COM S 578X: Optimization for Machine Learning

Lecture Note 4: Duality

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Outline

In this lecture:

- Lagrange dual problem
- Weak and strong duality
- Geometric interpretation
- Examples in machine learning

The Lagrangian

Standard optimization problem (may or may not be convex): Convex Optimization if: f convex. f c

$$L(\mathbf{x}, \mathbf{u}, \mathbf{v}) = f(\mathbf{x}) + \sum_{i=1}^{m} u_i g_i(\mathbf{x}) + \sum_{j=1}^{p} v_j h_j(\mathbf{x})$$

• weighted sum of objective and constraint functions

- $u_i \geq 0$ is dual variable (Lagrangian multiplier) associated with $g_i(\mathbf{x}) \leq 0$
- $v_j \in \mathbb{R}$ is dual variable (Lagrangian multiplier) associated with $h_j(\mathbf{x}) = 0$

Lagrangian Dual Function

Lagrangian dual function: $\Theta : \mathbb{R}^m \times \mathbb{R}^p \to \mathbb{R}$:

 $\Theta(\mathbf{u},\mathbf{v}) = \inf_{\mathbf{x}\in\mathcal{D}} L(\mathbf{x},\mathbf{u},\mathbf{v}) \text{ affine for w.r.t. } \mathbf{y},\mathbf{y}.$ $= \inf_{\mathbf{x}\in\mathcal{D}} \left(f(\mathbf{x}) + \sum_{i=1}^{m} u_i g_i(\mathbf{x}) + \sum_{i=1}^{p} \mathbf{v}_j h_j(\mathbf{x}) \right)$ $\Theta(\mathbf{u},\mathbf{v})$ is concave in \mathbf{u},\mathbf{v} , can be $-\infty$ for some \mathbf{u},\mathbf{v} by the second sec Lower bound property: If $\mathbf{u} \geq 0$, then $\Theta(\mathbf{u}, \mathbf{v}) \leq p^*$ opt. value of primal prob. Proof. If $\tilde{\mathbf{x}} \in \mathcal{D}$ and $\mathbf{u} \ge 0$, then doj. 01 $f(\tilde{\mathbf{x}}) \ge L(\tilde{\mathbf{x}}, \mathbf{u}, \mathbf{v}) \ge \inf_{\mathbf{x} \in \mathcal{D}} L(\mathbf{x}, \mathbf{u}, \mathbf{v}) = \Theta(\mathbf{u}, \mathbf{v}).$ duf. of Lagrangian dual Since this holds for any $\tilde{\mathbf{x}} \in \mathcal{D}$, minimizing over all $\tilde{\mathbf{x}}$ yields $p^* \geq \Theta(\mathbf{u}, \mathbf{v})$. JKL (CS@ISU) 4 / 21

Example: Least-norm solution of linear equations

Minimize
$$\mathbf{x}^{\top}\mathbf{x}$$

subject to $\mathbf{A}\mathbf{x} = \mathbf{b}$ \leftarrow $\mathbf{y} \in \mathbb{R}^{n}$

Dual function:

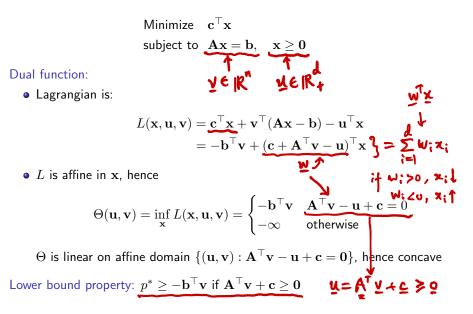
- Lagrangian is: $L(\mathbf{x}, \mathbf{v}) = \mathbf{x}^\top \mathbf{x} + \mathbf{v}^\top (\mathbf{A}\mathbf{x} \mathbf{b})$
- To minimize $L(\mathbf{x}, \mathbf{v})$ over \mathbf{x} , set gradient equal to zero

$$\nabla_{\mathbf{x}} L(\mathbf{x}, \mathbf{v}) = 2\mathbf{x} + \mathbf{A}^{\top} \mathbf{v} = 0 \quad \Longrightarrow \quad \mathbf{x} = -\frac{1}{2} \mathbf{A}^{\top} \mathbf{v}$$

