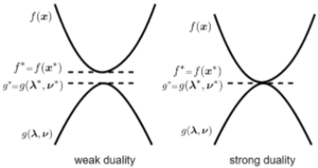
Optimization in Machine Learning

Duality in optimization



Learning goals

- Awareness of the concept of duality in optimization
- LP duality
- Weak and strong duality in LP

DUALITY: OVERVIEW

- Duality theory plays a fundamental role in (constrained) optimization. The concept of “duality" emerged in the context of LPs and dates back to the 1940s (works of Tucker and Wolfe).
- There are several different types of duality: LP duality, Lagrangian duality, Wolfe duality, Fenchel duality (which can lead to confusion).
- Key take-home message: The concepts of duality give you recipes to find **lower bounds** on your original “primal" constrained optimization problem. Under certain conditions, these lower bounds are actually identical to the optimal solution.
- Duality is also practical. It has been used to find **better algorithms** for solving constrained optimization problems

LP DUALITY: INTRODUCTORY EXAMPLE

Example:

A bakery sells brownies for 50 ct and mini cheesecakes for 80 ct each. The two products contain the following ingredients

	Chocolate	Sugar	Cream cheese
Brownie	3	2	2
Cheesecake	0	4	5

A student wants to minimize his expenses, but at the same time eat at least 6 units of chocolate, 10 units of sugar and 8 units of cream cheese.

LP DUALITY: INTRODUCTORY EXAMPLE

He is therefore confronted with the following optimization problem:

$$
\begin{aligned}
\min_{\mathbf{x}\in\mathbb{R}^2} \quad & 50x_1 + 80x_2 \\
\text{s.t.} \quad & 3x_1 \geq 6 \\
& 2x_1 + 4x_2 \geq 10 \\
& 2x_1 + 5x_2 \geq 8 \\
& \mathbf{x} \geq 0
\end{aligned}
$$

LP DUALITY: INTRODUCTORY EXAMPLE

The solution of the Simplex algorithm:

```
res = solveLP(cvec = c, bvec = b, Amat = A)
summary(res)
##
##
## Results of Linear Programming / Linear Optimization
##
## Objective function (Minimum): 220
##
## Solution
## opt
## 1 2.0
## 2 1.5
```

LP DUALITY: INTRODUCTORY EXAMPLE

The baker informs the supplier that he needs at least 6 units of chocolate, 10 units of sugar and 8 units of cream cheese to meet the student's requirements.

The supplier asks himself how he must set the prices for chocolate, sugar and cream cheese $(\alpha_1, \alpha_2, \alpha_3)$ such that he can

- maximize his revenue

$$\max_{\boldsymbol{\alpha} \in \mathbb{R}^3} 6\alpha_1 + 10\alpha_2 + 8\alpha_3$$

- and at the same time ensure that the baker buys from him (purchase cost $\leq$ selling price)

$$\begin{aligned} 3\alpha_1 + 2\alpha_2 + 2\alpha_3 &\leq 50 \qquad \text{Brownie} \\ 4\alpha_2 + 5\alpha_3 &\leq 80 \qquad \text{Cheesecake} \end{aligned}$$

LP DUALITY: INTRODUCTORY EXAMPLE

The presented example is known as a **dual problem**. The variables α_i are called **dual variables**.

In an economic context, dual variables can often be interpreted as **shadow prices** for certain goods.

If we solve the dual problem, we see that the dual problem has the same objective function value as the primal problem. This is later referred to as **strong duality**.

LP DUALITY: INTRODUCTORY EXAMPLE

```
res = solveLP(cvec = c, bvec = b, Amat = A, maximum = T)
summary(res)
##
##
## Results of Linear Programming / Linear Optimization
##
## Objective function (Maximum): 220
##
## Solution
## opt
## 1 3.333333
## 2 20.000000
## 3 0.000000
```

MATHEMATICAL INTUITION

The example explained duality from an economic point of view. But what is the mathematical intuition behind duality?

Idea: In minimization problems one is often interested in **lower bounds** of the objective function. How could we derive a lower bound for the problem above?

If we “skillfully” multiply the three inequalities by factors and add factors (similar to a linear system), we can find a lower bound.

MATHEMATICAL INTUITION

$$
\begin{aligned}
\min_{\mathbf{x}\in\mathbb{R}^2} \quad & 50x_1 + 80x_2 \\
\text{s.t.} \quad & 3x_1 \geq 6 \quad | \cdot 5 \\
& 2x_1 + 4x_2 \geq 10 \quad | \cdot 5 \\
& 2x_1 + 5x_2 \geq 8 \quad | \cdot 12 \\
& \mathbf{x} \geq 0
\end{aligned}
$$

If we add up the constraints we obtain

$$
\begin{aligned}
5 \cdot (3x_1) + 5 \cdot (2x_1 + 4x_2) + 12 \cdot (2x_1 + 5x_2) \\
&= 15x_1 + 10x_1 + 24x_1 + 20x_2 + 60x_2 \\
&= 49x_1 + 80x_2 \\
&\geq 30 + 50 + 96 = 176
\end{aligned}
$$

Since $x_1 \geq 0$ we found a lower bound because

$$50x_1 + 80x_2 \geq 49x_1 + 80x_2 \geq 176.$$

MATHEMATICAL INTUITION

Is our derived lower bound the best possible?

