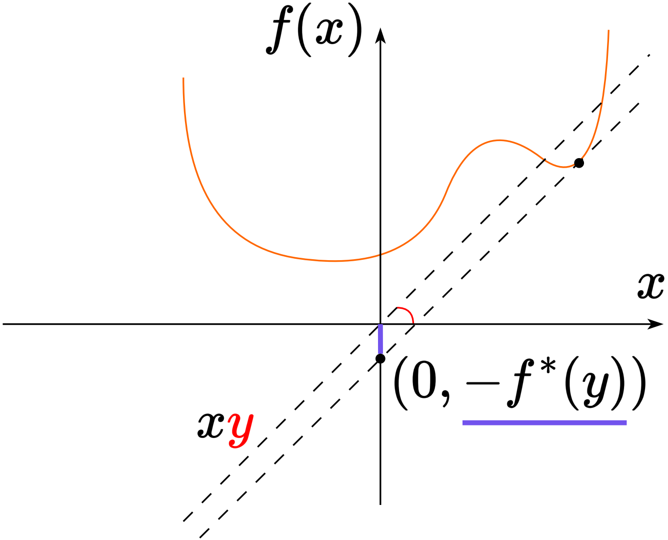
Conjugate functions. Dual (sub)gradient method. Augmented Lagrangian method. ADMM.

Seminar

Optimization for ML. Faculty of Computer Science. HSE University

Definition



Recall that given $f : \mathbb{R}^n \to \mathbb{R}$, the function defined by

$$f^*(y) = \max_x \left[y^T x - f(x) \right]$$

is called its conjugate.

Conjugate function properties

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- Conjugates appear frequently in dual programs, since

$$-f^*(y) = \min_x \left[f(x) - y^T x\right]$$

- If f is closed and convex, then $f^{**} = f$. Also,

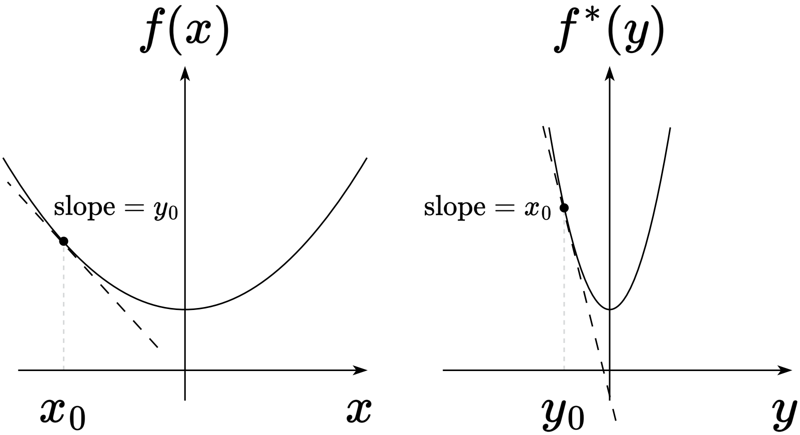
$$x \in \partial f^*(y) \Leftrightarrow y \in \partial f(x) \Leftrightarrow x \in \arg\min_z \left[f(z) - y^T z\right]$$

- If f is strictly convex, then

$$\nabla f^*(y) = \arg\min_z \left[f(z) - y^T z\right]$$

Slopes of f and f^*

Assume that f is a closed and convex function. Then f is strongly convex with parameter $\mu \Leftrightarrow \nabla f^*$ is Lipschitz with parameter $1/\mu$.



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Find the conjugate function for

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$$f^*(s) = \sup_{x \in \mathbb{R}^n} \left(s^T x - a^T x - b\right) = \begin{cases} -b, & \text{if } s = a \\ \infty, & \text{else} \end{cases} = \delta\left([s = a]\right) - b$$

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$$\left(\delta\left([s = a]\right) - b\right)^* = \sup_{s \in \operatorname{dom} f_2(s)} \left(y^T s - \delta\left([s = a]\right) + b\right) = a^T y + b$$

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$$f^*(s) = \sup_{x \in \mathbb{R}^n} (sx - \log(1 + \exp(x)))$$

$$f^*(s) = \begin{cases} \infty, & \text{if } s < 0 \\ 0, & \text{if } s = 0 \\ 0, & \text{if } s = 1 \\ \infty, & \text{if } s > 1 \\ \textbf{?}, & \text{if } 0 < s < 1 \end{cases}$$

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$s \in (0,1)$:

$$s - \frac{\exp(x)}{1+\exp(x)} = 0 \Leftrightarrow x_{opt} = \log \frac{s}{1-s}$$

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Thus,

$$f^*(s) = \begin{cases} 0, & \text{if } s \in \{0, 1\} \\ s \log s + (1 - s) \log(1 - s), & \text{if } 0 < s < 1 \\ \infty, & \text{else} \end{cases}$$

$$\text{dom} f^*(s) = [0, 1]$$

Dual (sub)gradient method

Even if we can't derive dual (conjugate) in closed form, we can still use dual-based gradient or subgradient methods.

Consider the problem:

$$\min_x \quad f(x) \quad \text{subject to} \quad Ax = b$$

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Its dual problem is:

$$\max_u \quad -f^*(-A^T u) - b^T u$$

where f^* is the conjugate of f. Defining $g(u) = -f^*(-A^T u) - b^T u$, note that:

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Dual ascent method for maximizing dual objective:

$$x_k \in \arg\min_x \left[f(x) + (u_{k-1})^T A x \right]$$

$$u_k = u_{k-1} + \alpha_k (A x_k - b)$$

- Step sizes α_k, $k = 1, 2, 3, \ldots$, are chosen in standard ways.
- Proximal gradients and acceleration can be applied as they would usually.