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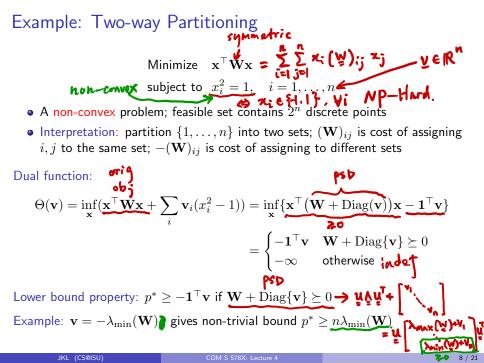
• Plug it in L to obtain Θ : $\Theta(\mathbf{v}) = L(-\frac{1}{2}\mathbf{A}^{\top}\mathbf{v}, \mathbf{v}) = -\frac{1}{4}\mathbf{v}^{\top}\mathbf{A}\mathbf{A}^{\top}\mathbf{v} - \mathbf{b}^{\top}\mathbf{v},$ which is clearly a concave function of \mathbf{v} . Lower bound property: $p^* \ge -\frac{1}{4}\mathbf{v}^{\top}\mathbf{A}\mathbf{A}^{\top}\mathbf{v} - \mathbf{b}^{\top}\mathbf{v}$ for all $\mathbf{v} \le -\frac{1}{2}\mathbf{v}^{\top}\mathbf{v}$ $\ge -\frac{1}{2}\mathbf{v}$ (largest UB).

Example: Linear Programming



Example: Equality Constrained Norm Minimization

$$\begin{aligned} & \text{Minimize } \|\mathbf{x}\| \\ & \text{subject to } \mathbf{A}\mathbf{x} = \mathbf{b} \leftarrow \mathbf{y} \in \mathbb{R}^{n} \\ & \text{Dual function: } \Theta(\mathbf{v}) = \inf(\|\mathbf{x}\| - \mathbf{v}^{\top}\mathbf{A}\mathbf{x} + \mathbf{b}^{\top}\mathbf{v}) = \begin{cases} \mathbf{b}^{\top}\mathbf{v} & \|\mathbf{A}^{\top}\mathbf{v}\|_{*} \leq 1 \\ -\infty & \text{otherwise} \end{cases} \\ & \text{where } \|\mathbf{v}\|_{*} \triangleq \sup_{\|\mathbf{u}\| \leq 1} \mathbf{u}^{\top}\mathbf{v} \text{ (referred to as drain norm of } \|\cdot\|) \end{cases} \\ & \text{Proof.} \\ & \text{It follows from the fact that } \inf_{\mathbf{x}}(\|\mathbf{x}\| - \mathbf{y}^{\top}\mathbf{x}) = 0 \text{ if } \|\mathbf{y}\|_{*} \leq 1, -\infty \text{ otherwise.} \end{cases} \\ & \text{otherwise} \quad \mathbf{h}^{\top}\mathbf{y}\|_{*} \leq 1, \text{ then } \|\mathbf{x}\| - \mathbf{y}^{\top}\mathbf{x} \geq 0, \forall \mathbf{x}, \text{ with equality if } \mathbf{x} = \mathbf{0} \\ & \text{otherwise} \quad \mathbf{h}^{\top}\mathbf{y}\|_{*} \leq 1, \text{ then } \|\mathbf{x}\| - \mathbf{y}^{\top}\mathbf{x} \geq 0, \forall \mathbf{x}, \text{ with equality if } \mathbf{x} = \mathbf{0} \\ & \text{otherwise} \quad \mathbf{h}^{\top}\mathbf{y}\|_{*} > 1, \text{ choose } \mathbf{x} = t\mathbf{u}, \text{ where } \mathbf{u} \text{ satisfies } \|\mathbf{u}\| \leq 1, \mathbf{u}^{\top}\mathbf{y} = \|\mathbf{y}\|_{*} > 1: \\ & \|\mathbf{x}\| - \mathbf{y}^{\top}\mathbf{x} = t(\|\mathbf{u}\| - \|\mathbf{y}\|_{*}) \rightarrow -\infty \text{ as } t \rightarrow \infty \end{aligned}$$



