CME 307 / MS&E 311: Optimization

Convex duality

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Announcements

facts:

- CME 307 has a qual (for ICME PhD students), and
- you want more lectures

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new plan for course:

1. KKT conditions and IPMs
2. first order methods
3. Bayesian optimization
4. two sessions of project presentations

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- Friday sessions will be research paper presentations
- next paper signups will open by this coming Friday.

Fenchel dual

Definition (Fenchel dual)

The **Fenchel dual** of a function $f : \mathcal{X} \to \mathbf{R}$ is

$$f^*(w) = \sup_{x \in \mathcal{X}} \langle w, x \rangle - f(x)$$

also called the **conjugate function**. draw picture!
https://remilepriol.github.io/dualityviz/

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example: $f(x) = \|x\|_1$, $x \in \mathbf{R}^n$

$$f^*(w) = \sup_{x \in \mathbf{R}^n} \langle w, x \rangle - \|x\|_1 = \begin{cases} 0 & \|w\|_\infty \leq 1 \\ \infty & \text{otherwise} \end{cases}$$

$\implies$ fenchel dual of ℓ_1 norm is indicator of ℓ_∞ ball

Biconjugate

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The **biconjugate** of a function $f : \mathcal{X} \to \mathbf{R}$ is

$$f^{**}(x) = \sup_{w \in \mathcal{X}^*} \langle w, x \rangle - f^*(w)$$

- for convex $f : \mathbf{R} \to \mathbf{R}$, $f^{**} = f$
- for nonconvex f, f^{**} is convex hull of f

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example: consider $f : \mathbf{R} \to \mathbf{R}$ defined by

$$f(x) = \begin{cases} 0 & x \in \{-1, 1\} \\ \infty & \text{otherwise} \end{cases}$$

what is f^*? f^{**}?

Outline

Lagrange duality

Why duality?

- certify optimality
  - turn $\forall$ into $\exists$
  - use dual lower bound to derive stopping conditions
- new algorithms based on the dual
  - solve dual, then recover primal solution

Nonlinear duality

primal problem with solution $x^\star \in \mathbf{R}^n$, optimal value $p^\star$:

$$\begin{array}{lll} \text{minimize} & f(x) & \\ \text{subject to} & Ax = b: & \text{dual } y \\ \text{variable} & x \in \mathbf{R}^n & \end{array} \qquad (\mathcal{P})$$

if x is feasible, then $Ax = b$, so $\langle y, Ax - b \rangle = 0$.

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define the **Lagrangian**

$$\mathcal{L}(x, y) \;:=\; f(x) - \langle y, b - Ax\rangle$$

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$$\begin{aligned} \mathcal{L}(x,y) &:= f(x) - \langle y, b - Ax\rangle \\ p^\star &= \inf_{x:Ax=b} \mathcal{L}(x,y) \geq \inf_x \mathcal{L}(x,y) \end{aligned}$$

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Lagrange duality

inequality holds for any $y \in \mathbf{R}^m$, so we have proved **weak duality**

$$\begin{aligned} p^\star &\geq g(y) \quad \forall y \in \mathbf{R}^m \\ &\geq \underbrace{\sup_y g(y)}_{\mathcal{D}} =: d^\star \end{aligned} \tag{1}$$

dual optimal value $d^\star \leq p^\star$

Strong duality

Definition (Duality gap)

The **duality gap** for a primal-dual pair (x, y) is $f(x) - g(y)$

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strong duality holds

- for feasible LPs
- for convex problems under **constraint qualification** aka **Slater's condition**. feasible region has an **interior point** x so that all inequality constraints hold strictly

strong duality fails if either primal or dual problem is infeasible or unbounded

Lagrange duality with inequality constraints

primal problem with solution $x^\star \in \mathbf{R}^n$, optimal value $p^\star$:

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to construct Lagrangian $\mathcal{L}(x, y) = f(x) - \langle y, b - Ax \rangle$, ensure value is **better** (lower) when x and y are feasible

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this holds for all $y \geq 0$, so we have weak duality

$$p^\star \geq \sup_{y \geq 0} g(y) =: d^\star$$

SVM dual

support vector machine: for $x_i \in \mathbf{R}^n$, $y_i \in \{-1, 1\}$, $i = 1, \ldots, m$

$$\begin{array}{lll} \text{minimize} & \frac{1}{2}\|w\|^2 + 1^T s & \\ \text{subject to} & y_i w^T x_i + s_i \geq 1 \quad i = 1, \ldots, m : & \alpha \geq 0 \\ & s \geq 0 : & \mu \geq 0 \end{array} \qquad \text{(SVM)}$$

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verify Slater's condition. strong duality holds!

