

COMP9501: Machine Learning

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Duality

Tools prepared for SVM

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 Suppose we want to find lower bound on the optimal value in our convex problem:

$$B \le \min_{x \in C} f(x)$$

For instance, consider the simple LP:

$$\min_{x,y} x + y$$

subject to $x + y \ge 2$
 $x, y \ge 0$

Luckily, the lower bound here is easy: take B = 2

Try again

$$\min_{x,y} x + 3y$$

subject to $x + y \ge 2$
 $x, y \ge 0$

$$x + y \ge 2$$

$$+ 2y \ge 0$$

$$= x + 3y \ge 2$$

Lower bound B = 2

More general

$$\min_{x,y} px + qy$$

subject to $x + y \ge 2$
 $x, y \ge 0$

$$a + b = p$$
$$a + c = q$$
$$a, b, c \ge 0$$

Lower bound B = 2a, for any a, b, c satisfying above³

 What is the best we can do? Maximize our lower bound over all possible a, b, c

$$\min_{x,y} px + qy$$

subject to $x + y \ge 2$
 $x, y \ge 0$

$$\max_{a,b,c} 2a$$
subject to $a + b = p$

$$a + c = q$$

$$a, b, c \ge 0$$

called primal LP

called dual LP

Note: the number of dual variables is the number of primal constraints

Try another one

$$\min_{x,y} px + qy$$
subject to $x \ge 0$

$$y \le 1$$

$$3x + y = 2$$

$$\max_{a,b,c} 2c - b$$
 subject to $a + 3c = p$
$$-b + c = q$$

$$a, b \ge 0$$

called primal LP

called dual LP

- Note: for the ≤ constraints, need to convert them first into ≥ constraints
- Note: for = constraints, the corresponding dual variables are not constrained
- Note: for max program, the dual program is min, and since we need to find the minimum upper bound, ≤ constraint unchanged , but ≥ converts to ≤

Given $c \in \mathcal{R}^n, A \in \mathcal{R}^{m \times n}, b \in \mathcal{R}^m, G \in \mathcal{R}^{r \times n}, h \in \mathcal{R}^r$

$$\min_{x} c^{T} x$$

subject to $Ax = b$
$$Gx \le h$$

called primal LP

$$\max_{u,v} -b^T u - h^T v$$
 subject to
$$-A^T u - G^T v = c$$

$$v \ge 0$$

called dual LP

• Explanation #1: for any u and $v \ge 0$, and x primal feasible,

$$-u^T(Ax - b) - v^T(Gx - h) \ge 0$$

- Or $(-A^Tu G^Tv)^Tx \ge -b^Tu h^Tv$
- So if let $c = -A^T u G^T v$, we get a lower bound on primal optimal value

Another "deeper" perspective on LP duality

$$\min_{x} c^{T} x$$

subject to $Ax = b$
$$Gx \le h$$

called primal LP

$$\max_{u,v} - b^T u - h^T v$$
 subject to
$$-A^T u - G^T v = c$$

$$v \ge 0$$

called dual LP

- Explanation #2: for any u and $v \ge 0$, and x primal feasible:
- $c^T x \ge c^T x + u^T (Ax b) + v^T (Gx h) := L(x, u, v)$
- So if C denotes the unknown primal feasible set, f^* primal optimal value, then for any u and $v \ge 0$,
- $f^* = \min_{x \in C} c^T x \ge \min_{x \in C} L(x, u, v) \ge \min_{x \in R^n} L(x, u, v) \coloneqq g(u, v)$

Another "deeper" perspective on LP duality

In other words,

$$g(u, v) = \min_{x \in \mathbb{R}^n} c^T x + u^T (Ax - b) + v^T (Gx - h)$$

is a lower bound on f^* for any u and $v \ge 0$

Note that:

$$g(u,v) = \begin{cases} -b^T u - h^T v & \text{if } c = -A^T u - G^T v \\ -\infty & \text{otherwise} \end{cases}$$