Lagrangian Dual and Conjugate Function

$$\begin{array}{c} \text{Minimize} \quad f(\mathbf{x}) \\ \text{subject to} \quad \mathbf{A}\mathbf{x} \leq \mathbf{b}, \\ \textbf{X} \in \mathbf{R}^{\mathsf{M}} \end{array} \quad \mathbf{C}\mathbf{x} = \mathbf{d} \\ \textbf{x} \in \mathbf{R}^{\mathsf{N}} \end{array}$$

Dual function:

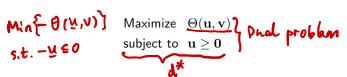
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$$\Theta(\mathbf{u}, \mathbf{v}) = \inf_{\mathbf{x} \in \text{dom}(f)} \left(f(\mathbf{x}) + (\mathbf{A}^{\top}\mathbf{u} + \mathbf{C}^{\top}\mathbf{v})^{\top}\mathbf{x} - \mathbf{b}^{\top}\mathbf{u} - \mathbf{d}^{\top}\mathbf{v} \right)$$
$$= -f^*(-\mathbf{A}^{\top}\mathbf{u} - \mathbf{C}^{\top}\mathbf{v}) - \mathbf{b}^{\top}\mathbf{u} - \mathbf{d}^{\top}\mathbf{v}$$
Legendre – Fenchel conjugate (convex conjugate)
Definition of conjugate function: $f^*(\mathbf{y}) = \sup_{x \in \text{dom}(f)} (\mathbf{y}^{\top}\mathbf{x} - f(\mathbf{x}))$ Simplifies derivation of dual if conjugate of f is known

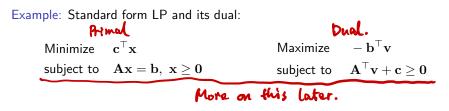
Example: Entropy maximization

$$f(\mathbf{x}) = \sum_{i=1}^{n} x_i \log x_i, \quad f^*(\mathbf{y}) = \sum_{i=1}^{n} \exp(y_i - 1)$$

The Lagrangian Dual Problem



- Finds largest lower bound on p^* , obtained from Lagrangian dual function
- A convex optimization problem; optimal value denoted d^*
- \mathbf{u}, \mathbf{v} are dual feasible if $\mathbf{u} \ge \mathbf{0}$, $(\mathbf{u}, \mathbf{v}) \in \operatorname{dom}(\Theta)$
- Often simplified by making implicit constraint $\mathbf{u}\geq\mathbf{0},\;(\mathbf{u},\mathbf{v})\in\mathrm{dom}(\Theta)$ explicit



Weak and Strong Duality

Weak duality: $d^* \leq p^*$

- Always holds (for convex and non-convex problems)
- Can be used to find non-trivial lower bounds for difficult problems
- · For example, solving SDP Semidefinite Programming.

 $\begin{aligned} \mathsf{Maximize} \quad & -\mathbf{1}^{\top}\mathbf{v} \\ \mathsf{subject to} \quad & \mathbf{W} + \mathrm{Diag}\{\mathbf{v}\} \succeq 0 \end{aligned}$

yields a lower bound for the two-way partitioning problem

Strong duality: $d^* = p^*$

- Does not hold in general
- Usually hold for convex problems
- Conditions that guarantee strong duality in convex problems are called constraint qualifications

(CQ)

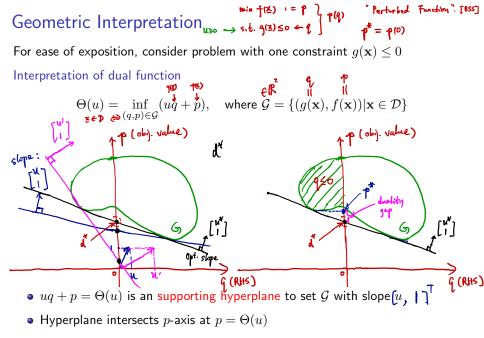
Slater's Constraint Qualification

Strong duality holds for a convex problem

- Also guarantees that the dual optimum is attained (if $p^* > -\infty$)
- Can be further relaxed: e.g., can replace int \mathcal{D} with relint \mathcal{D} (interior relative to affine hull); linear inequalities do not need to hold with strict inequality, ...
- There exist many other types of constraint qualifications (see [BSS, Ch. 5])