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$$\mathcal{L}(w, s, \alpha, \mu) = \frac{1}{2}\|w\|^2 + 1^T s - \sum_{i=1}^{m} \alpha_i (y_i w^T x_i + s_i - 1) - \mu^T s$$

- minimize $\mathcal{L}(w, s, \alpha, \mu)$ over w to eliminate w

$$w = \sum_{i=1}^{m} \alpha_i y_i x_i$$

- minimize $\mathcal{L}(w, s, \alpha, \mu)$ over s $\implies$ $\alpha + \mu = 1$
- $\implies$ can eliminate $\mu = 1 - \alpha$, with resulting constraints $0 \leq \alpha \leq 1$

SVM dual

so simplify:

$$
\begin{aligned}
g(\alpha) &= \inf_{w,s} \mathcal{L}(w, s, \alpha, 1-\alpha) \\
&= \frac{1}{2}\|w\|^2 - w^T \sum_{i=1}^{m} \alpha_i y_i x_i + 1^T \alpha \\
&= -\frac{1}{2}\| \sum_{i=1}^{m} \alpha_i y_i x_i \|^2 + 1^T \alpha
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define $K \in \mathbf{R}^m$ so $K_{ij} = y_i y_j x_i^T x_j$. then

$$\| \sum_{i=1}^{m} \alpha_i y_i x_i \|^2 = \sum_{i=1}^{m} \sum_{j=1}^{m} \alpha_i \alpha_j y_i y_j x_i^T x_j = \alpha^T K \alpha$$

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dual problem:

$$\begin{array}{ll} \text{maximize} & -\frac{1}{2}\alpha^T K \alpha + 1^T \alpha \\ \text{subject to} & 0 \leq \alpha \leq 1 \end{array} \qquad \text{(SVM-dual)}$$

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new solution ideas! proj grad, coord descent (SMO), kernel trick

Generalize Lagrangian duality

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$$0 \geq Ax - b \quad \text{with} \quad 0 \geq g(x)$$

(harder to derive explicit form for dual problem)

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- **conic duality:** for cone K, replace

$$b - Ax \geq 0 \quad \text{with} \quad b - Ax \in K$$

  define **slack vector** $s = b - Ax \in K$
  for weak duality, dual y must satisfy

$$\langle y, s \rangle \geq 0 \quad \forall s \in K$$

Dual cones

this inequality defines the **dual cone** K^*:

Definition (dual cone)

the dual cone K^* of a cone K is the set of vectors y such that

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examples of cones and their duals:

- K acute, K^* obtuse
- $K = \mathbf{R}^m_+$, $K^* = \mathbf{R}^m_+$
- $K = \{x \in \mathbf{R}^n \mid \|x\| \leq x_0\}$, $K^* = \{y \in \mathbf{R}^n \mid \|y\| \leq y_0\}$
- $K = \{X \in \mathbf{S}^n \mid X \succeq 0\}$, $K^* = \{Y \in \mathbf{S}^n \mid Y \succeq 0\}$

inner product $\langle X, Y \rangle = \mathbf{tr}(X^T Y) = \sum_{ij} X_{ij} Y_{ij}$ for $X, Y \in \mathbf{S}^n$

Conic duality

primal problem with solution $x^\star \in \mathbf{R}^n$, optimal value $p^\star$:

$$\begin{array}{ll} \text{minimize} & \langle c, x \rangle \\ \text{subject to} & b - Ax \in K : \quad y \in K^* \\ \text{variable} & x \in \mathbf{R}^n \end{array} \qquad (\mathcal{P})$$

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for $y \in K^*$, construct Lagrangian $\mathcal{L}(x, y) = \langle c, x\rangle - \langle y, b - Ax\rangle$, ensure value is **better** (lower) when x and y are feasible

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which is $-\infty$ unless $c + A^* y = 0$, so ...

Conic duality

define the **dual problem**

$$\begin{array}{ll} \text{maximize} & \langle y, -b \rangle \\ \text{subject to} & c + A^* y = 0 \\ \text{variable} & y \in K^* \end{array} \qquad (\mathcal{D})$$

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again, we have weak duality $p^\star \geq d^\star$ and,
(under a constraint qualification) strong duality $p^\star = d^\star$

Strong duality and complementary slackness

Definition (complementary slackness)

The primal-dual pair x and y are **complementary** if

$$\langle y, b - Ax \rangle = 0 \qquad \Longleftrightarrow \qquad y_i(b_i - a_i^T x) = 0, \quad i = 1, \ldots, n$$

They satisfy **strict complementary slackness** if for each $i = 1, \ldots, n$, exactly one of the following holds:

$$y_i = 0 \qquad \text{or} \qquad (b_i - a_i^T x) = 0.$$

for conic problem, strong duality $\Longleftrightarrow$ complementary slackness

$$\begin{aligned} \langle y, b - Ax \rangle &= \langle y, b \rangle - \langle A^T y, x \rangle \\ &= \langle y, b \rangle + \langle c, x \rangle \\ &= \langle c, x \rangle - \langle y, -b \rangle \end{aligned}$$

First-order optimality condition

The KKT conditions are first-order **necessary** conditions for optimality of optimization problem.

