UVA CS 4501: Machine Learning

Lecture 16 Extra: Support Vector Machine Optimization with Dual

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Today Extra

- Optimization of SVM
  - ✓ SVM as QP
  - ✓ A simple example of constrained optimization
  - ✓ SVM Optimization with dual form
  - ✓ KKT condition
  - ✓ SMO algorithm for fast SVM dual optimization

Optimization with Quadratic programming (QP)

Quadratic programming solves optimization problems of the following form:

$$\min_U \boxed{\frac{u^T R u}{2} + d^T u + c}$$

subject to n inequality constraints:

$$\left.\begin{array}{l} a_{11}u_1 + a_{12}u_2 + \ldots \le b_1 \\ \vdots \qquad\quad \vdots \qquad\quad \vdots \\ a_{n1}u_1 + a_{n2}u_2 + \ldots \le b_n \end{array}\right\}$$

and k equivalency constraints:

$$a_{n+1,1}u_1 + a_{n+1,2}u_2 + \ldots = b_{n+1}$$

$$\vdots \qquad\quad \vdots \qquad\quad \vdots$$

$$a_{n+k,1}u_1 + a_{n+k,2}u_2 + \ldots = b_{n+k}$$

$u \rightarrow$ variable

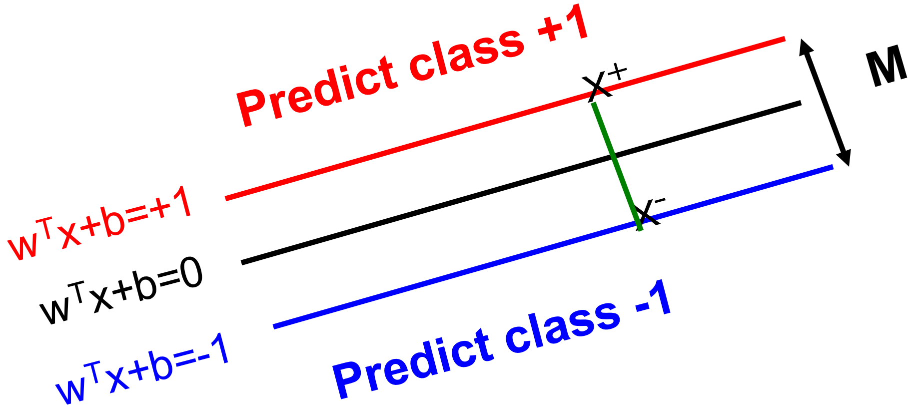
$f(u) \rightarrow$ object

Quadratic term

$g_i(u) \rightarrow$ constraints

When a problem can be specified as a QP problem we can use solvers that are better than gradient descent or simulated annealing

SVM as a QP problem



$$M = \frac{2}{\sqrt{w^T w}}$$

R as I matrix, d as zero vector, c as 0 value

$$\min_U \frac{u^T R u}{2} + d^T u + c$$

subject to n inequality constraints:

$$a_{11}u_1 + a_{12}u_2 + \ldots \le b_1$$
$$\vdots \qquad \vdots \qquad \vdots$$
$$a_{n1}u_1 + a_{n2}u_2 + \ldots \le b_n$$

and k equivalency constraints:

$$a_{n+1,1}u_1 + a_{n+1,2}u_2 + \ldots = b_{n+1}$$
$$\vdots \qquad \vdots \qquad \vdots$$
$$a_{n+k,1}u_1 + a_{n+k,2}u_2 + \ldots = b_{n+k}$$

Min $(w^T w)/2$

subject to the following inequality constraints:

For all x in class + 1

$w^T x + b >= 1$

For all x in class - 1

$w^T x + b <= -1$

A total of n constraints if we have n input samples

Optimization Review:
Ingredients

- Objective function
- Variables
- Constraints

Find values of the variables
that minimize or maximize the objective function
while satisfying the constraints

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  - ✓ A simple example of constrained optimization and dual
  - ✓ Optimization with dual form
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  - ✓ SMO algorithm for fast SVM dual optimization

Optimization Review:
Lagrangian Duality

- The Primal Problem

Primal:

$$\min_w \quad f_0(w)$$
$$\text{s.t.} \quad f_i(w) \le 0, \quad i = 1,\ldots,k$$

The generalized Lagrangian:

"Method of Lagrange multipliers"
convert to a higher-dimensional problem

$$\mathcal{L}(w,\alpha) = f_0(w) + \sum_{i=1}^{k} \alpha_i f_i(w)$$

the α's ($\alpha_i \ge 0$) are called the Lagarangian multipliers

Lemma:

$$\max_{\alpha,\alpha_i \ge 0} \mathcal{L}(w,\alpha) = \begin{cases} f_0(w) & \text{if } w \text{ satisfies primal constraints} \\ \infty & \text{o/w} \end{cases}$$

A re-written Primal:

$$\min_w \max_{\alpha,\alpha_i \ge 0} \mathcal{L}(w,\alpha)$$

Optimization Review:
Lagrangian Duality, cont.