We replace the multipliers $5, 5, 12$ by $\alpha_1, \alpha_2, \alpha_3$ and compute:

$$\begin{aligned} 50x_1 + 80x_2 &\geq \alpha_1(3x_1) + \alpha_2(2x_1 + 4x_2) + \alpha_3(2x_1 + 5x_2) \\ &= (3\alpha_1 + 2\alpha_2 + 2\alpha_3)x_1 + (4\alpha_2 + 5\alpha_3)x_2 \\ &\geq 6\alpha_1 + 10\alpha_2 + 8\alpha_3 \end{aligned}$$

But: We have to demand that

$$\begin{aligned} 3\alpha_1 + 2\alpha_2 + 2\alpha_3 &\leq 50 \\ 4\alpha_2 + 5\alpha_3 &\leq 80 \end{aligned}$$

MATHEMATICAL INTUITION

We are interested in a **largest possible** lower bound.

This yields the **dual problem**:

$$\begin{aligned}
\max_{\boldsymbol{\alpha}\in\mathbb{R}^3} \quad & 6\alpha_1 + 10\alpha_2 + 8\alpha_3 \\
\text{s.t.} \quad & 3\alpha_1 + 2\alpha_2 + 2\alpha_3 \leq 50 \\
& 4\alpha_2 + 5\alpha_3 \leq 80 \\
& \boldsymbol{\alpha} \geq 0
\end{aligned}$$

DUALITY

Dual problem:

$$\begin{aligned} \max_{\boldsymbol{\alpha} \in \mathbb{R}^m} \quad & g(\boldsymbol{\alpha}) := \boldsymbol{\alpha}^\top \mathbf{b} \\ \text{s.t.} \quad & \boldsymbol{\alpha}^\top \mathbf{A} \leq \mathbf{c}^\top \\ & \boldsymbol{\alpha} \geq 0 \end{aligned}$$

Primal problem:

$$\begin{aligned} \min_{\mathbf{x} \in \mathbb{R}^n} \quad & f(\mathbf{x}) := \mathbf{c}^\top \mathbf{x} \\ \text{s.t.} \quad & \mathbf{A}\mathbf{x} \geq \mathbf{b} \\ & \mathbf{x} \geq 0 \end{aligned}$$

DUALITY

Connection of primal and dual problem:

	Primal (minimize)	Dual (maximize)	
condition	$\leq$ $\geq$ $=$	≤ 0 ≥ 0 unconstrained	variable
variable	≥ 0 ≤ 0 unconstrained	$\leq$ $\geq$ $=$	condition

DUALITY THEOREM

In general, the **weak duality theorem** applies to all feasible $\mathbf{x}, \boldsymbol{\alpha}$

$$g(\boldsymbol{\alpha}) = \boldsymbol{\alpha}^\top \mathbf{b} \leq \mathbf{c}^\top \mathbf{x} = f(\mathbf{x})$$

The value of the dual function is therefore **always** a lower bound for the objective function value of the primal problem.

Proof:

$$\boldsymbol{\alpha}^\top \mathbf{b} \overset{\mathbf{Ax} \geq \mathbf{b}}{\leq} \boldsymbol{\alpha}^\top \mathbf{A}\mathbf{x} \overset{\boldsymbol{\alpha}^\top \mathbf{A} \leq \mathbf{c}^\top}{\leq} \mathbf{c}^\top \mathbf{x}$$

DUALITY THEOREM

The **strong duality theorem** states that if one of the two problems has a constrained solution, then the other also has a constrained solution. The objective function values are the same in this case:

$$g(\boldsymbol{\alpha}^*) = (\boldsymbol{\alpha}^*)^\top \mathbf{b} = \mathbf{c}^\top \mathbf{x}^* = f(\mathbf{x}^*)$$

In this case, the dual problem can be solved instead of the primal problem, which can lead to enormous run time advantages, especially with many constraints and few variables.

The **dual simplex algorithm**, which has emerged as a standard procedure for linear programming, is based on this idea.