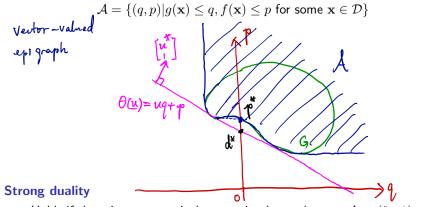
Other Well-Known CQs

- LICQ (Linear independence CQ): Gradients of active inequality constraints and gradients of equality constraints are linearly independent at x*
 - MFCQ (Manasarian-Fromovitz CQ): Gradients of equality constraints are LI at \mathbf{x}^* , $\exists \mathbf{d} \in \mathbb{R}^n$ such that $\nabla g_i^\top(\mathbf{x}^*)\mathbf{d} < 0$ for active inequality constraints, $\nabla h_i^\top(\mathbf{x}^*)\mathbf{d} = 0$ for equality constraints
 - CRCQ (Constant rank CQ): For each subset of gradients of active inequality constraints & gradients of equality constraints, the rank at x^* 's vicinity is constant
 - CPLD (Constant positive linear dependence CQ): For each subset of gradients of active inequality constraints & gradients of equality constraints, if it's positive-linear dep. at x^* then it's positive-linear dependent in x^* 's vicinity
 - QNCQ (Quasi-normality CQ): If gradients of active inequality constraints and gradients of equality constraints are positively-linearly dependent at \mathbf{x}^* with duals u_i for inequalities and v_j for equalities, then there is no sequence $\mathbf{x}_k \to \mathbf{x}^*$ such that $v_j \neq 0 \Rightarrow v_j h_j(\mathbf{x}_k) > 0$ and $u_i \neq 0 \Rightarrow u_i g_i(\mathbf{x}_k) < 0$

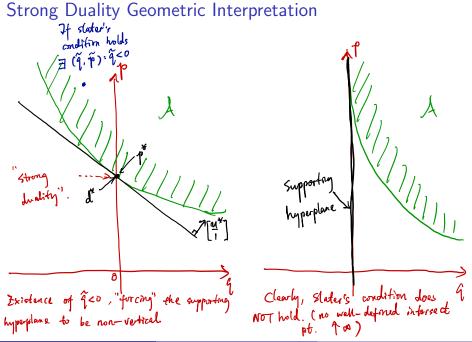


Geometric Interpretation

Epigraph variation: Same interpretation if \mathcal{G} is replaced with



- $\bullet\,$ Holds if there is a non-vertical supporting hyperplane to ${\cal A}$ at $(0,p^*)$
- For convex problem, ${\cal A}$ is convex, hence has supporting hyperplane at $(0,p^*)$
- Slater's condition: If there exist $(\tilde{q}, \tilde{p}) \in \mathcal{A}$ with $\tilde{q} < 0$, then supporting hyperplanes at $(0, p^*)$ must be non-vertical



Example: Inequality Form of LP

Assume A is full row rank. Primal problem: Minimize $\mathbf{c}^{\top}\mathbf{x}$ subject to $Ax < b \leftarrow \mathcal{U} \geq \mathcal{Q}$ $\Theta(\mathbf{u}) = \inf_{\mathbf{x}} \left((\mathbf{c} + \mathbf{A}^{\top} \mathbf{u})^{\top} \mathbf{x} - \mathbf{b}^{\top} \mathbf{u} \right) = \begin{cases} -\mathbf{b}^{\top} \mathbf{u} & \mathbf{A}^{\top} \mathbf{u} + \mathbf{c} = \mathbf{0} \\ -\infty & \text{otherwise} \end{cases}$ Dual function: Dual problem: $\begin{array}{ll} \mathsf{M}\mathsf{aximize} & -\mathbf{b}^{\top}\mathbf{u} \\ \mathsf{subject to} & \mathbf{A}^{\top}\mathbf{u} + \mathbf{c} = \mathbf{0}, \quad \mathbf{u} \geq \mathbf{0} \end{array} \begin{array}{l} \mathsf{L} \\ \end{array}$

• From Slater's condition: $p^* = d^*$ if $A\tilde{\mathbf{x}} < \mathbf{b}$ for some $\tilde{\mathbf{x}}$

• In fact, $p^* = d^*$ except when primal and dual are infeasible (LICR)

