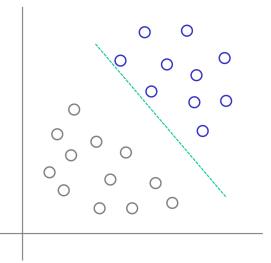
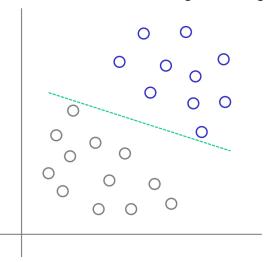
Support Vector Machines (SVM)

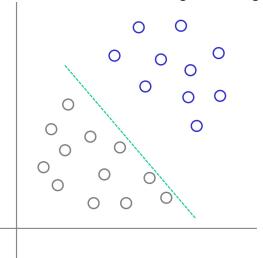
Yingming Li yingming@zju.edu.cn

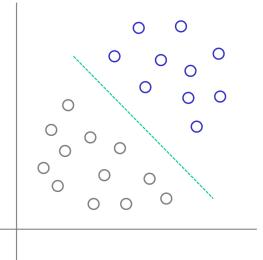
Data Science & Engineering Research Center, ZJU

29th March 2018



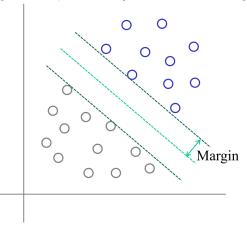






But the maximum margin hyperplane generalizes the best to new data

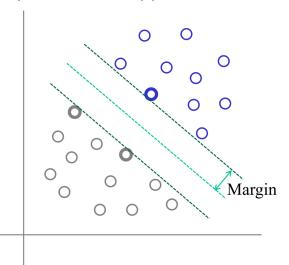
According to computational/statistical learning theory



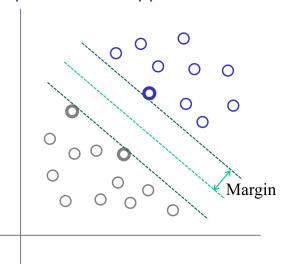
But the maximum margin hyperplane generalizes the best to new data

- According to computational learning theory
- Also known as statistical learning theory
- We won't get into the details of that
- Recall from the perceptron convergence proof
 - We assumed the existance of a best hyperplane \mathbf{w}_0
 - Which provided the maximum margin α
 - Such that $d_p \mathbf{w}_0^T \mathbf{x}_p \leqslant \alpha$ for all training points p
- The SVM actually finds this hyperplane

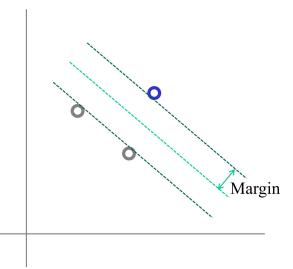
The maximum margin only depends on certain points, the support vectors



The maximum margin only depends on certain points, the support vectors



The maximum margin only depends on certain points, the support vectors



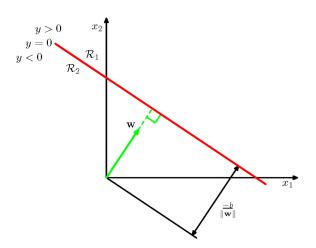
Maximum margin problem

- Given a set of data from two classes $\{\mathbf{x}_p,\,d_p\}$
 - $\mathbf{x}_p \in \mathbb{R}^D$ and $d_p \in \{-1, 1\}$
 - Assume the classes are linearly separable for now
- Find the hyperplane that separates them
 - with maximum margin
- Equation of general linear discriminant function

$$y(\mathbf{x}) = \mathbf{w}^T \mathbf{x} + b$$

- Find w and b that give maximum margin
- How can we quantify margin?

