UVA CS 6316: Machine Learning

Lecture 11 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

Quadratic programming solves optimization problems of the following form:

$$\min_{U} \frac{u^{T}Ru}{2} + d^{T}u + c$$

subject to n inequality constraints:

and k equivalency constraints:

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

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

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

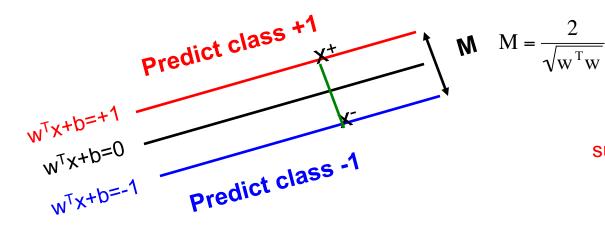
$$f(u) \rightarrow object$$

Quadratic term

 $g(u) \rightarrow consmits$

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



Min $(w^Tw)/2$

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

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:

$$a_{11}u_1 + a_{12}u_2 + \dots \le b_1$$

 \vdots \vdots \vdots
 $a_{n1}u_1 + a_{n2}u_2 + \dots \le b_n$

and k equivalency constraints:

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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Optimization Review:

Lagrangian Duality

The Primal Problem

$$\min_{w} f_0(w)$$

Primal:

s.t.
$$f_i(w) \le 0, i = 1,...,k$$

The generalized Lagrangian:

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

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

the α 's (α ₂>0) are called the Lagarangian multipliers

Lemma:

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

A re-written Primal:

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

Optimization Review:

Lagrangian Duality, cont. • Recall the Primal Problem:

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

The Dual Problem:

$$\max_{\alpha,\alpha,\geq 0} \min_{w} \angle(w,\alpha)$$

Theorem (weak duality):

$$d^* = \max_{\alpha,\alpha_i \ge 0} \min_{w} \angle(w,\alpha) \le \min_{w} \max_{\alpha,\alpha_i \ge 0} \angle(w,\alpha) = p^*$$

Theorem (strong duality):

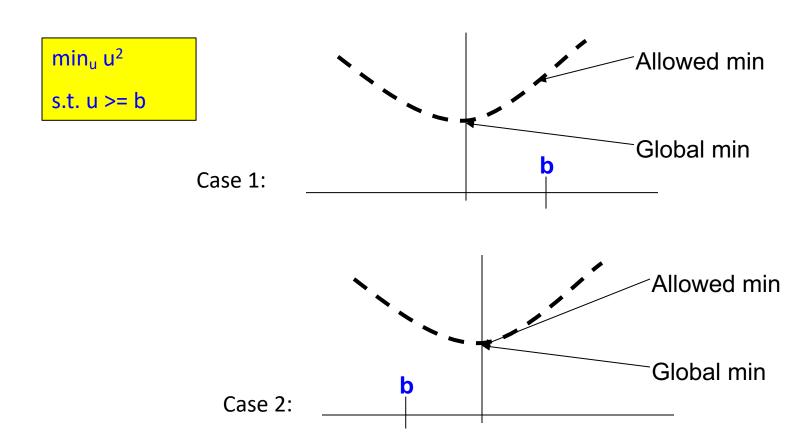
 $L(w,\alpha)$ Iff there exist a saddle point of