- Thus, if we maximize g(u, v) over u and $v \ge 0$ and get the tightest bound, the result gives exactly the dual LP as before
- This last perspective is actually completely general, and applies to arbitrary optimization problems (even nonlinear and nonconvex ones)

Lagrangian

Consider general minimization problem

$$\min_{x \in \mathcal{R}^n} f(x)$$

subject to
$$h_i(x) \le 0, i = 1, \dots, m$$

$$l_j(x) = 0, j = 1, \dots, r$$

- Need not to be convex, but for sure we will pay special attention to convex cases
- We define the Lagrangian as

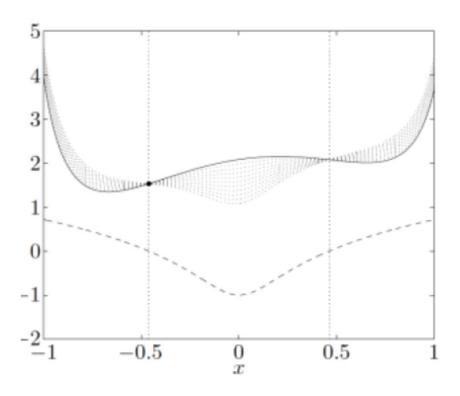
$$L(x, u, v) = f(x) + \sum_{i=1}^{m} u_i h_i(x) + \sum_{j=1}^{r} v_j l_j(x)$$

• New variables $u \in R^m$, $v \in R^r$ with $u \ge 0$ (implicitly we define $L(x, u, v) = -\infty$ for u < 0

Lagrangian

• For any $u \ge 0$ and v, at each feasible x, there is

$$L(x, u, v) = f(x) + \sum_{i=1}^{m} u_i \underbrace{h_i(x)}_{\leq 0} + \sum_{j=1}^{r} v_j \underbrace{l_j(x)}_{=0} \leq f(x)$$



- Solid line is *f*
- Dashed line is h, hence feasible set $\approx [-0.46, 0.46]$
- Each dotted line shows L(x, u, v) for different choices of u and v

Lagrange dual function

- Same relaxation as before
- Let C denote primal feasible set, f* denote primal optimal value
- Minimizing L(x, u, v) over all $x \in \mathbb{R}^n$ gives a lower bound:

$$f^* \ge \min_{x \in \mathcal{C}} L(x, u, v) \ge \min_{x \in \mathcal{R}^n} L(x, u, v) := g(u, v)$$

• We call g(u, v) the Lagrange dual function, and it gives a lower bound on f^* for any $u \ge 0$ and v (called the dual feasible u, v)

Example: Quadratic program

Consider quadratic program (QP)

$$\min_{x \in \mathcal{R}^n} \frac{1}{2} x^T Q x + c^T x$$

subject to $Ax = b, x \ge 0$

where $Q \succ 0$ is a positive definite matrix

• Lagrangian:

$$L(x, u, v) = \frac{1}{2}x^{T}Qx + c^{T}x - u^{T}x + v^{T}(Ax - b)$$

Lagrange dual function:

$$\begin{split} g(u,v) &= \min_{x \in \mathcal{R}^n} L(x,u,v) \\ &= -\frac{1}{2} (c - u + A^T v)^T Q^{-1} (c - u + A^T v) - b^T v \\ &< f^* \end{split}$$

Example: Quadratic program

Consider quadratic program (QP)

$$\min_{x \in \mathcal{R}^n} \frac{1}{2} x^T Q x + c^T x$$

subject to $Ax = b, x \ge 0$

where $Q \succeq 0$ is a positive semidefinite matrix

Lagrangian is the same

$$L(x, u, v) = \frac{1}{2}x^{T}Qx + c^{T}x - u^{T}x + v^{T}(Ax - b)$$

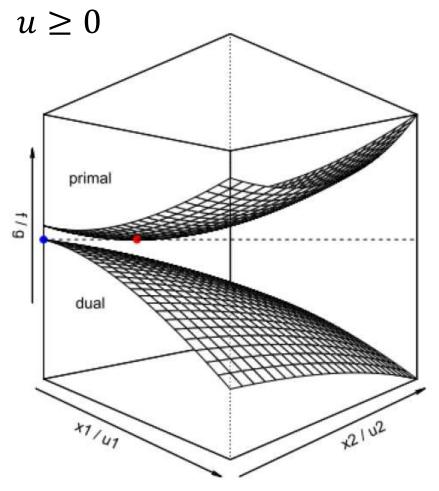
Lagrange dual function:

$$g(u,v) = \begin{cases} -\frac{1}{2}(c-u+A^Tv)^T Q^+(c-u+A^Tv) - b^Tv & \text{if } c-u+A^Tv \perp \text{null}(Q) \\ -\infty & \text{otherwise} \end{cases}$$

 Q^+ denotes generalized inverse of Q

QP in 2D

- Choose f(x) to be quadratic in 2 variables, s.t $x \ge 0$
- Dual function g(u) is also quadratic in 2 variables, s.t.



- Dual function g(u)
 provides a lower bound
 on f* for every u ≥ 0
- The computed largest bound turns out to be exactly f*
- Is this coincidence?
- More on this later

General Lagrange dual problem

Given primal problem

$$\min_{x \in \mathcal{R}^n} f(x)$$
subject to $h_i(x) \le 0, i = 1, \dots, m$

$$l_j(x) = 0, j = 1, \dots, r$$

- Our constructed dual function g(u, v) satisfies $f^* \ge g(u, v)$ for all dual feasible (u, v)
- Hence the best lower bound is given by maximizing g(u, v) over all dual feasible (u, v), yielding the Lagrange dual problem:

$$\max_{u \in \mathcal{R}^m, v \in \mathcal{R}^r} g(u, v)$$

subject to $u \ge 0$

Duality property

- Weak duality: the dual optimal value g^* and the primal optimal value f^* satisfy: $f^* \ge g^*$ (holds for general f)
- Dual problem is a convex optimization problem (i.e. a concave maximization problem)

$$g(u,v) = \min_{x \in \mathcal{R}^n} \left\{ f(x) + \sum_{i=1}^m u_i h_i(x) + \sum_{j=1}^n v_j l_j(x) \right\}$$

$$= -\max_{x \in \mathcal{R}^n} \left\{ -f(x) - \sum_{i=1}^m u_i h_i(x) - \sum_{j=1}^r v_j l_j(x) \right\}$$

linear function in (u,v)

pointwise maximization of convex functions in $(u,v)_{10}$

Weak duality and minimax/maximin

The original problem can be rewritten as

$$\min_{x \in \mathcal{R}^n} \max_{u \ge 0, v} L(x, u, v)$$

The dual problem is actually

$$\max_{u>0,v} \min_{x\in\mathcal{R}^n} L(x,u,v)$$

- Since minimax is always larger than maximin
- Hence,

$$f^* = \min_{x \in \mathcal{R}^n} \max_{u \ge 0, v} L(x, u, v)$$
$$\ge \max_{u \ge 0, v} \min_{x \in \mathcal{R}^n} L(x, u, v)$$
$$= q^*$$

Strong duality

- Weak duality always holds: $f^* \ge g^*$
- In QP, we have observed that actually $f^* = g^*$, which is called the strong duality.

Slater's condition: if the primal is a convex problem (i.e. f and h_1, \dots, h_m are convex, l_1, \dots, l_r are affine), and there exists at least one strictly feasible $x \in R^n$, meaning that $h_1(x) < 0, \dots, h_m(x) < 0$, and $l_1(x) = 0, \dots, l_r(x) = 0$, then strong duality holds

• This is a pretty weak condition. And it can be further refined by requiring strict inequalities only over functions h_i that are not affine

Strong duality of LPs

- For linear programs:
 - Easy to check that the dual of the dual LP is the primal LP
 - Refined version of Slater's condition: strong duality holds for an LP if it is feasible
 - Apply the same logic to its dual LP: strong duality holds if it is feasible
 - Hence strong duality holds for LPs, except when both primal and dual are infeasible
- In other words, we pretty much always have strong duality for LPs