${f w}$ is perpendicular to the hyperplane, b defines its distance from the origin



w is perpendicular to the hyperplane

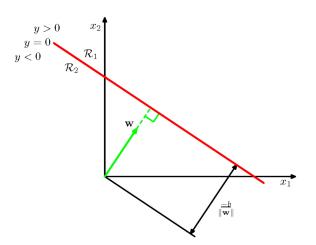
- Consider two points on the hyperplane \mathbf{x}_A and \mathbf{x}_B
- Then $y(\mathbf{x}_A) = y(\mathbf{x}_B) = 0$ by definition
- So $0 = y(\mathbf{x}_A) y(\mathbf{x}_B) = \mathbf{w}^T(\mathbf{x}_A \mathbf{x}_B)$
- $\mathbf{x}_A \mathbf{x}_B$ is a vector pointing along the hyperplane
- So w is perpendicular to the hyperplane

b defines the hyerplane's distance from the origin

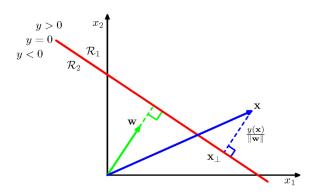
- Consider a general point x
- Its distance to the origin is $D = \frac{\mathbf{w}^T x}{||\mathbf{w}||}$
- If \mathbf{x} is on the hyperplane, then $y(\mathbf{x}) = 0$
 - So $\mathbf{w}^T x = -b$
- So the distance from the hyperplane to the origin is

$$D = -\frac{b}{||\mathbf{w}||}$$

${f w}$ is perpendicular to the hyperplane, b defines its distance from the origin



The distance from point ${\bf x}$ to the hyperplane is $y({\bf x})/||{\bf w}||$

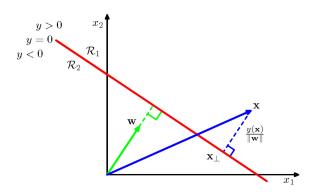


The distance from point \mathbf{x} to the hyperplane is $y(\mathbf{x})/||\mathbf{w}||$

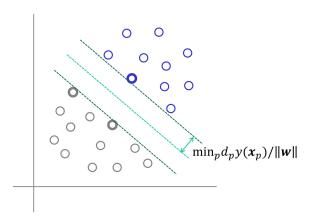
- Consider a point ${\bf x}$ and its projection onto the hyperplane ${\bf x}_{\perp}$ so that ${\bf x}={\bf x}_{\perp}+r\frac{{\bf w}}{||{\bf w}||}$
- We want to find r, the distance to the hyperplane
- Multiply both sides by \mathbf{w}^T and add b

$$\mathbf{w}^{T}\mathbf{x} + b = \mathbf{w}^{T}\mathbf{x}_{\perp} + b + r\frac{||\mathbf{w}||^{2}}{||\mathbf{w}||}$$
$$y(\mathbf{x}) = y(\mathbf{x}_{\perp}) + r||\mathbf{w}||$$
$$r = \frac{y(\mathbf{x})}{||\mathbf{w}||}$$

The distance from point ${\bf x}$ to the hyperplane is $y({\bf x})/||{\bf w}||$



The maximum margin hyperplane is farthest from all of the data points



The maximum margin hyperplane is farthest from all of the data points

• The margin is defined as

$$\alpha = \min_{p} d_{p} \frac{y(\mathbf{x}_{p})}{||\mathbf{w}||}$$
$$= \frac{1}{||\mathbf{w}||} \min_{p} d_{p} y(\mathbf{x}_{p})$$

- We want to find ${\bf w}$ and that maximize the margin $\mathop{\rm argmax}_{{\bf w},b} \frac{1}{||{\bf w}||} \min_p d_p y({\bf x}_p)$
- Solving this problem is hard as it is written



We are free to choose a rescaling of \mathbf{w}

- If we replace \mathbf{w} by $a\mathbf{w}$ and b with ab
- Then the margin is unchanged

$$\min_{p} d_{p} \frac{a \mathbf{w}^{T} \mathbf{x}_{p} + ab}{a||\mathbf{w}||} = \min_{p} d_{p} \frac{\mathbf{w}^{T} \mathbf{x}_{p} + b}{||\mathbf{w}||}$$

