CS189/CS289A Introduction to Machine Learning Lecture 13: A Little Convex Optimization and SVMs Revisited

Peter Bartlett

March 5, 2015

• Convex optimization ideas: primal, Lagrangian, dual.

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- Weak and strong duality

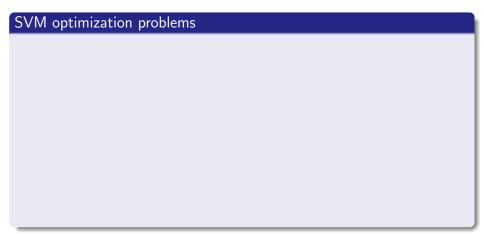
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SVM optimization problems Hard margin SVM $\|\theta\|^2$ min such that $y^i \theta \cdot x^i \ge 1$ (i = 1, ..., n)

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Hard margin SVM

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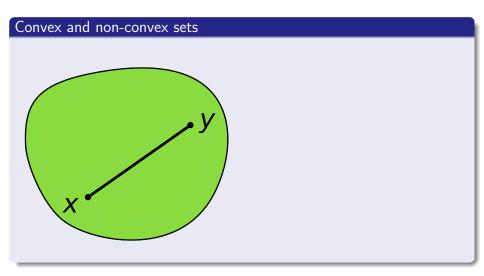
$$\min_{ heta} \qquad \| heta\|^2$$
 such that $\qquad y^i heta \cdot x^i \geq 1 \qquad (i=1,\ldots,n)$

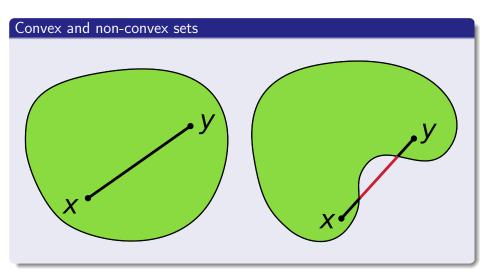
Soft margin SVM

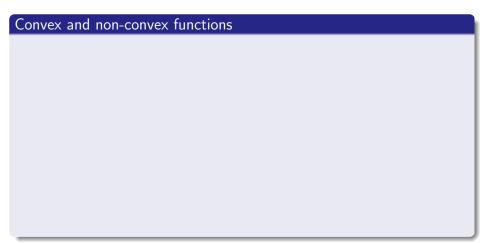
$$\min_{\substack{\theta,\xi}} \qquad \|\theta\|^2 + C \sum_{i=1}^n \xi_i$$
 such that
$$\xi_i \geq 0,$$

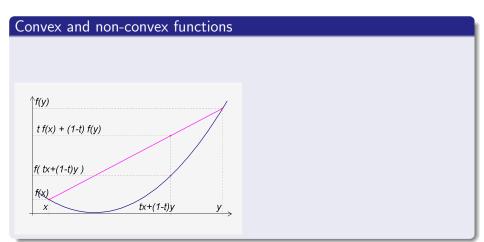
$$\xi_i > 1 - y^i \theta \cdot x^i.$$

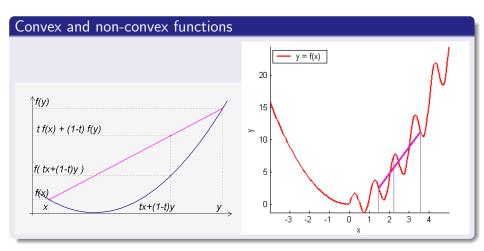


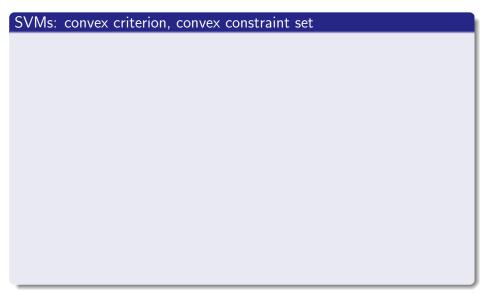












SVMs: convex criterion, convex constraint set

Hard margin SVM

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s.t. $f_i(x) \le 0, \qquad i = 1, 2, \dots, m.$

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Then replace that constraint penalty with something smaller: Introduce Lagrange multipliers (dual variables) $\lambda_1,\ldots,\lambda_m\geq 0$, and define the Lagrangian $L:\mathbb{R}^{n+m}\to\mathbb{R}$ as

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

The Lagrangian

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Joseph-Louis Lagrange 1736-1813

The Lagrangian

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- Think of the λ_i as the cost of violating the constraint $f_i(x) \leq 0$.
- L defines a saddle point game: one player (MIN) chooses x to minimize L, the other player (MAX) chooses λ to maximize L. If MIN violates a constraint, $f_i(x) > 0$, then MAX can drive L to infinity.