- Recall the Primal Problem:

$$\min_{w} \max_{\alpha, \alpha_i \geq 0} \mathcal{L}(w, \alpha)$$

- The Dual Problem:

$$\max_{\alpha, \alpha_i \geq 0} \min_{w} \mathcal{L}(w, \alpha)$$

- **Theorem (weak duality):**

$$d^* = \max_{\alpha, \alpha_i \geq 0} \min_{w} \mathcal{L}(w, \alpha) \quad \leq \quad \min_{w} \max_{\alpha, \alpha_i \geq 0} \mathcal{L}(w, \alpha) = p^*$$

- **Theorem (strong duality):**

Iff there exist a saddle point of $\mathcal{L}(w, \alpha)$

we have $d^* = p^*$

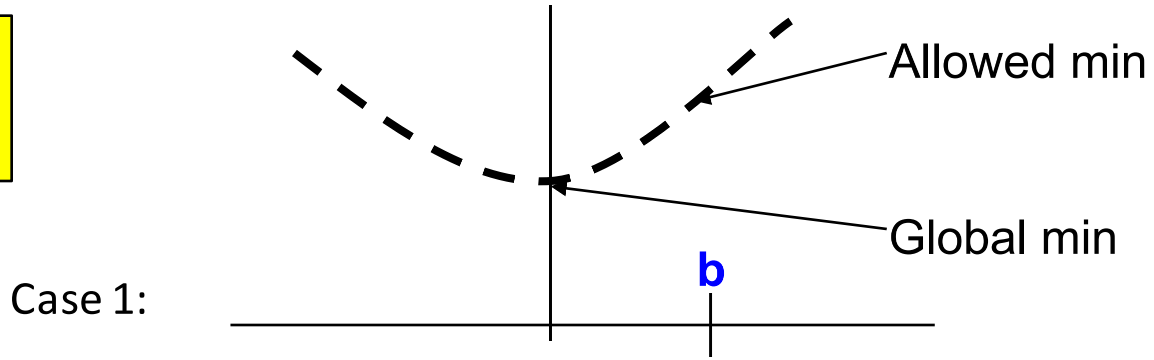
$\min_u u^2$

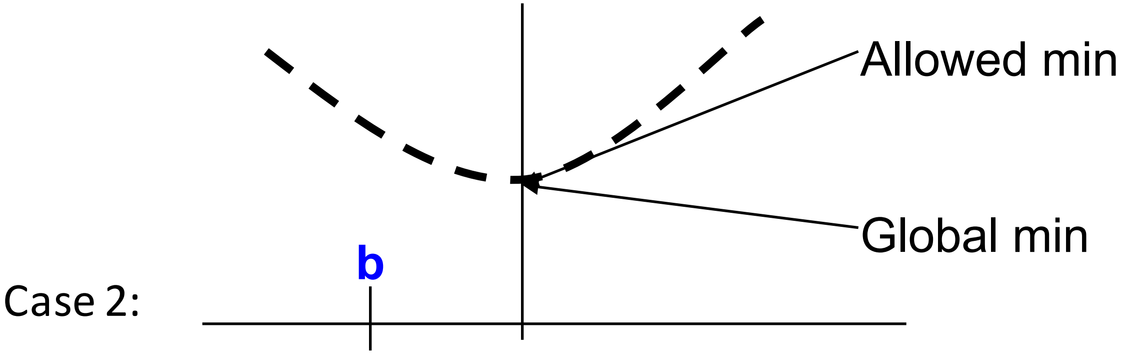
s.t. $u >= b$

Optimization Review:
Constrained Optimization

$\min_u u^2$

s.t. $u >= b$



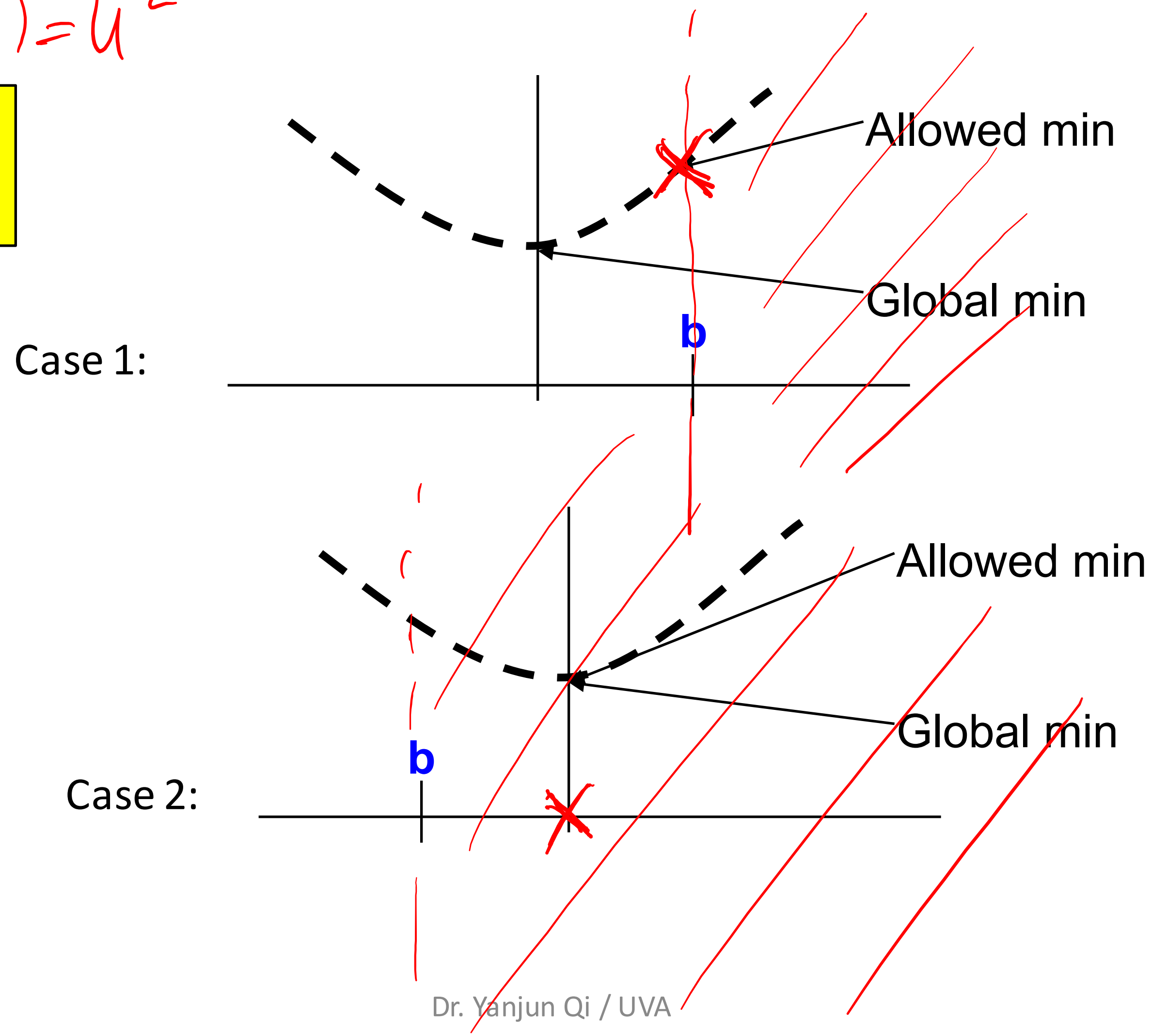


Optimization Review:
Constrained Optimization

$f(u) = u^2$

$\min_u u^2$

s.t. $u >= b$



Optimization Review:
Constrained Optimization

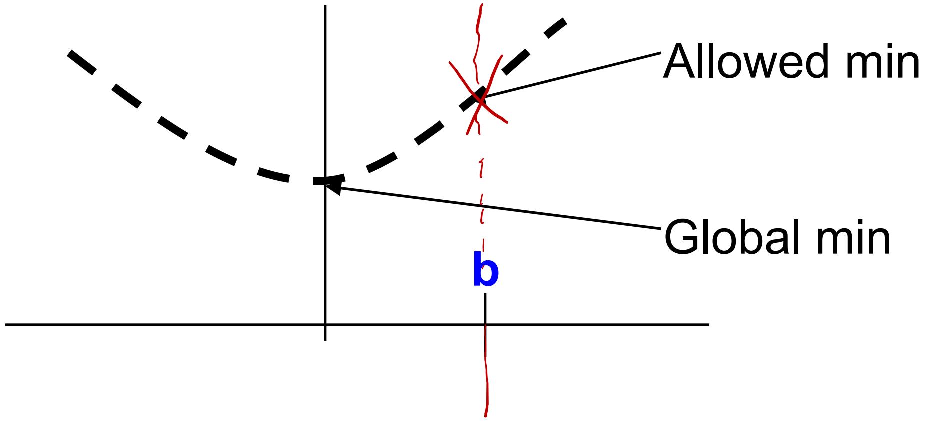
$f(u)$

$\min_u u^2$

s.t. $u >= b$

[Subject to]