- So choose a such that $\min_p d_p(a\mathbf{w}^T\mathbf{x}_p + ab) = 1$
- Which means that for all points

$$d_p(\mathbf{w}^T\mathbf{x}_p + b) \geqslant 1$$

Maximum margin constrained optimization problem

• Then the maximum margin optimization becomes

$$\operatorname{argmax}_{\mathbf{w},b} \frac{1}{||\mathbf{w}||} \min_{p} d_{p} y(\mathbf{x}_{p})$$
$$= \operatorname{argmax}_{\mathbf{w},b} \frac{1}{||\mathbf{w}||}$$

• With the constraints $d_p(\mathbf{w}^T\mathbf{x}_p + b) \geqslant 1$

Maximum margin constrained optimization problem

- Which is equivalent to $\underset{\mathbf{w},b}{\operatorname{argmin}}_{\mathbf{w},b} \frac{1}{2} ||\mathbf{w}||^2$, subject to $d_p(\mathbf{w}^T \mathbf{x}_p + b) \geqslant 1$
- This is a well studied type of problem
 - A quadratic program with linear inequality constraints

Detour: Lagrange multipliers solve constrained optimization problems

- Want to maximize a function $f(x_1, x_2)$
- Subject to the equality constraint $g(x_1, x_2) = 0$
- Could solve $g(x_1, x_2) = 0$ for x_1 in terms of x_2
 - But that is hard to do in general (i.e., on computers)
- Or could use Lagrange multipliers
 - Which are easier to use in general (i.e., on computers)

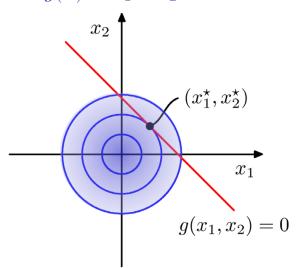
Lagrange multipliers with general x

In general, we can write

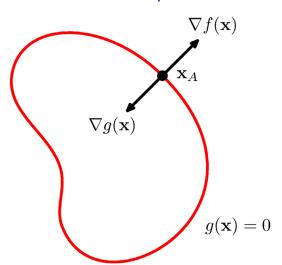
$$\max_x f(\mathbf{x})$$
 subject to $g(\mathbf{x}) = 0$

• Constraint $g(\mathbf{x}) = 0$ defines a D-1 dimensional surface for D dimensional \mathbf{x}

Example: Maximize $f(\mathbf{x}) = 1 - x_1^2 - x_2^2$ subject to $g(\mathbf{x}) = x_1 + x_2 - 1 = 0$



Gradients of g and f are orthogonal to surface at solution point



Gradients of g and f are orthogonal to surface at maximum of f

- For g because on all points on the surface $g(\mathbf{x}) = 0$
- For f because if it wasn't, you could move along the surface in the direction of the gradient to find a better maximum
- Thus ∇f and ∇g parallel.
 - If g is inequality constraint , ∇f and ∇g are of oppsite direction.
 - If *g* is equality constraint, we only know that they are parallel.
- And there must exist a scalar λ such that

$$\nabla f + \lambda \nabla g = 0$$



The Lagrangian function captures the constraints on x and on the gradients

$$L(\mathbf{x}, \lambda) = f(\mathbf{x}) + \lambda g(\mathbf{x})$$

Setting gradient of L with respect to x to 0 gives

$$\nabla f + \lambda \nabla g = 0$$

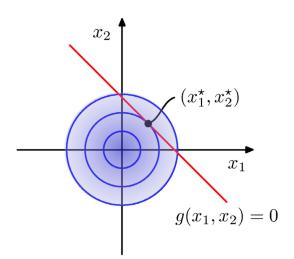
• Setting partial of L with respect to λ to 0 gives

$$g(\mathbf{x}) = 0$$

 Thus stationary points of L solve the constrained optimization problem



Example: Maximize $f(\mathbf{x}) = 1 - x_1^2 - x_2^2$ subject to $g(\mathbf{x}) = x_1 + x_2 - 1 = 0$