What we have seen so far

Given a minimization problem

$$\min_{x \in \mathcal{R}^n} f(x)$$
subject to $h_i(x) \le 0, i = 1, \dots, m$

$$l_j(x) = 0, j = 1, \dots, r$$

We defined the Lagrangian:

$$L(x, u, v) = f(x) + \sum_{i=1}^{m} u_i h_i(x) + \sum_{j=1}^{r} v_j l_j(x)$$

And the Lagrange dual function

$$g(u,v) = \min_{x \in \mathcal{R}^n} L(x, u, v)$$

What we have seen so far

The subsequent dual problem is:

$$\max_{u \in \mathcal{R}^m, v \in \mathcal{R}^r} g(u, v)$$
subject to $u \ge 0$

- Important properties:
 - Dual problem is always convex, i.e. g is always concave (even if primal problem is not convex)
 - The primal and dual optimal values, f^* and g^* , always satisfy weak duality $f^* \ge g^*$
 - Slater's condition: for convex primal, if there is an x such that $h_1(x) < 0, \dots, h_m(x) < 0$, and $l_1(x) = 0, \dots, l_r(x) = 0$, then strong duality holds: $f^* = g^*$ (can be further refined)

Duality gap

• Given primal feasible x and dual feasible u, v, the quantity f(x) - q(u, v)

is called the duality gap between x and u, v.

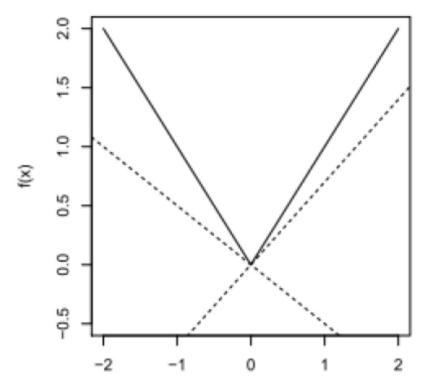
- Note that $f(x) f^* \le f(x) g(u, v)$
- so if the duality gap is zero, then x is primal optimal (and similarly, u, v are dual optimal)
- From an algorithmic viewpoint, provides a stopping criterion: if $f(x)-g(u,v)\leq \epsilon$, then we are guaranteed that $0\leq f(x)-f^*\leq \epsilon$
- Very useful, especially in conjunction with iterative methods.

Subgradients

- Recall that for convex $f: R^n \to R$ $f(y) \ge f(x) + \nabla f(x)^T (y - x)$ for all x, y
- i..e linear approximation always underestimates *f*
- A subgradient of convex f at x is any $g \in \mathbb{R}^n$ such that
- $f(y) \ge f(x) + g^T(y x)$, for all y
- Subgradient
 - Always exists
 - If f differentiable at x, then $g = \nabla f(x)$ uniquely
 - Otherwise, subgradient can be among a set of vectors
 - Actually, the same definition works for nonconvex f (though subgradients need not exist for such f)

Subgradients: example

• Consider $f: R \to R$, f(x) = |x|



- For $x \neq 0$, unique subgradient $g = \operatorname{sgn}(x)$
- For x = 0, subgradient g is any element of [-1, 1]

Subdifferential

• Set of all subgradients of convex *f* is called the subdifferential:

$$\partial f(x) = \{g \in \mathbb{R}^n : g \text{ is a subgradient of } f \text{ at } x\}$$

- $\partial f(x)$ is closed and convex (even for nonconvex f)
- Nonempty (can be empty for nonconvex f)
- If f is differentiable at x, then $\partial f(x) = \{\nabla f(x)\}$
- If $\partial f(x) = \{g\}$, then f is differentiable at x and $\nabla f(x) = g$