Theorem (KKT conditions)

Suppose $x^\star$ and $y^\star$ are primal and dual optimal, respectively. Then

- **stationarity.** *$x^\star$ minimizes the Lagrangian at $y^\star$. If $\mathcal{L}$ is differentiable, then*

$$\nabla_x \mathcal{L}(x^\star, y^\star) = 0.$$

- **feasibility.** *$x^\star$ is primal feasible; $y^\star$ is dual feasible.*
- **complementary slackness.** *dual variable $y_i^\star$ is nonzero only if the ith constraint is active at $x^\star$.*

- KKT conditions are named after Karush, Kuhn, and Tucker.
- KKT conditions turn optimization problem into a system of equations.
- If the problem is convex, then the KKT conditions are also **sufficient** for optimality.

KKT conditions: example

nonlinear optimization with inequality constraints:

$$\begin{array}{ll} \text{minimize} & f(x) \\ \text{subject to} & Ax \leq b: \quad y \geq 0 \end{array}$$

Lagrangian $\mathcal{L}(x, y) = f(x) - \langle y, Ax - b \rangle$.

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- **stationarity.** $x^\star$ minimizes the Lagrangian at $y^\star$:

$$\nabla_x \mathcal{L}(x^\star, y^\star) = 0 \implies \nabla f(x^\star) = A^T y^\star$$

- **feasibility.** $Ax^\star \leq b$ is primal feasible; $y^\star \geq 0$ is dual feasible.
- **complementary slackness.** dual variable $y_i^\star$ is nonzero only if the ith constraint is active at $x^\star$:

$$\langle y^\star, b - Ax^\star \rangle = 0$$

KKT Example

Consider the following optimization problem:

$$\begin{aligned} \text{minimize} \quad & x^2 + y^2 \\ \text{subject to} \quad & x + y \leq -1 : \quad \lambda \geq 0 \\ & x - y = 0 : \quad \mu \end{aligned}$$

Lagrangian:

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Lagrangian:

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KKT conditions:

1. stationarity: $\nabla_x L(x, y, \lambda, \mu) = 0$, $\nabla_y L(x, y, \lambda, \mu) = 0$, ie,

$$\frac{\partial \mathcal{L}}{\partial x} = 2x + \lambda + \mu = 0$$
$$\frac{\partial \mathcal{L}}{\partial y} = 2y + \lambda - \mu = 0$$

2. feasibility:
   - primal: $x + y \leq -1$ and $x - y = 0$
   - dual: $\lambda \geq 0$
3. complementary slackness: $\lambda = 0$ or $x + y = -1$ (or both)

Lagrangian:

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   - dual: $\lambda \geq 0$
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solve!

Lagrangian:

$$\mathcal{L}(x, y, \lambda, \mu) = x^2 + y^2 + \lambda(x + y + 1) + \mu(x - y)$$

KKT conditions:

1. stationarity: $\nabla_x L(x, y, \lambda, \mu) = 0$, $\nabla_y L(x, y, \lambda, \mu) = 0$, ie,

$$\frac{\partial \mathcal{L}}{\partial x} = 2x + \lambda + \mu = 0$$
$$\frac{\partial \mathcal{L}}{\partial y} = 2y + \lambda - \mu = 0$$

2. feasibility:
   - primal: $x + y \leq -1$ and $x - y = 0$
   - dual: $\lambda \geq 0$
3. complementary slackness: $\lambda = 0$ or $x + y = -1$ (or both)

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- primal feasibility (PF) $\implies x = y$

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- so use stationarity to solve for optimal dual: $\lambda^\star = \frac{1}{2}$, $\mu^\star = 0$

Summary

- Duality provides lower bounds on the optimal value of an optimization problem.
- Construct the Lagrangian for any optimization problem by
  1. adding a linear combination of the constraints to the objective,
  2. restricting the associated dual variables to ensure Lagrangian provides a lower bound when primal is feasible.
- Duality can be used to certify optimality or as a stopping condition.
- KKT conditions give necessary (and for convex problems, sufficient) conditions for optimality,
  - ...and hence new ways to solve the problem by solving the KKT system.
  - Solving KKT conditions reduces to a linear system for problems with equality constraints,
  - but more complex for problems with inequality (or conic) constraints.