Joseph-Louis Lagrange

• We call the original optimization the *primal* problem. It has value

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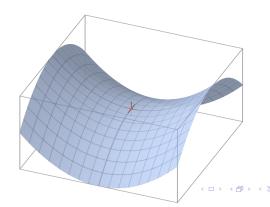
$$d^* = \max_{\lambda \geq 0} g(\lambda) = \max_{\lambda \geq 0} \min_{x} L(x, \lambda).$$

• In a zero sum game, it's always better to play second:

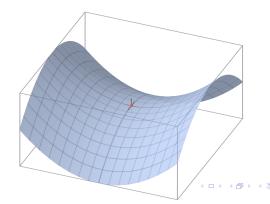
$$p^* = \min_{\substack{x \ \lambda \geq 0}} \max_{\lambda \geq 0} L(x, \lambda) \geq \max_{\substack{\lambda \geq 0 \ x}} \min_{\substack{x}} L(x, \lambda) = d^*.$$

This is called weak duality.

• If there is a saddle point (x^*, λ^*) , so that for all x and $\lambda \geq 0$, $L(x^*, \lambda^*)$

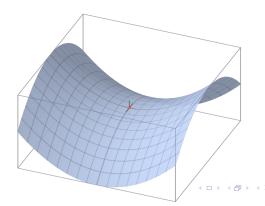


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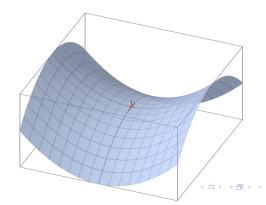


• If there is a saddle point (x^*, λ^*) , so that for all x and $\lambda \ge 0$,

$$L(x^*, \lambda) \le L(x^*, \lambda^*) \le L(x, \lambda^*),$$

then we have strong duality: the primal and dual have same value,

$$p^* = \min_{x} \max_{\lambda > 0} L(x, \lambda) = \max_{\lambda > 0} \min_{x} L(x, \lambda) = d^*.$$



Outline

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- Weak and strong duality
- Complementary slackness
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Suppose $p^* = d^*$. (This will be true for all of our examples.)

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Complementary slackness

If $p^*=d^*$ and we have primal solution x^* and dual solution λ^* , then for the *i*th constraint $(f_i(x) \leq 0)$,

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$$\lambda_i^* f_i(x^*) = 0.$$

That is, if $f_i(x^*) < 0$ then $\lambda_i = 0$. And if $\lambda_i > 0$ then $f_i(x^*) = 0$.

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Why?

$$f_0(x^*) = g(\lambda^*) = \min_{x} \left(f_0(x) + \sum_{i=1}^m \lambda_i^* f_i(x) \right) \le f_0(x^*) + \sum_{i=1}^m \lambda_i^* f_i(x^*).$$

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$$f_0(x^*) = g(\lambda^*) = \min_{x} \left(f_0(x) + \sum_{i=1}^m \lambda_i^* f_i(x) \right) \le f_0(x^*) + \sum_{i=1}^m \lambda_i^* f_i(x^*).$$

That is,

$$\sum_{i=1}^m \lambda_i^* f_i(x^*) \geq 0.$$

But $\lambda_i^* \geq 0$ and $f_i(x^*) \leq 0$, so every term in the sum must be zero.

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Karush-Kuhn-Tucker optimality conditions

Suppose f_0 , f_i are convex and differentiable.

Then x and λ are optimal (and $f_0(x) = p^* = d^* = g(\lambda)$) if and only if

• Primal feasibility: $f_i(x) \leq 0$.

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- Primal feasibility: $f_i(x) \leq 0$.
- ② Dual feasibility: $\lambda_i \geq 0$.
- **3** Complementary slackness: $\lambda_i f_i(x) = 0$.
- **4** Stationarity: $\nabla f_0(x) + \sum_i \lambda_i \nabla f_i(x) = 0$.

William Karush 1917-1997



1925-2014



Albert W. Tucker

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\min_{\theta} \qquad \|\theta\|^2 such that y^i\theta \cdot x^i \geq 1 \qquad (i=1,\dots,n)
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Hard margin SVM

 $\min_{ heta} \qquad \| heta\|^2$ such that $\qquad y^i heta \cdot x^i \geq 1 \qquad (i=1,\ldots,n)$

$$L(\theta,\alpha) = \frac{1}{2} \|\theta\|^2 + \sum_{i=1}^n \alpha_i (1 - y_i \theta' x_i)$$

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$$g(\alpha) = \min_{\theta} L(\theta, \alpha)$$

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$$\begin{split} L(\theta,\alpha) &= \frac{1}{2} \|\theta\|^2 + \sum_{i=1}^n \alpha_i (1 - y_i \theta' x_i) \\ g(\alpha) &= \min_{\theta} L(\theta,\alpha) \\ \text{setting} \qquad \theta^* &= \sum_{i=1}^n \alpha_i y_i x_i, \end{split}$$

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

$$g(\alpha) = \sum_{i=1}^n \alpha_i - \frac{1}{2} \sum_{i=1}^n \alpha_i \alpha_j y_i y_j x_i' x_j.$$

It turns out that, if there is a feasible θ (that is, the data are separable), we have strong duality.