$$d^* = p^*$$

 $\min_{u} u^2$

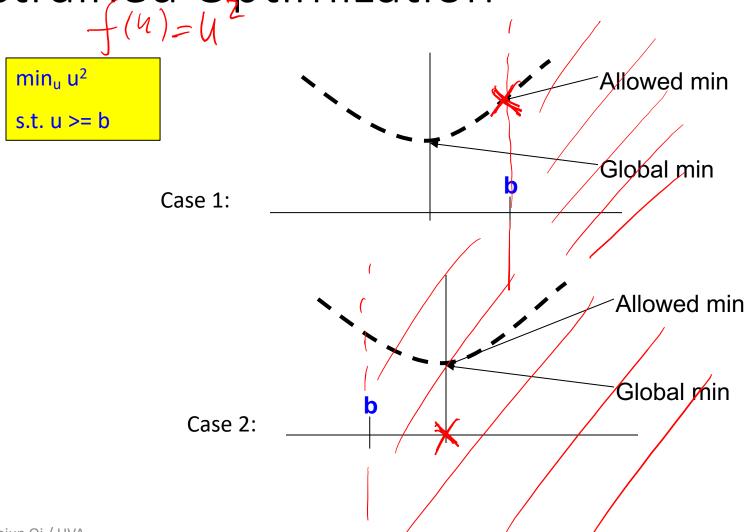
s.t. u >= b

Optimization Review: Constrained Optimization



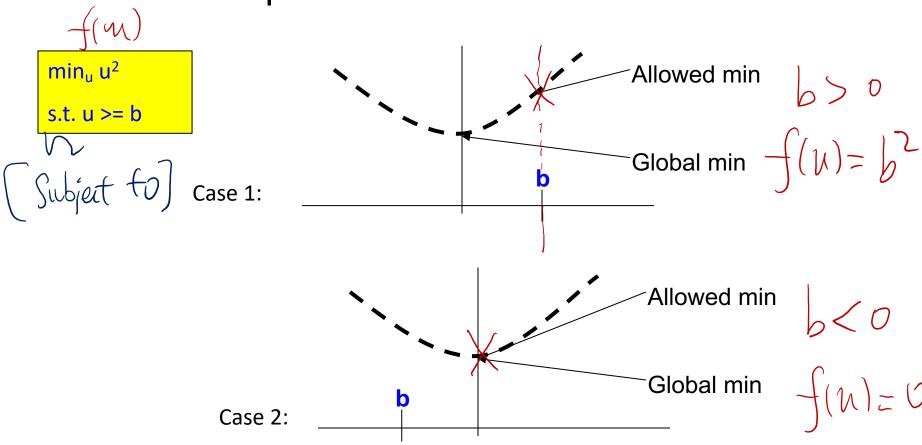
Optimization Review:

Constrained Optimization



Optimization Review:

Constrained Optimization



 $\frac{\min_{u} u^{2}}{s.t. u >= b}$ Signature $\int_{u} W(u) = u^{2}$ Prima $\int_{u} V(u) = u^{2}$ Problem

$$\min_{\mathbf{u}} \mathbf{u}^{2}$$
s.t. $\mathbf{u} >= \mathbf{b}$

$$0 \begin{cases} Min & fo(\mathbf{u}) = \mathbf{u}^{2} \\ N \\ S,f. & b - \mathbf{u} \leq 0 \end{cases}$$

$$\Rightarrow \text{multiplier variable}$$

$$2 L(\mathbf{u}, \mathbf{x}) = \mathbf{u}^{2} + \mathbf{x}(b-\mathbf{u})$$

$$= \mathbf{u}^{2} + \mathbf{x}(b-\mathbf{u})$$

$$= \mathbf{u}^{2} + \mathbf{x}(b-\mathbf{u})$$

$$\frac{\min_{u} u^{2}}{s.t. u >= b}$$

$$\int_{0}^{\infty} \left(\mathcal{U} \right) = \mathcal{U}^{2}$$

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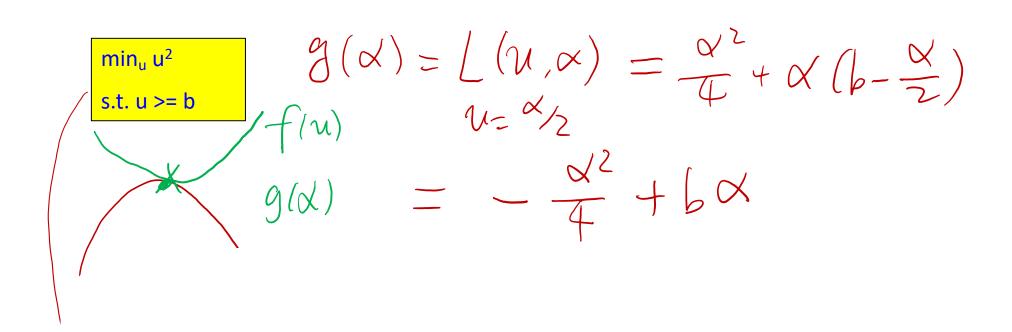
$$\int_{0}^{\infty} \left(\mathcal{U} \right) = \mathcal{U}^{2}$$

3
$$\frac{\partial L(u, \lambda)}{\partial u} = 2u - \lambda = 0$$

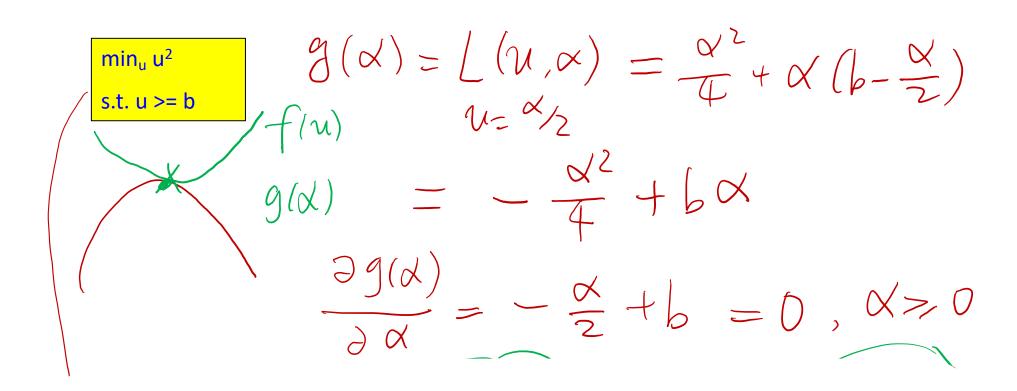
 $u = \frac{\alpha}{2}$
 $\frac{\partial L(u, \lambda)}{\partial u} = 2u - \lambda = 0$
 $\frac{\partial L(u, \lambda)}{\partial u} = 2u - \lambda = 0$