Example: Maximize
$$f(\mathbf{x}) = 1 - x_1^2 - x_2^2$$
 subject to $g(\mathbf{x}) = x_1 + x_2 - 1 = 0$

So the Lagrangian function is

$$L(\mathbf{x}, \lambda) = f(\mathbf{x}) + \lambda g(\mathbf{x}) = 1 - x_1^2 - x_2^2 + \lambda (x_1 + x_2 - 1)$$

The conditions for L to be stationary are

$$\partial L/\partial x_1 = -2x_1 + \lambda = 0$$

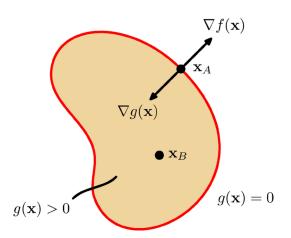
$$\partial L/\partial x_2 = -2x_2 + \lambda = 0$$

$$\partial L/\partial \lambda = x_1 + x_2 - 1 = 0$$

• Can solve to find $\lambda = 1, x_1 = x_2 = \frac{1}{2}$



Lagrange multipliers can also be used with inequality constraints $g(\mathbf{x}) \geqslant 0$



Lagrange multipliers can also be used with inequality constraints $g(\mathbf{x}) \geqslant 0$

- Now two kinds of solutions:
- If $g(\mathbf{x}) > 0$, then the solution only depends on $f(\mathbf{x})$
 - Inside constraint surface with $\nabla f = 0$
 - Stationary point of $L(\mathbf{x}, \lambda)$ with $\lambda = 0$
 - Constraint $g(\mathbf{x})$ is said to be inactive
- If $g(\mathbf{x}) = 0$, then same as before (with equality constraint)
 - On boundary of constraint surface with ∇f pointing out
 - Stationary point of $L(\mathbf{x}, \lambda)$ with $\lambda > 0$
 - Constraint $q(\mathbf{x})$ is said to be active

Lagrange multipliers can also be used with inequality constraints $g(\mathbf{x}) \geqslant 0$

- In either case, $\lambda g(\mathbf{x}) = 0$
- Thus maximizing $f(\mathbf{x})$ subject to $g(\mathbf{x}) \geqslant 0$ is obtained by optimizing $L(\mathbf{x},\lambda)$ w.r.t. \mathbf{x} and λ subject to

$$g(\mathbf{x}) \geqslant 0$$

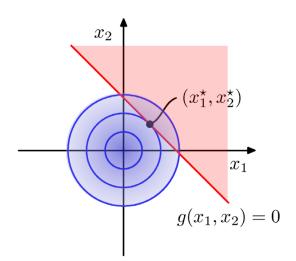
$$\lambda \geqslant 0$$

$$\lambda g(\mathbf{x}) = 0$$

These are known as the Karush-Kuhn-Tucker (KKT) conditions



Example: Maximize $f(\mathbf{x}) = 1 - x_1^2 - x_2^2$ subject to $g(\mathbf{x}) = x_1 + x_2 - 1 \geqslant 0$



Example: Maximize
$$f(\mathbf{x}) = 1 - x_1^2 - x_2^2$$
 subject to $g(\mathbf{x}) = x_1 + x_2 - 1 \geqslant 0$

So the Lagrangian function is

$$L(\mathbf{x}, \lambda) = 1 - x_1^2 - x_2^2 + \lambda(x_1 + x_2 - 1)$$

The conditions for L to be stationary are

$$\partial L/\partial x_1 = -2x_1 + \lambda = 0$$

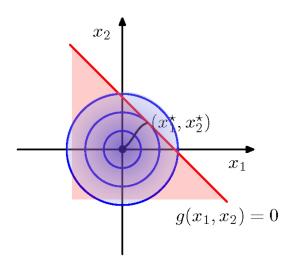
$$\partial L/\partial x_2 = -2x_2 + \lambda = 0$$

$$\partial L/\partial \lambda = x_1 + x_2 - 1 = 0$$

- Can solve to find $\lambda=1, x_1=x_2=rac{1}{2}$
 - Which still satisfies KKT conditions