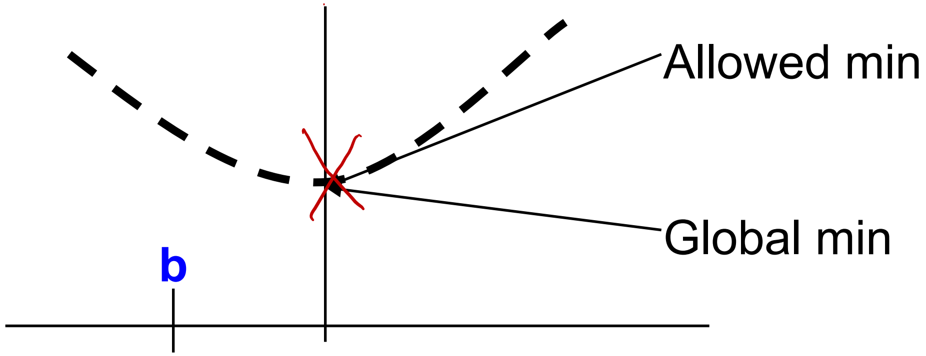
Case 1:



$b > 0$

$f(u) = b^2$

Case 2:



$b < 0$

$f(u) = 0$

$\boxed{\begin{array}{l} \min_u u^2 \\ \text{s.t. } u >= b \end{array}}$

$$\textcircled{1} \begin{cases} \min_{u} f_0(u) = u^2 \\ \text{s.t.} \quad b - u \leq 0 \end{cases}$$

primal problem

$\min_u u^2$

s.t. $u >= b$

① $\begin{cases} \min\limits_{u} f_0(u) = u^2 \\ \text{s.t.} \quad b - u \leq 0 \end{cases}$

⇒ multiplier variable

② $L(\underset{1\times 1}{u}, \underset{1\times 1}{\alpha}) = u^2 + \underbrace{\alpha}_{\geq 0} \underbrace{(b-u)}_{\leq 0}$

$\min_u u^2$

s.t. $u >= b$

① $\begin{cases} \min\limits_{u} f_0(u) = u^2 \\ \text{s.t.} \quad b - u \le 0 \end{cases}$

② $L(\underset{1\times 1}{u}, \underset{1\times 1}{\alpha}) = u^2 + \underbrace{\alpha}_{\geq 0}\underbrace{(b-u)}_{\leq 0}$

③ $\dfrac{\partial L(u,\alpha)}{\partial u} = 2u - \alpha = 0$

$$u = \frac{\alpha}{2}$$

$\rightarrow \operatorname{argmin}_u L(u, \alpha)$

$\min_u u^2$

s.t. $u >= b$

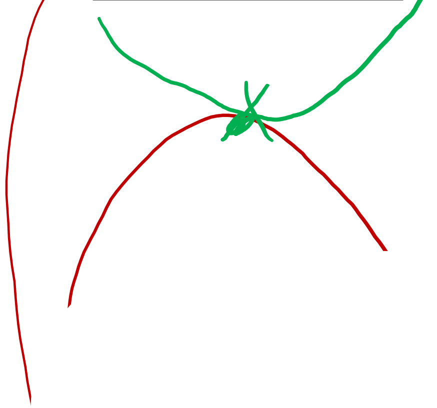
$$g(\alpha) = L(u, \alpha) = \frac{\alpha^2}{4} + \alpha\left(b - \frac{\alpha}{2}\right)$$

min$_u$ u^2

s.t. $u \geq b$

$$g(\alpha) = L(u,\alpha) = \frac{\alpha^2}{4} + \alpha\left(b - \frac{\alpha}{2}\right)$$

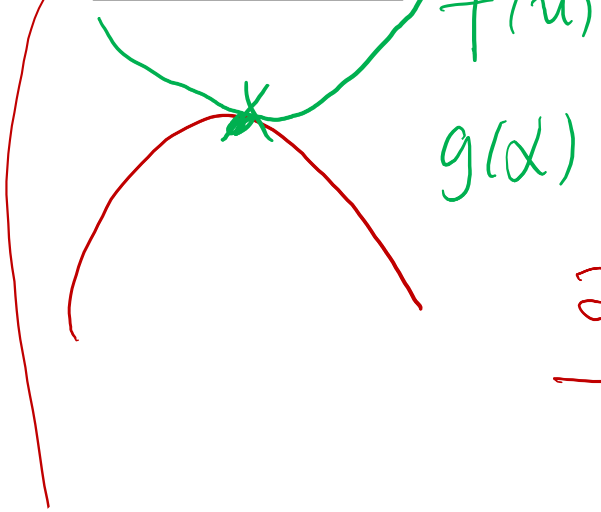
$$u = \alpha/2$$



$$g(\alpha) = -\frac{\alpha^2}{4} + b\alpha$$

$\min_u u^2$

s.t. $u >= b$



$$g(\alpha) = L(u,\alpha) = \frac{\alpha^2}{4} + \alpha\left(b - \frac{\alpha}{2}\right)$$