Optimality condition

For any f (convex or not),

$$f(x^*) = \min_{x \in R^n} f(x) \Leftrightarrow 0 \in \partial f(x^*)$$

• i.e., x^* is a minimizer if and only if 0 is a subgradient of f at x^*

Proof: g is a subgradient means that for all y:

$$f(y) \ge f(x^*) + 0^T (y - x^*)$$

Karush-Kuhn-Tucker (KKT) conditions

Given a general problem

$$\min_{x \in \mathcal{R}^n} f(x)$$
subject to $h_i(x) \le 0, i = 1, \dots, m$

$$l_j(x) = 0, j = 1, \dots, r$$

- The KKT conditions are:
 - Stationarity: $0 \in \partial f(x) + \sum_{i=1}^m u_i \partial h_i(x) + \sum_{j=1}^r v_j \partial l_j(x)$
 - Complementary slackness: $u_i \cdot h_i(x) = 0, \forall i$
 - Primal feasibility: $h_i(x) \leq 0, l_j(x) = 0, \forall i, j$
 - Dual feasibility: $u_i \geq 0, \forall i$

Necessity – Part 1

- Let x^* and u^* , v^* be primal and dual solutions with zero duality gap (strong duality holds, e.g., under Slater's condition)
- Then $f(x^*) = g(u^*, v^*) = \min_{x \in \mathcal{R}^n} L(x, u^*, v^*)$ $= \min_{x \in \mathcal{R}^n} f(x) + \sum_{i=1}^m u_i^* h_i(x) + \sum_{j=1}^r v_j^* l_j(x)$ $\leq f(x^*) + \sum_{i=1}^m u_i^* h_i(x^*) + \sum_{j=1}^r v_j^* l_j(x^*)$ $\leq f(x^*)$
- In other words, all these inequalities are actually equalities

Necessity – Part 2

Two things to learn from this:

- The point x^* minimizes $L(x, u^*, v^*)$ over $x \in \mathbb{R}^n$. Hence, the subdifferential of $L(x, u^*, v^*)$ must contain 0 at $x = x^*$ this is exactly the stationary condition
- We must have $\sum_{i=1}^m u_i^*h_i(x^*)=0$ so that the inequalities becomes equalities. And since each term here is ≤ 0 , this implies $u_i^*h_i(x^*)=0$ for all i. this is exactly the complementary slackness
- Primal and dual feasibility obviously hold. Hence:

If x^* and u^* , v^* be primal and dual solutions with zero duality gap, then x^* and u^* , v^* satisfy the KKT conditions

 Note that this statement assumes nothing a priori about the convexity

Sufficiency

• If there exist x^* and u^* , v^* that satisfy the KKT conditions, then

$$g(u^*, v^*) = f(x^*) + \sum_{i=1}^{m} u_i^* h_i(x^*) + \sum_{j=1}^{r} v_j^* l_j(x^*)$$
$$= f(x^*)$$

- Where the first equality holds from stationarity, and the second holds from complementary slackness
- Therefore duality gap is zero (and x^* and u^* , v^* are primal and dual feasible), so x^* and u^* , v^* are primal and dual optimal

If x^* and u^* , v^* satisfy the KKT conditions, then x^* and u^* , v^* are primal and dual solutions

Putting everything together

- In summary, KKT conditions
 - Always sufficient
 - Necessary under strong duality
- Putting it together

For a problem with strong duality (e.g., assume Slater's condition: convex problem and there exists x strictly satisfying non-affine inequality constraints x^* and u^* , v^* are primal and dual solutions $\Leftrightarrow x^*$ and u^* , v^* satisfy the KKT conditions

• (Warning, concerning the stationarity condition: for a differentiable function f, we cannot use $\partial f(x) = \{\nabla f(x)\}$ until f is convex)

Example: quadratic with equality constraints

• Consider for $Q \ge 0$ $\min_{x \in \mathcal{R}^n} \ \frac{1}{2} x^T Q x + c^T x$

subject to
$$Ax = 0$$

- This is a core sub-problem used in Newton step for $\min_{x \in \mathbb{R}^n} f(x)$ subject to Ax = b
- Convex problem, no inequality constraints, so by KKT conditions, x is a solution if and only if

$$\begin{pmatrix} Q & A^T \\ A & 0 \end{pmatrix} \begin{pmatrix} x \\ u \end{pmatrix} = \begin{pmatrix} -c \\ 0 \end{pmatrix}$$

• For some *u*. Linear system combines stationary and primal feasibility.