Example: Maximize $f(\mathbf{x}) = 1 - x_1^2 - x_2^2$ subject to $g(\mathbf{x}) = -x_1 - x_2 + 1 \geqslant 0$



Example: Maximize
$$f(\mathbf{x}) = 1 - x_1^2 - x_2^2$$
 subject to $g(\mathbf{x}) = -x_1 - x_2 + 1 \geqslant 0$

So the Lagrangian function is

$$L(\mathbf{x}, \lambda) = 1 - x_1^2 - x_2^2 + \lambda(-x_1 - x_2 + 1)$$

The conditions for L to be stationary are

$$\frac{\partial L/\partial x_1 = -2x_1 - \lambda = 0}{\partial L/\partial x_2 = -2x_2 - \lambda = 0}$$
$$\frac{\partial L/\partial \lambda = x_1 + x_2 - 1 = 0}{\partial L/\partial \lambda = x_1 + x_2 - 1 = 0}$$

- Can solve to find $\lambda = -1$
 - which does not satisfy KKT condition $\lambda \geqslant 0$
- Instead use unconstrained solution $x_1 = x_2 = 0$
 - which does satisfy KKT conditions



Multiple constraints each get their own Lagrange multiplier

- Maximize $f(\mathbf{x})$ subject to $h_i(\mathbf{x}) = 0$ and $g_i(\mathbf{x}) \geqslant 0$
- Leads to the Lagrangian function

$$L(\mathbf{x}, \lambda, \nu) = f(\mathbf{x}) + \sum_{i} \lambda_{i} g_{i}(\mathbf{x}) + \sum_{j} u_{j} h_{j}(\mathbf{x})$$

- Still solve for $\nabla L(\mathbf{x}, \lambda, \nu) = 0$
- Trickier in general to figure out which $h_j(\mathbf{x})$ constraints should be active

Minimizing $f(\mathbf{x})$ with an inequality constraint requires a slightly different Lagrange

Subject to

$$g(\mathbf{x}) \leq 0$$

Minimize w.r.t. x

$$L(\mathbf{x}, \lambda) = f(\mathbf{x}) + \lambda g(\mathbf{x})$$

Summary of Lagrange multipliers with multiple inequality constraints

- Goal: maximize $f(\mathbf{x})$ subject to $g_i(\mathbf{x}) \geqslant 0$
- Write down Lagrangian function

$$L(\mathbf{x}, \lambda) = f(x) + \sum_{i} \lambda_{i} g_{i}(\mathbf{x})$$

- Find points where $\nabla L(\mathbf{x}, \lambda) = 0$
- Keep points that satisfy constraints $g_x(\mathbf{x}) \geqslant 0$
- Figure out which KKT conditions should be active
 - Don't need to try all 2^I combinations for SVMs
 - Because $f(\mathbf{x})$ and $g(\mathbf{x})$ form a "quadratic program"

Recap: Lagrange dual problem

Primal Problem

$$\max_{\mathbf{x}} f(\mathbf{x})$$
s.t. $g_i(\mathbf{x}) \ge 0, \quad i = 1, \dots, m$

$$h_j(\mathbf{x}) = 0, \quad j = 1, \dots, p$$

$$\mathbf{x} \in D$$

$$(1)$$

Dual Problem

$$\min_{\boldsymbol{\lambda}, \boldsymbol{\nu}} \quad \tilde{L}(\boldsymbol{\lambda}, \boldsymbol{\nu})
\text{s.t.} \quad \boldsymbol{\lambda} \ge 0$$
(2)