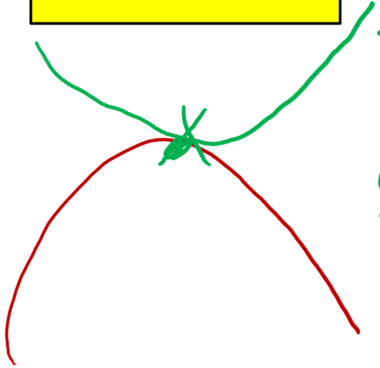
$$u = \alpha/2$$

$$g(\alpha) = -\frac{\alpha^2}{4} + b\alpha$$

$$\frac{\partial g(\alpha)}{\partial \alpha} = -\frac{\alpha}{2} + b = 0, \quad \alpha \geq 0$$

$\min_u u^2$

s.t. $u >= b$



$f(u)$

$$g(\alpha) = L(u,\alpha) = \frac{\alpha^2}{4} + \alpha\left(b - \frac{\alpha}{2}\right)$$

$u = \alpha/2$

$$g(\alpha) = -\frac{\alpha^2}{4} + b\alpha$$

$$\frac{\partial g(\alpha)}{\partial \alpha} = -\frac{\alpha}{2} + b = 0, \quad \alpha \geq 0$$

$\Rightarrow$ Dual

$$\begin{cases} b > 0, & \alpha = 2b, \quad g(\alpha) = b^2 \\ b < 0, & \alpha = 0, \quad g(\alpha) = 0 \end{cases}$$

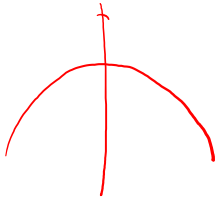
$\Rightarrow$ Primal

$$\begin{cases} b > 0, & f(u) = b^2 \quad u = b \\ b < 0, & f(u) = 0 \quad u = 0 \end{cases}$$

primal : $\min_{w} \max_{\alpha} L(w, \alpha)$

Dual : $\underbrace{\max_{\alpha} \min_{w} L(w, \alpha)}$

$\Rightarrow \max_{\alpha} g(\alpha)$



$$f(u): \begin{cases} \min u^2 \\ \text{s.t. } u \geq b \end{cases}$$

$$g(\alpha): \begin{cases} \max -\dfrac{\alpha^2}{4} + b\alpha = \max\left\{ \underbrace{-\left(\cancel{\tfrac{\alpha}{2}} - b\right)^2} + \underbrace{b^2} \right\} \\ \text{s.t. } \alpha \geq 0 \end{cases}$$

$$\begin{cases} \text{if}_{\,b \geq 0} \quad b = \alpha/2, \quad u = b, \quad g = b^2 \\ \text{if}_{\,b < 0} \quad b \neq \alpha/2, \quad \alpha = 0, \quad g = 0 \end{cases}$$

$$\Rightarrow \quad \alpha(b - u) = 0 \qquad \text{KKT condition}$$

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$$\min_{w,b} \max_{\alpha} \frac{\mathrm{w}^T\mathrm{w}}{2} - \sum_i \alpha_i [(\mathrm{w}^T x_i + b) y_i - 1]$$

$$\alpha_i \geq 0 \qquad \forall i$$

train

$$\frac{\partial L}{\partial w} = 0 \Rightarrow w - \sum_i \alpha_i x_i y_i = 0$$

$$\min_{w,b} \max_{\alpha} \left\{ \frac{\mathrm{w}^{\mathrm{T}}\mathrm{w}}{2} - \sum_i \alpha_i [(\mathrm{w}^{\mathrm{T}} x_i + b) y_i - 1] \right\} \Rightarrow \max_{\alpha} \min_{w,b} L(w,b,\alpha)$$

$$\alpha_i \geq 0 \qquad \forall i$$

train

$$\begin{cases} \dfrac{\partial L}{\partial w} = 0 \Rightarrow w - \sum_i \alpha_i x_i y_i = 0 \\ \dfrac{\partial L}{\partial b} = 0 \Rightarrow \sum \alpha_i y_i = 0 \end{cases}$$

$$L_{primal} = \frac{1}{2}\|\mathbf{w}\|^2 - \sum_{i=1}^{N} \alpha_i \left(y_i(\mathbf{w}\cdot\mathbf{x}_i + b) - 1 \right)$$