ALTERNATIVE LP FORMULATION

Unfortunately, many slightly different (but ultimately equivalent) formulations of primal and dual LPs exist in the literature.
One common alternative with inequality and equality constraints is often formulated as follows. Let $\mathbf{c} \in \mathbb{R}^d$, $\mathbf{b} \in \mathbb{R}^l$, $\mathbf{A} \in \mathbb{R}^{l \times d}$, $\mathbf{h} \in \mathbb{R}^k$, and $\mathbf{G} \in \mathbb{R}^{k \times d}$.
Then the primal LP is defined as

$$
\begin{aligned}
\min_{\mathbf{x} \in \mathbb{R}^d} \quad & \mathbf{c}^\top \mathbf{x} \\
\text{s.t.} \quad & \mathbf{G}\mathbf{x} = \mathbf{h} \\
& \mathbf{A}\mathbf{x} \leq \mathbf{b}
\end{aligned}
$$

ALTERNATIVE LP FORMULATION

and the corresponding dual LP

$$\begin{aligned} \max_{\alpha \in \mathbb{R}^l, \beta \in \mathbb{R}^k} \quad & -\mathbf{b}^\top \boldsymbol{\alpha} - \mathbf{h}^\top \boldsymbol{\beta} \\ \text{s.t.} \quad & -\mathbf{A}^\top \boldsymbol{\alpha} - \mathbf{G}^\top \boldsymbol{\beta} = \mathbf{c} \\ & \boldsymbol{\alpha} \geq 0 \end{aligned}$$

The following argument again highlights the interpretation of the dual LP as a lower bound. Here, for $\boldsymbol{\alpha} \geq 0$ and any $\boldsymbol{\beta}$, and $\mathbf{x}$ primal feasible, it holds that

$$\boldsymbol{\alpha}^\top(\mathbf{Ax}-\mathbf{b})+\boldsymbol{\beta}^\top(\mathbf{Gx}-\mathbf{h}) \leq 0 \iff (-\mathbf{A}^\top\boldsymbol{\alpha}-\mathbf{G}^\top\boldsymbol{\beta})^\top\mathbf{x} \geq -\mathbf{b}^\top\boldsymbol{\alpha}-\mathbf{h}^\top\boldsymbol{\beta}$$

So if $\mathbf{c} = -\mathbf{A}^\top\boldsymbol{\alpha} - \mathbf{G}^\top\boldsymbol{\beta}$, we get a lower bound on the primal optimal value.

ALTERNATIVE LP FORMULATION

Another perspective on this formulation will connect LP duality to the more general notion of **Lagrangian duality**. Again, for $\boldsymbol{\alpha} \geq 0$, any $\boldsymbol{\beta}$, and **x** primal feasible, it holds that

$$\mathbf{c}^\top \mathbf{x} \geq \mathbf{c}^\top \mathbf{x} + \boldsymbol{\alpha}^\top (\mathbf{A}\mathbf{x} - \mathbf{b}) + \boldsymbol{\beta}^\top (\mathbf{G}\mathbf{x} - \mathbf{h}) =: \mathcal{L}(\mathbf{x}, \boldsymbol{\alpha}, \boldsymbol{\beta})$$

If $\mathcal{S}$ denotes the primal feasible set, $f(\mathbf{x}^*)$ the primal optimal value, then for $\boldsymbol{\alpha} \geq 0$ and any $\boldsymbol{\beta}$, it holds that

$$f(\mathbf{x}^*) \geq \min_{\mathbf{x} \in \mathcal{S}} \mathcal{L}(\mathbf{x}, \boldsymbol{\alpha}, \boldsymbol{\beta}) \geq \min_{\mathbf{x} \in \mathbb{R}^d} \mathcal{L}(\mathbf{x}, \boldsymbol{\alpha}, \boldsymbol{\beta}) =: g(\boldsymbol{\alpha}, \boldsymbol{\beta})$$

This shows that the function $g(\boldsymbol{\alpha}, \boldsymbol{\beta})$ is a lower bound on $f(\mathbf{x}^*)$ for $\boldsymbol{\alpha} \geq 0$ and any $\boldsymbol{\beta}$. It is the *Lagrange (dual) function* and defined as

$$g(\boldsymbol{\alpha}, \boldsymbol{\beta}) = \begin{cases} -\mathbf{b}^\top \boldsymbol{\alpha} - \mathbf{h}^\top \boldsymbol{\beta} & \text{if } \mathbf{c} = -\mathbf{A}^\top \boldsymbol{\alpha} - \mathbf{G}^\top \boldsymbol{\beta} \\ -\infty & \text{otherwise} \end{cases}$$

ALTERNATIVE LP FORMULATION

- Maximizing $g(\alpha, \beta)$ leads again to the first dual formulation
- **Note:** Lagrangian perspective is completely general
  $\Rightarrow$ applicable to arbitrary (non-linear) problems

Final remarks:

- We introduced key concepts of duality for Linear Programming as the simplest instance of a constrained optimization problem.
- We refer to the excellent course of L. Vandenberghe ▸ EE236A - Linear Programming for many more details.
- We have skipped algorithmic approaches for solving linear programs: Dantzig's Simplex Algorithm, Interior point methods, and the Ellipsoid method.