, where

$$\tilde{L}(\boldsymbol{\lambda}, \boldsymbol{\nu}) = \sup_{\mathbf{x} \in D} L(\mathbf{x}, \boldsymbol{\lambda}, \boldsymbol{\nu}) = \sup_{\mathbf{x} \in D} \left\{ f(\mathbf{x}) + \sum_{i} \lambda_{i} g_{i}(\mathbf{x}) + \sum_{j} \nu_{j} h_{j}(\mathbf{x}) \right\}$$

Recap: Lagrange dual problem

Primal Problem

$$\min_{\mathbf{x}} \quad f(\mathbf{x})$$
s.t. $g_i(\mathbf{x}) \le 0, \quad i = 1, \dots, m$

$$h_j(\mathbf{x}) = 0, \quad j = 1, \dots, p$$

$$\mathbf{x} \in D$$
(3)

Dual Problem

$$\max_{\boldsymbol{\lambda}, \boldsymbol{\nu}} \quad \tilde{L}(\boldsymbol{\lambda}, \boldsymbol{\nu})$$
s.t. $\boldsymbol{\lambda} \ge 0$ (4)

, where

$$\tilde{L}(\boldsymbol{\lambda}, \boldsymbol{\nu}) = \inf_{\mathbf{x} \in D} L(\mathbf{x}, \boldsymbol{\lambda}, \boldsymbol{\nu}) = \inf_{\mathbf{x} \in D} \left\{ f(\mathbf{x}) + \sum_{i} \lambda_{i} g_{i}(\mathbf{x}) + \sum_{j} \nu_{j} h_{j}(\mathbf{x}) \right\}$$

Example

Primal Problem

$$\min_{x} \quad \mathbf{c}^{T} \mathbf{x}$$
s.t. $\mathbf{A}_{1} \mathbf{x} \succeq \mathbf{b}_{1}$

$$\mathbf{A}_{2} \mathbf{x} = \mathbf{b}_{2}$$

$$\mathbf{x} \succeq 0$$
(5)

Example

Primal Problem

$$\min_{x} \quad \mathbf{c}^{T} \mathbf{x}$$
s.t. $\mathbf{A}_{1} \mathbf{x} \succeq \mathbf{b}_{1}$

$$\mathbf{A}_{2} \mathbf{x} = \mathbf{b}_{2}$$

$$\mathbf{x} \succeq 0$$
(5)

Dual Problem

$$\begin{split} \tilde{L}(\boldsymbol{\lambda}, \boldsymbol{\nu}) &= \inf_{\mathbf{x} \in D} L(\mathbf{x}, \boldsymbol{\lambda}, \boldsymbol{\nu}) \\ &= \inf_{\mathbf{x} \succeq 0} \left\{ (\mathbf{c}^T - \boldsymbol{\lambda}^T \mathbf{A}_1 - \boldsymbol{\nu}^T \mathbf{A}_2) \mathbf{x} + \boldsymbol{\lambda}^T \mathbf{b}_1 + \boldsymbol{\nu}^T \mathbf{b}_2 \right\} \\ &= \begin{cases} \boldsymbol{\lambda}^T \mathbf{b}_1 + \boldsymbol{\nu}^T \mathbf{b}_2 & \mathbf{c}^T - \boldsymbol{\lambda}^T \mathbf{A}_1 - \boldsymbol{\nu}^T \mathbf{A}_2 \succeq 0 \\ -\infty & \mathbf{c}^T - \boldsymbol{\lambda}^T \mathbf{A}_1 - \boldsymbol{\nu}^T \mathbf{A}_2 \prec 0 \end{cases} \end{split}$$

Example

Dual Problem

LP as a special case

Primal

$$\min_{x} c^{T}x$$
s.t. $Ax \ge b$ (7)
$$x \ge 0$$

LP as a special case

Primal

Dual

$$\min_{x} c^{T}x \qquad \max_{\lambda} b^{T}\lambda$$
s.t. $Ax \ge b$ (7) s.t. $A^{T}\lambda \le c$ (8)
$$x \ge 0 \qquad \qquad \lambda \ge 0$$

$$\tilde{L}(\lambda) = \inf_{x \ge 0} L(x, \lambda)$$

$$= \inf_{x \ge 0} \left\{ (c^{T} - \lambda^{T}A)x + \lambda^{T}b \right\}$$

$$= \begin{cases} \lambda^{T}b \quad \lambda^{T}A \le c^{T} \\ -\infty \quad \lambda^{T}A > c^{T} \end{cases}$$

Q1: Raw materials A1, A2 and A3 will be made into products X and Y. The ingredients and requirements for products are show in table.