 $g(\alpha) = L(\alpha, \alpha) = \alpha^{2} + \alpha(b - \frac{\alpha}{2})$ s.t. u >= b

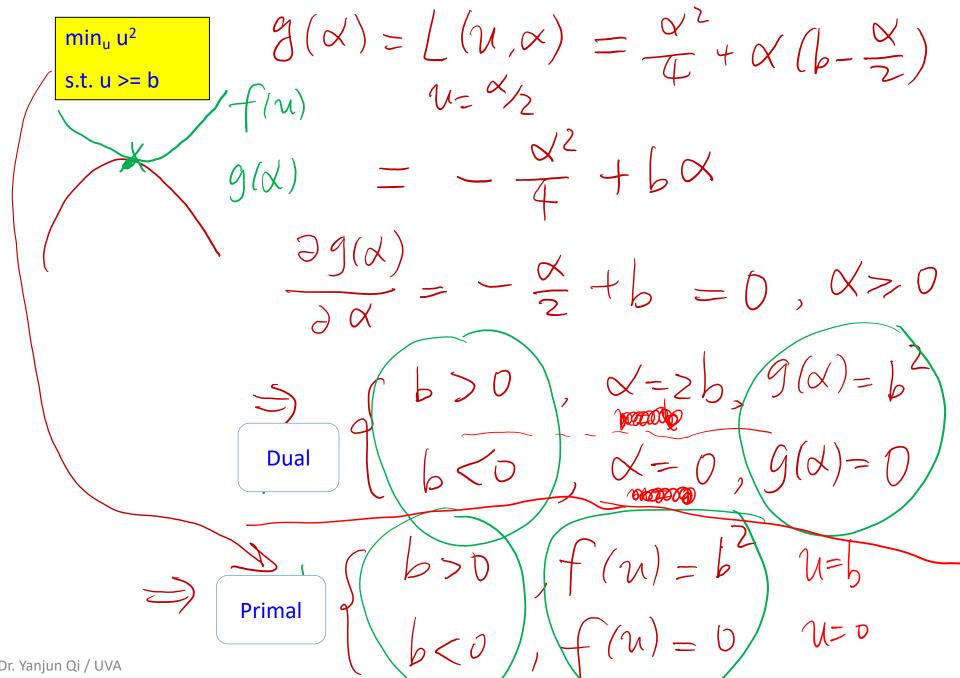
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PHMU: Min Max L(W, X) WDual : max min L(w,x)

$$f(n): \begin{cases} \min n^{2} \\ st. & u > b \end{cases}$$

$$g(x): \begin{cases} \max - \frac{x^{2}}{4} + b x = \max \{-(x-b)^{2} + b^{2}\} \\ st. & x > 0 \end{cases}$$

$$\int_{b < 0}^{b} \frac{d^{2}}{d^{2}} d^{2} d^{2}$$

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$$\min_{w,b} \max_{\alpha} \frac{\sqrt{v^{T}w}}{2} - \sum_{i} \alpha_{i} [(w^{T}x_{i} + b)y_{i} - 1]$$

$$\alpha_{i} \ge 0 \qquad \forall i$$

$$0 \qquad \text{train}$$

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$$\min_{w,b} \max_{\alpha} \frac{w^{T}w}{2} - \sum_{i} \alpha_{i} [(w^{T}x_{i} + b)y_{i} - 1]$$

$$\alpha_{i} \ge 0 \qquad \forall i \qquad \text{train}$$

$$\frac{\partial L}{\partial w} = 0 \implies w - \sum_{i} x_{i} \times y_{i} = 0$$

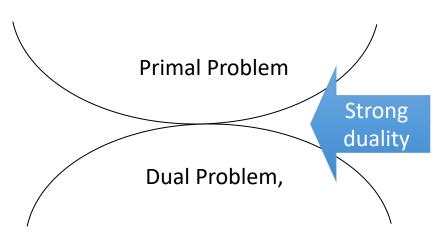
$$\frac{\partial L}{\partial w} = 0 \implies w \times y_{i} = 0$$