Example: Quadratic Program positive definite. Primal problem ($\mathbf{P} \in \mathbb{S}^n_{++}$): Minimize $\mathbf{x}^{\top} \mathbf{P} \mathbf{x}$ subject to $Ax < b \longleftarrow \mathcal{V} \geq \mathcal{O}$ Dual function: Lagrangian $\Theta(\mathbf{\hat{x}}) = \inf_{\mathbf{x}} \left(\underbrace{\mathbf{x}^{\top} \mathbf{P} \mathbf{x} + \mathbf{u}^{\top} (\mathbf{A} \mathbf{x} - \mathbf{b})}_{\text{quadratic}} \right) = -\frac{1}{4} \mathbf{u}^{\top} \mathbf{A} \mathbf{P}^{-1} \mathbf{A}^{\top} \mathbf{u} - \mathbf{b}^{\top} \mathbf{u}$ take der, set to $0 \Rightarrow LES: 2PX + A^T Y = 0 \Rightarrow X = - EPATY$ Dual problem: $\mathsf{Maximize} \qquad -\frac{1}{4}\mathbf{u}^{\top}\mathbf{A}\mathbf{P}^{-1}\mathbf{A}^{\top}\mathbf{u} - \mathbf{b}^{\top}\mathbf{u}$ invertible subject to $\mathbf{u} \geq \mathbf{0}$

• From Slater's condition: $p^* = d^*$ if $A\tilde{x} < b$ for some \tilde{x}

• In fact, $p^* = d^*$ always (stater's condition is autometric).

Example: Support Vector Machine

Given labels $y \in \{-1, 1\}^n$, feature vectors $\mathbf{x}_1, \ldots, \mathbf{x}_m$. Let $\mathbf{X} \triangleq [\mathbf{x}_1, \ldots, \mathbf{x}_m]^\top$ Recall from Lecture 1 that the support vector machine problem:

Introducing dual variables $\mathbf{u},\mathbf{v}\geq\mathbf{0}$ to obtain the Lagrangian:

$$L(\mathbf{w}, b, \boldsymbol{\epsilon}, \mathbf{u}, \mathbf{v}) = \underbrace{\frac{1}{2} \|\mathbf{w}\|_{2}^{2} + C \sum_{i=1}^{m} \epsilon_{i} + \sum_{i=1}^{n} u_{i}(1 - \epsilon_{i} - y_{i}(\mathbf{w}^{\top}\mathbf{x}_{i} + b)) - \sum_{i=1}^{n} v_{i}\epsilon_{i}}_{\text{drig: obj. obj.}}$$

Minimizing over $\mathbf{w}, b, \boldsymbol{\epsilon}$ yields the Lagrangian dual function .

Example: Support Vector Machine

$$\Theta(\mathbf{u}, \mathbf{v}) = \begin{cases} \mathbf{v}^{\mathsf{NSD}} \\ -\frac{1}{2} \mathbf{u}^{\top} \tilde{\mathbf{X}}^{\top} \tilde{\mathbf{X}} \mathbf{u} + \mathbf{1}^{\top} \mathbf{u} & \text{if } \mathbf{u} = C\mathbf{1} - \mathbf{v}, \mathbf{u}^{\top} \mathbf{y} = 0 \\ -\infty & \text{otherwise} \end{cases}$$

where $\tilde{\mathbf{X}} \triangleq \mathbf{X} \text{Diag}\{y_1, \dots, y_m\}$. The dual problem, after eliminating \mathbf{v} , becomes:

$$\begin{array}{ll} \underset{\boldsymbol{\alpha}}{\text{Minimize}} & \frac{1}{2} \mathbf{u}^{\top} \tilde{\mathbf{X}}^{\top} \tilde{\mathbf{X}} \mathbf{u} - \mathbf{1}^{\top} \mathbf{u} \\ \text{subject to} & \mathbf{u}^{\top} \mathbf{y} = 0, \quad 0 \leq u_i \leq C, \ i = 1, \dots, m. \end{array}$$

- Slater's condition is satisfied \Rightarrow strong duality
- In ML literature, more common to work with the dual: Quadratic having PSD Hessian with simple bounds, plus a single linear & simple box constraints
- At optimality, we can verify that $\mathbf{w} = \tilde{\mathbf{X}}\mathbf{u}$ (this is not a coincidence! will be proved by KKT conditions in next class)

Next Class

Optimality Conditions