Ingredients	Products		Minimal requirements
	X	Υ	willilliai requirements
A1	0.1	0.15	1
A2	1.7	0.75	7.5
А3	1.2	1.3	10
cost	3	2	

Ingredients	Products		- Minimal requirements
	X	Υ	
A1	0.1	0.15	1
A2	1.7	0.75	7.5
А3	1.2	1.3	10
cost	3	2	

min
$$z = 3x_1 + 2x_2$$

s.t. $0.1x_1 + 0.15x_2 \ge 1$
 $1.7x_1 + 0.75x_2 \ge 7.5$
 $1.2x_1 + 1.3x_2 \ge 10$
 $x_1, x_2 > 0$

Q1: Raw materials A1, A2 and A3 will be made into products X and Y. The ingredients and requirements for products are show in table.

Q2: The company is selling raw materials A1, A2 and A3. How to make the price for A1, A2 and A3 to maximize profit of the company and make sure the price is acceptable comparing to products X and Y?

Ingredients	Products		Minimal requirements
	Χ	Υ	willina requirements
A1	0.1	0.15	1
A2	1.7	0.75	7.5
А3	1.2	1.3	10
cost	3	2	

$$\max \quad w = 1y_1 + 7.5y_2 + 10y_3$$
s.t.
$$0.1y_1 + 1.7y_2 + 1.2y_3 \le 3$$

$$0.15y_1 + 0.75y_2 + 1.3y_3 \le 2$$

$$y_1, y_2, y_3 \ge 0$$

Karush-Kuhn-Tucker (KKT) Conditions

KKT conditions for differentiable g_i , h_i

- Primal feasible: $g_i(x) \le 0, h_i(x) = 0$
- Dual feasible: $\lambda > 0$
- Complementary slackness: $\lambda_i^* f_i(x^*) = 0$
- Zero gradient of Lagrangian w.r.t. x

$$\nabla f(x) + \sum_{i} \lambda_{i} \nabla g_{i}(x) + \sum_{j} \nu_{j} \nabla h_{j}(x) = 0$$

KKT for LP

Primal

Dual

$$\min_{x} c^{T}x \qquad \max_{\lambda} b^{T}\lambda$$
s.t. $Ax \ge b$ (9) s.t. $A^{T}\lambda \le c$ (10)
$$x > 0 \qquad \lambda \ge 0$$

Theorem (KKT for LP)

If x' is feasible for Primal Problem 9 and λ' is feasible for Dual Problem 10 and $c^Tx'=b^T\lambda'$, then x' and λ' is optimal for Problem 9 and 10 respectively.

Back to SVMs: Maximum margin solution is a fixed point of the Lagrangian function

- Recall, the maximum margin hyperplane is $\underset{\mathbf{w},b}{\operatorname{argmin}}_{\mathbf{w},b} \frac{1}{2} ||\mathbf{w}||^2$ subject to $d_p(\mathbf{w}^T \mathbf{x}_p + b) \geqslant 1$
 - Minimization of a quadratic function subject to multiple linear inequality constraints
- Will use Lagrange multipliers, a_p , to write Lagrangian function

$$L(\mathbf{w}, b, \mathbf{a}) = \frac{1}{2} ||\mathbf{w}||^2 - \sum_{p} a_p (d_p(\mathbf{w}^T \mathbf{x}_p + b) - 1)$$

• Note that \mathbf{x}_p and d_p are fixed for the optimization



Thank you!