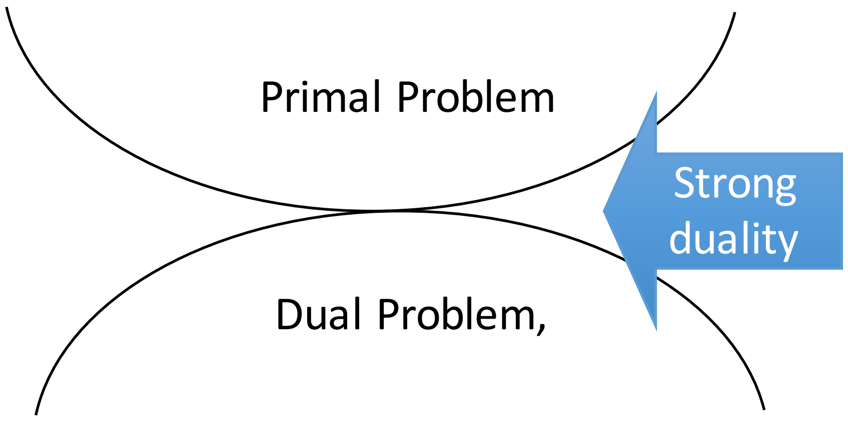
$$L_{dual} = \frac{1}{2}\left(\sum \alpha_i x_i y_i\right)^T \left(\sum_j \alpha_j x_j y_j\right) - \sum_i \alpha_i y_i \left(\sum_j \alpha_j x_j y_j\right)^T x_i$$

$$- \underbrace{\sum \alpha_i y_i}_{0} b + \underbrace{\sum \alpha_i}$$

$$= \sum_i \alpha_i - \frac{1}{2} \sum_i \sum_j \alpha_i \alpha_j y_i y_j \left(x_i^T x_j \right)$$

Optimization Review: Dual Problem

- Solving dual problem if the dual form is easier than primal form
- Need to change primal minimization to dual maximization (OR → Need to change primal maximization to dual minimization)
- Only valid when the original optimization problem is convex/concave (strong duality)



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KKT Condition for Strong Duality

$\min_w \max_\alpha L(w,\alpha)$

Primal Problem

Strong duality

Dual Problem,

$\max_\alpha \min_w L(w,\alpha)$

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

Lagrangian: $L : \mathbf{R}^n \times \mathbf{R}^m \times \mathbf{R}^p \to \mathbf{R}$, with $\mathbf{dom}\, L = \mathcal{D} \times \mathbf{R}^m \times \mathbf{R}^p$,

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

complementary slackness: $\lambda_i f_i(x) = 0,\ i = 1, \dots, m$

Key for SVM Dual

Optimization Review: Lagrangian (even more general standard form)

standard form problem (not necessarily convex)

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

variable $x \in \mathbf{R}^n$, domain $\mathcal{D}$, optimal value $p^\star$

Lagrangian: $L : \mathbf{R}^n \times \mathbf{R}^m \times \mathbf{R}^p \to \mathbf{R}$, with $\mathbf{dom}\, L = \mathcal{D} \times \mathbf{R}^m \times \mathbf{R}^p$,

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

- weighted sum of objective and constraint functions
- λ_i is Lagrange multiplier associated with $f_i(x) \leq 0$
- ν_i is Lagrange multiplier associated with $h_i(x) = 0$

From Stanford "Convex Optimization — Boyd & Vandenberghe

Optimization Review: Lagrange dual function

Lagrange dual function: $g : \mathbf{R}^m \times \mathbf{R}^p \to \mathbf{R}$,

$$\begin{aligned} g(\lambda, \nu) &= \inf_{x \in \mathcal{D}} L(x, \lambda, \nu) \\ &= \inf_{x \in \mathcal{D}} \left(f_0(x) + \sum_{i=1}^{m} \lambda_i f_i(x) + \sum_{i=1}^{p} \nu_i h_i(x) \right) \end{aligned}$$

g is concave, can be $-\infty$ for some λ, ν

lower bound property: if $\lambda \succeq 0$, then $g(\lambda, \nu) \leq p^\star$

Inf(.): greatest lower bound

proof: if $\tilde{x}$ is feasible and $\lambda \succeq 0$, then

$$f_0(\tilde{x}) \geq L(\tilde{x}, \lambda, \nu) \geq \inf_{x \in \mathcal{D}} L(x, \lambda, \nu) = g(\lambda, \nu)$$

minimizing over all feasible $\tilde{x}$ gives $p^\star \geq g(\lambda, \nu)$

Optimization Review:

Complementary slackness

assume strong duality holds, $x^\star$ is primal optimal, $(\lambda^\star, \nu^\star)$ is dual optimal

inf (.): greatest lower bound

$$
\begin{aligned}
f_0(x^\star) = g(\lambda^\star, \nu^\star) &= \inf_x \left(f_0(x) + \sum_{i=1}^m \lambda_i^\star f_i(x) + \sum_{i=1}^p \nu_i^\star h_i(x) \right) \\
&\le f_0(x^\star) + \sum_{i=1}^m \lambda_i^\star f_i(x^\star) + \sum_{i=1}^p \nu_i^\star h_i(x^\star) \\
&\le f_0(x^\star)
\end{aligned}
$$

hence, the two inequalities hold with equality

- $x^\star$ minimizes $L(x, \lambda^\star, \nu^\star)$
- $\lambda_i^\star f_i(x^\star) = 0$ for $i = 1, \ldots, m$ (known as complementary slackness):

$$
\lambda_i^\star > 0 \Longrightarrow f_i(x^\star) = 0, \qquad f_i(x^\star) < 0 \Longrightarrow \lambda_i^\star = 0
$$

Optimization Review:

Complementary slackness

assume strong duality holds, $x^\star$ is primal optimal, $(\lambda^\star, \nu^\star)$ is dual optimal

inf (.): greatest lower bound

$$
\begin{aligned}
f_0(x^\star) = g(\lambda^\star, \nu^\star) &= \inf_x \left(f_0(x) + \sum_{i=1}^m \lambda_i^\star f_i(x) + \sum_{i=1}^p \nu_i^\star h_i(x) \right) \\
&\le f_0(x^\star) + \sum_{i=1}^m \lambda_i^\star f_i(x^\star) + \sum_{i=1}^p \nu_i^\star h_i(x^\star) \\
&\le f_0(x^\star)
\end{aligned}
$$

obj $\Rightarrow f(u^*)$ $\qquad g(\alpha^*)$

$u^* \begin{cases} b>0 & u^* = b \\ b<0 & u^* = 0 \end{cases}$ $\qquad \alpha^* = 2b$, $\alpha^* = 0$

≥ 0 $\quad \le 0$ $\quad = 0$

hence, the two inequalities hold with equality

$\Rightarrow \alpha_i(1-(w^T x_i + b)y_i)$

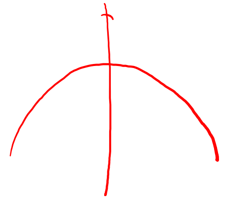
- $x^\star$ minimizes $L(x, \lambda^\star, \nu^\star)$
- $\lambda_i^\star f_i(x^\star) = 0$ for $i = 1, \ldots, m$ (known as complementary slackness):

① $\alpha_i = 0$

② $\alpha_i > 0$

$$\lambda_i^\star > 0 \Longrightarrow f_i(x^\star) = 0, \qquad f_i(x^\star) < 0 \Longrightarrow \lambda_i^\star = 0$$

$$f(u): \begin{cases} \min u^2 \\ s.t. \quad u \geq b \end{cases}$$



$$g(\alpha): \begin{cases} \max -\frac{\alpha^2}{4} + b\alpha = \max\left\{-\underbrace{\left(\frac{\alpha}{2}-b\right)^2}+\underbrace{b^2}\right\} \\ s.t. \quad \alpha \geq 0 \end{cases}$$

$$\begin{cases} \text{if}_{\,b \geq 0} \quad b = \alpha/2, \quad u = b, \quad g = b^2 \\ \text{if}_{\,b < 0} \quad b \neq \alpha/2, \quad \alpha = 0, \quad g = 0 \end{cases}$$

$$\Rightarrow \quad \alpha(b-u) = 0$$

KKT condition

Optimization Review:

Karush-Kuhn-Tucker (KKT) conditions

the following four conditions are called KKT conditions (for a problem with differentiable f_i, h_i):

1. primal constraints: $f_i(x) \leq 0$, $i = 1, \ldots, m$, $h_i(x) = 0$, $i = 1, \ldots, p$
2. dual constraints: $\lambda \succeq 0$
3. complementary slackness: $\lambda_i f_i(x) = 0$, $i = 1, \ldots, m$
4. gradient of Lagrangian with respect to x vanishes:

Key for SVM Dual

$$\nabla f_0(x) + \sum_{i=1}^{m} \lambda_i \nabla f_i(x) + \sum_{i=1}^{p} \nu_i \nabla h_i(x) = 0$$

~~from page 5–17~~: if strong duality holds and x, λ, ν are optimal, then they must satisfy the KKT conditions