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

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)

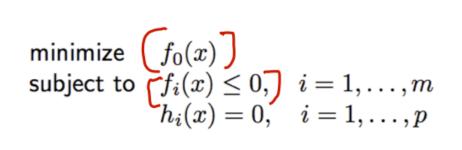


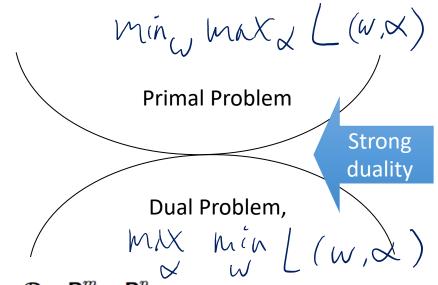
 Only valid when the original optimization problem is convex/concave (strong duality)

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KKT Condition for Strong Duality





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

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

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)

minimize
$$f_0(x)$$
 subject to $f_i(x) \leq 0$, $i=1,\ldots,m$ $h_i(x)=0, \quad i=1,\ldots,p$

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

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

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

- weighted sum of objective and constraint functions
- λ_i is Lagrange multiplier associated with $f_i(x) \leq 0$
- $_{_{10/16/19~Dr.~Yanjun~Qi}}
 u_i$ is Lagrange multiplier associated with $h_i(x)=0$

Optimization Review: Lagrange dual function

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

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

$$= \inf_{x \in \mathcal{D}} \left(f_0(x) + \sum_{i=1}^m \lambda_i f_i(x) + \sum_{i=1}^p \nu_i h_i(x) \right)$$

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

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

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

Inf(.): greatest lower bound

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

Optimization Review:

Complementary slackness

assume strong duality holds, x^* is primal optimal, (λ^*, ν^*) is dual optimal

inf (.): greatest lower bound

$$f_0(x^*) = g(\lambda^*, \nu^*) = \inf_{x} \left(f_0(x) + \sum_{i=1}^m \lambda_i^* f_i(x) + \sum_{i=1}^p \nu_i^* h_i(x) \right)$$

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

$$\leq f_0(x^*)$$

hence, the two inequalities hold with equality

- x^* minimizes $L(x, \lambda^*, \nu^*)$
- $\lambda_i^{\star} f_i(x^{\star}) = 0$ for $i = 1, \dots, m$ (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^* is primal optimal, (λ^*, ν^*) is dual optimal

$$f_0(x^\star) = g(\lambda^\star, \nu^\star)$$

$$= \inf_x \left(f_0(x) + \sum_{i=1}^m \lambda_i^\star f_i(x) + \sum_{i=1}^p \nu_i^\star h_i(x) \right)$$

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

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

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hence, the two inequalities hold with equality
$$= x^\star \text{ minimizes } I(x, \lambda^\star, \nu^\star)$$

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

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

10/16/19

$$f(n): \begin{cases} \min n^{2} \\ st. & u > b \end{cases}$$

$$g(x): \begin{cases} \max - \frac{x^{2}}{4} + b x = \max \{-(x-b)^{2} + b^{2}\} \\ st. & x > 0 \end{cases}$$

$$\int_{b < 0}^{b} \frac{d^{2}}{dt} dt = b, g = b^{2}$$

$$\int_{b < 0}^{c} \frac{d^{2}}{dt} dt = b, g = 0$$

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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: $\lambda_i f_i(x) = 0$, $i = 1, \dots, m$ Key for SVM Dual
- 4. gradient of Lagrangian with respect to x vanishes:

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

for page ν : 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:

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

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

- Support vectors are
 - Samples on the margin: $y_i(\mathbf{x}_i \cdot \mathbf{w} + b) = 1$, $0 < \alpha_i < C$

• Sample violate (mostly inside the margin area):

$$y_i (\mathbf{x}_i \cdot \mathbf{w} + b) < 1,$$

$$\alpha_i = C$$

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✓ SMO algorithm for fast SVM dual optimization

Fast SVM Implementations

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

J. Platt (1999),

Fast Training of Support Vector Machines Using Sequential Minimal Optimization https://pdfs.semanticscholar.org/d1fa/8485ad749d51e7470d801bc1931706597601.pdf

SMO: Sequential Minimal Optimization

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 timeconsuming 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.

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
- <u>Elements of Statistical Learning, by Hastie, Tibshirani</u> and <u>Friedman</u>
- Prof. Andrew Moore @ CMU's slides
- Tutorial slides from Dr. Tie-Yan Liu, MSR Asia
- A Practical Guide to Support Vector Classification Chih-Wei Hsu, Chih-Chung Chang, and Chih-Jen Lin, 2003-2010
- Tutorial slides from Stanford "Convex Optimization I Boyd & Vandenberghe