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We can express the optimal θ^* in terms of the solution, α^* , to the dual problem:

$$\max_{\alpha} \qquad \sum_{i=1}^{n} \alpha_{i} - \frac{1}{2} \sum_{i,j} \alpha_{i} \alpha_{j} y_{i} y_{j} x_{i}' x_{j}$$
s.t.
$$\alpha_{i} \geq 0, \qquad i = 1, 2, \dots, n.$$

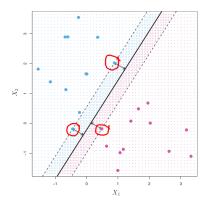
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Complementary slackness demonstrates the role of the α_i :

$$\alpha_i > 0$$
 implies $y_i \theta^{*'} x_i = 1$,

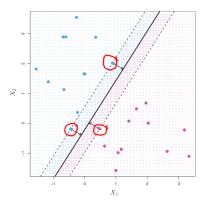
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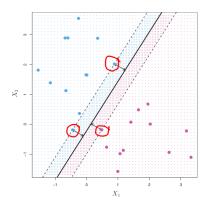
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That is, only the points for which the constraints are tight (support vectors) appear in the sum defining θ^* .



$$\hat{y}(x) = \operatorname{sign}(\langle \theta, \Phi(x) \rangle)$$

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$$= \operatorname{sign}\left(\sum_{i=1}^{n} \alpha_{i} y_{i} \langle \Phi(x_{i}), \Phi(x) \rangle\right)$$

$$\begin{split} \hat{y}(x) &= \operatorname{sign} \left(\langle \theta, \Phi(x) \rangle \right) \\ &= \operatorname{sign} \left(\sum_{i=1}^{n} \alpha_{i} y_{i} \langle \Phi(x_{i}), \Phi(x) \rangle \right) \\ &= \operatorname{sign} \left(\sum_{i=1}^{n} \alpha_{i} y_{i} k(x_{i}, x) \right), \end{split}$$

And we can express the solution in terms of an arbitrary kernel k:

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where α solves the dual problem

$$\min_{\alpha} \frac{1}{2} \alpha^{T} \operatorname{diag}(y) K \operatorname{diag}(y) \alpha - \alpha^{T} 1$$
s.t. $\alpha \ge 0$.

Soft margin SVM

$$\min_{\theta} \qquad \frac{1}{2} \|\theta\|^2 + \frac{C}{n} \sum_{i=1}^{n} \left(1 - y^i \theta \cdot x^i\right)_+.$$

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$$\begin{split} \min_{\theta,\xi} & \quad \frac{1}{2}\|\theta\|^2 + \frac{C}{n}\sum_{i=1}^n \xi_i \\ \text{such that} & \quad \xi_i \geq 0, \\ & \quad \xi_i > 1 - v^i\theta \cdot x^i. \end{split}$$

Soft margin SVM

$$\min_{\theta} \qquad \frac{1}{2} \|\theta\|^2 + \frac{C}{n} \sum_{i=1}^{n} \left(1 - y^i \theta \cdot x^i \right)_+.$$

As a QP

$$\min_{\substack{\theta,\xi}} \qquad \frac{1}{2}\|\theta\|^2 + \frac{C}{n}\sum_{i=1}^n \xi_i$$
 such that
$$\xi_i \geq 0,$$

$$\xi_i \geq 1 - y^i\theta \cdot x^i.$$

The optimal slack variables ξ_i satisfy $\xi_i = (1 - y_i \theta^T x_i)_+$.

$$L(\theta, \xi, \alpha, \lambda)$$

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$$g(\alpha, \lambda) = \sum_{i} \alpha_{i} - \frac{1}{2} \sum_{i,j} \alpha_{i} \alpha_{j} y_{i} y_{j} x_{i}^{T} x_{j}.$$

The dual problem is:

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

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Consider the consequences of complementary slackness:

$$\alpha_i^* \left(1 - y_i x_i^T \theta^* - \xi_i^* \right) = 0.$$
$$\lambda_i^* \xi_i^* = 0.$$

• $\alpha_i^* > 0$ implies $y_i x_i^T \theta^* = 1 - \xi_i^* \le 1$. That is, the 'support vectors' $(y_i x_i \text{ with } \alpha_i^* > 0)$ are in the wrong halfspace $\{x : x^T \theta^* \le 1\}$.

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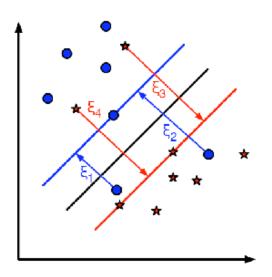
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- ② If $y_i x_i^T \theta^* < 1$, $\xi_i^* > 0$, so $\lambda_i^* = 0$, and $\alpha_i^* = C/n$. That is, the support vectors in the open halfspace $\{x : x^T \theta^* < 1\}$ have $\alpha_i^* = C/n$.



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- In the primal, increasing C penalizes errors more (and puts less emphasis on minimizing $\|\theta\|$, that is, maximizing the margin).
- In the dual, decreasing C forces the α_i s to be small. So the solution is not strongly influenced by a single outlier.

Outline

- Optimization ideas: primal, Lagrangian, dual.
- Weak and strong duality
- Complementary slackness
- Karush-Kuhn-Tucker optimality conditions
- SVMs
 - Complementary slackness and support vectors
 - Dual problem and kernels