The dual variables often have interesting and relevant interpretations.
- The dual variables provide certificate for optimality.

Weak Duality

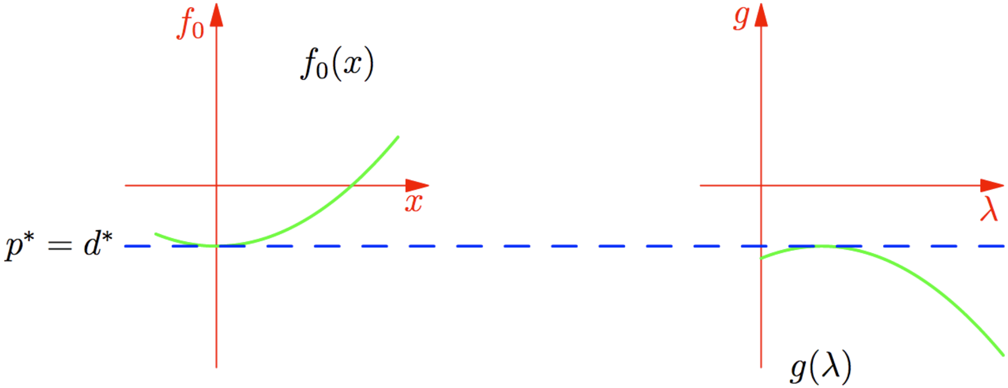
We always have **weak duality:** $p^* \geqslant d^*$.



Plot courtesy of Brett Bernstein.

Strong Duality

For some problems, we have **strong duality**: $p^* = d^*$.



For convex problems, strong duality is fairly typical.

Plot courtesy of Brett Bernstein.

Complementary Slackness

- Assume strong duality. Let x^* be primal optimal and λ^* be dual optimal. Then:

$$
\begin{aligned}
\underset{p^*}{f_0(x^*)} &= \overset{d^*}{g(\lambda^*)} = \inf_x L(x, \lambda^*) \quad \text{(strong duality and definition)} \\
&\leqslant L(x^*, \lambda^*) \\
&= f_0(x^*) + \underbrace{\sum_{i=1}^{m} \lambda_i^* f_i(x^*)}_{\leq 0} \\
&\leqslant f_0(x^*).
\end{aligned}
$$

Each term in sum $\sum_{i=1} \lambda_i^* f_i(x^*)$ must actually be 0. That is

$$
\lambda_i > 0 \implies f_i(x^*) = 0 \quad \text{and} \quad f_i(x^*) < 0 \implies \lambda_i = 0 \quad \forall i
$$

This condition is known as **complementary slackness**.

The SVM Dual Problem

SVM Lagrange Multipliers

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

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

$$L(w,b,\xi,\alpha,\lambda) = \underbrace{\frac{1}{2}||w||^2 + \frac{c}{n}\sum_{i=1}^{n}\xi_i}_{f_0(x)} + \sum_{i=1}^{n}\alpha_i\left(1 - y_i\left[w^T x_i + b\right] - \xi_i\right) + \sum_{i=1}^{n}\lambda_i\left(-\xi_i\right)$$

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

Strong Duality by Slater's Constraint Qualification

The SVM optimization problem:

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

$1 - \xi_i \le 0$

Slater's constraint qualification:

- Convex problem + affine constraints $\Longrightarrow$ strong duality iff problem is feasible
- Do we have a feasible point? Find one w, b, ξ that satisfy all constraints. $0 \quad 0 \quad 1$
- For SVM, we have strong duality.

SVM Dual Function: First Order Conditions

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

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

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

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

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

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

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

SVM Dual Problem

- The **dual function** is

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

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

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

Insights from the Dual Problem

KKT Conditions

For convex problems, if Slater's condition is satisfied, then **KKT conditions** provide necessary and sufficient conditions for the optimal solution.

- Primal feasibility: $f_i(x) \leqslant 0 \quad \forall i$
- Dual feasibility: $\lambda \succeq 0$
- Complementary slackness: $\lambda_i f_i(x) = 0$
- First-order condition:

$$\frac{\partial}{\partial x} L(x, \lambda) = 0$$

The SVM Dual Solution

- We found the SVM dual problem can be written as:

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

$\alpha_i + \lambda_i = \frac{c}{n} \quad \lambda_i \geq 0$

$\alpha_i = \frac{c}{n} - \lambda_i \leq \frac{c}{n}$

- Given solution α^* to dual, primal solution is $w^* = \sum_{i=1}^{n} \alpha_i^* y_i x_i$.
- The solution is in the space spanned by the inputs.
- Note $\alpha_i^* \in [0, \frac{c}{n}]$. So c controls max weight on each example. (**Robustness**!)
  - What's the relation between c and regularization?

Complementary Slackness Conditions

- Recall our primal constraints and Lagrange multipliers:

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

- 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**.

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

Recall "**slack variable**" $\xi_i^* = \max(0, 1 - y_i f^*(x_i))$ is the hinge loss on (x_i, y_i).

margin

- 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 $y_i f^*(x) \geqslant 1$.
- 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

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

$$w^* = \sum_{i=1}^{n} \alpha_i^* y_i x_i \quad \text{where} \alpha_i^* \in [0, \frac{c}{n}].$$

Relation between margin and example weights (α_i's):

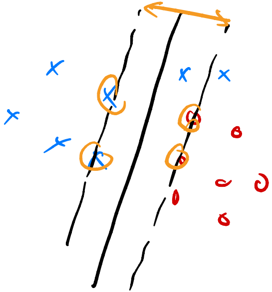
$$\begin{aligned}
\alpha_i^* = 0 \quad &\implies \quad y_i f^*(x_i) \geqslant 1 \\
\alpha_i^* \in \left(0, \frac{c}{n}\right) \quad &\implies \quad y_i f^*(x_i) = 1 \\
\alpha_i^* = \frac{c}{n} \quad &\implies \quad y_i f^*(x_i) \leqslant 1
\end{aligned}$$

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

- 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 $\Longrightarrow$ sparsity in input examples.

The Bias Term: b

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

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

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

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

- We get the same b^* for any choice of i with $\alpha_i^* \in \left(0, \frac{c}{n}\right)$

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

- 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.

Teaser for Kernelization

Dual Problem: Dependence on x through inner products

- SVM Dual Problem:

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

- 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 $x_j^T x_i$ by other products...
- This is a "kernelized" objective function.