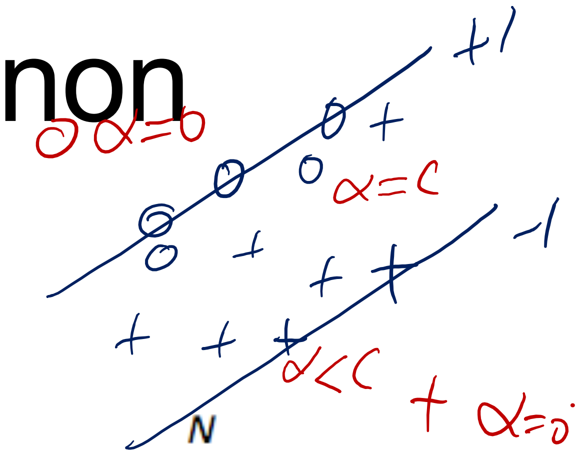
Dual formulation for linearly non separable case (soft SVM)

Substituting (1), (2), and (3) into the Lagrange, we have:

$$L(\boldsymbol{\alpha}) = \sum_{i=1}^{N} \alpha_i - \frac{1}{2}\sum_{i=1}^{N}\sum_{k=1}^{N} \alpha_i \alpha_k y_i y_k x_i^T x_k, \text{ with } 0 \leq \alpha_i \leq C \text{ and } \sum_{i=1}^{N} \alpha_i y_i = 0. \quad (4)$$

- $\hat{\alpha}_i > 0$: which implies $y_i(x_i^T \hat{\mathbf{w}} + \hat{b}) - 1 + \hat{\xi}_i = 0$ according to (5). These points are the *support vectors*.
  - $\hat{\xi}_i = 0$: which implies $\hat{\mu}_i > 0$ from (6) and so $\hat{\alpha}_i < C$ from (3). There are the support points which lie on the edge of the margin.
  - $\hat{\xi}_i > 0$: which implies $\hat{\mu}_i = 0$ from (6) and so $\hat{\alpha}_i = C$ from (3). There are the support points which violate the margin.
- $\hat{\alpha}_i = 0$: These points are not support vectors, which play no role in determining the hyperplane.

Dual formulation for linearly non separable case



Substituting (1), (2), and (3) into the Lagrange, we have:

$$L(\alpha) = \sum_{i=1}^{N} \alpha_i - \frac{1}{2}\sum_{i=1}^{N}\sum_{k=1}^{N} \alpha_i \alpha_k y_i y_k x_i^T x_k, \text{ with } 0 \le \alpha_i \le C \text{ and } \sum_{i=1}^{N} \alpha_i y_i = 0. \quad (4)$$

- $\hat{\alpha}_i > 0$: which implies $y_i(x_i^T \hat{\mathbf{w}} + \hat{b}) - 1 + \hat{\xi}_i = 0$ according to (5). These points are the *support vectors*.
  - $\hat{\xi}_i = 0$: which implies $\hat{\mu}_i > 0$ from (6) and so $\hat{\alpha}_i < C$ from (3). There are the support points which lie on the edge of the margin.
  - $\hat{\xi}_i > 0$: which implies $\hat{\mu}_i = 0$ from (6) and so $\hat{\alpha}_i = C$ from (3). There are the support points which violate the margin.
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Fast SVM Implementations

- SMO: Sequential Minimal Optimization
- SVM-Light
- LibSVM
- BSVM
- ……

SMO: Sequential Minimal Optimization

$$\underset{\alpha_1,\alpha_2,\dots,\alpha_n}{\operatorname{argmax}} \left\{ \sum \alpha_i - \sum_{i=1}^{n} \sum_{j=1}^{n} \underline{\alpha_i \alpha_j} \, y_i y_j \, \underline{x_i^T x_j} \right\}$$

- Key idea
  - Divide the large QP problem of SVM into a series of smallest possible QP problems, which can be solved analytically and thus avoids using a time-consuming numerical QP in the loop (a kind of SQP method).
  - Space complexity: O(n).
  - Since QP is greatly simplified, most time-consuming part of SMO is the evaluation of decision function, therefore it is very fast for linear SVM and sparse data.

$$\alpha_i \left(y_i (\underline{w^T x_i + b}) - 1 \right) = 0$$

SMO

- At each step, SMO chooses 2 Lagrange multipliers to jointly optimize, find the optimal values for these multipliers and updates the SVM to reflect the new optimal values.
- Three components
  - An analytic method to solve for the two Lagrange multipliers
  - A heuristic for choosing which (next) two multipliers to optimize
  - A method for computing b at each step, so that the KTT conditions are fulfilled for both the two examples (corresponding to the two multipliers)

Choosing Which Multipliers to Optimize

- First multiplier
  - Iterate over the entire training set, and find an example that violates the KTT condition.
- Second multiplier
  - Maximize the size of step taken during joint optimization.
  - $|E_1 - E_2|$, where E_i is the error on the *i*-th example.

References

- Big thanks to Prof. Ziv Bar-Joseph and Prof. Eric Xing @ CMU for allowing me to reuse some of his slides
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