Convergence guarantees

The following results hold from combining the last fact with what we already know about gradient descent:[1]

- If f is strongly convex with parameter μ, then dual gradient ascent with constant step sizes $\alpha_k = \mu$ converges at sublinear rate $O(\frac{1}{\epsilon})$.
- If f is strongly convex with parameter μ and ∇f is Lipschitz with parameter L, then dual gradient ascent with step sizes $\alpha_k = \frac{2}{\frac{1}{\mu} + \frac{1}{L}}$ converges at linear rate $O(\log(\frac{1}{\epsilon}))$.

Note that this describes convergence in the dual. (Convergence in the primal requires more assumptions)

[1]This is ignoring the role of A, and thus reflects the case when the singular values of A are all close to 1. To be more precise, the step sizes here should be: $\frac{\mu}{\sigma_{\text{max}}(A)^2}$ (first case) and $\frac{2}{\frac{\sigma_{\text{max}}(A)^2}{\mu} + \frac{\sigma_{\text{min}}(A)^2}{L}}$ (second case).

Dual decomposition

Consider

$$\min_x \sum_{i=1}^{B} f_i(x_i) \quad \text{subject to} \quad Ax = b$$

Here $x = (x_1, \ldots, x_B) \in \mathbb{R}^n$ divides into B blocks of variables, with each $x_i \in \mathbb{R}^{n_i}$. We can also partition A accordingly:

$$A = [A_1 \ldots A_B], \text{ where } A_i \in \mathbb{R}^{m \times n_i}$$

Simple but powerful observation, in calculation of subgradient, is that the minimization decomposes into B separate problems:

$$x^{\text{new}} \in \arg\min_x \left(\sum_{i=1}^{B} f_i(x_i) + u^T A x \right)$$

$$\Rightarrow x_i^{\text{new}} \in \arg\min_{x_i} \left(f_i(x_i) + u^T A_i x_i \right), \quad i = 1, \ldots, B$$

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$$x_i^k \in \arg\min_{x_i} \left(f_i(x_i) + (u^{k-1})^T A_i x_i \right), \quad i = 1, \dots, B$$

$$u_i^k = u_i^{k-1} + \alpha_k \left(A_i x_i^k - b_i \right), \quad i = 1, \dots, B$$

Can think of these steps as:

- **Broadcast:** Send u to each of the B processors, each optimizes in parallel to find x_i.
- **Gather:** Collect $A_i x_i$ from each processor, update the global dual variable u.

Inequality constraints

Consider the optimization problem:

$$\min_x \sum_{i=1}^B f_i(x_i) \quad \text{subject to} \quad \sum_{i=1}^B A_i x_i \leq b$$

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Using **dual decomposition**, specifically the **projected subgradient method**, the iterative steps can be expressed as:

- The primal update step:

$$x_i^k \in \arg\min_{x_i} \left[f_i(x_i) + \left(u^{k-1}\right)^T A_i x_i \right], \quad i = 1, \dots, B$$

- The dual update step:

$$u^k = \left(u^{k-1} + \alpha_k \left(\sum_{i=1}^B A_i x_i^k - b \right) \right)_+$$

where $(u)_+$ denotes the positive part of u, i.e., $(u_+)_i = \max\{0, u_i\}$, for $i = 1, \dots, m$.

Augmented Lagrangian method aka method of multipliers

Dual ascent disadvantage: convergence requires strong conditions. Augmented Lagrangian method transforms the primal problem:

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\begin{aligned}
&\min_x f(x) + \frac{\rho}{2}\|Ax - b\|^2 \\
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Dual gradient ascent: The iterative updates are given by:

$$
\begin{aligned}
x_k &= \arg\min_x \left[f(x) + (u_{k-1})^T Ax + \frac{\rho}{2}\|Ax - b\|^2 \right] \\
u_k &= u_{k-1} + \rho(Ax_k - b)
\end{aligned}
$$

- **Advantage:** The augmented Lagrangian gives better convergence.
- **Disadvantage:** We lose decomposability! (Separability is ruined)
- **Notice** step size choice $\alpha_k = \rho$ in dual algorithm.

Colab Example

- Dual subgradient and Augmented Lagrangian methods Comparison Open in Colab.

Alternating Direction Method of Multipliers (ADMM)

Alternating direction method of multipliers or ADMM aims for the best of both worlds. Consider the following optimization problem:

Minimize the function:

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where $\rho > 0$ is a parameter. The augmented Lagrangian for this problem is defined as:

$$L_\rho(x, z, u) = f(x) + g(z) + u^T(Ax + Bz - c) + \frac{\rho}{2}\|Ax + Bz - c\|^2$$

Alternating Direction Method of Multipliers (ADMM)

ADMM repeats the following steps, for $k = 1, 2, 3, \dots$:

1. Update x:

$$x_k = \arg\min_x L_\rho(x, z_{k-1}, u_{k-1})$$

2. Update z:

$$z_k = \arg\min_z L_\rho(x_k, z, u_{k-1})$$

3. Update u:

$$u_k = u_{k-1} + \rho(Ax_k + Bz_k - c)$$

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Note: The usual method of multipliers would replace the first two steps by a joint minimization:

$$(x^{(k)}, z^{(k)}) = \arg\min_{x,z} L_\rho(x, z, u^{(k-1)})$$

ADMM Summary

- ADMM is one of the key and popular recent optimization methods.
- It is implemented in many solvers and is often used as a default method.
- The non-standard formulation of the problem itself, for which ADMM is invented, turns out to include many important special cases. "Unusual" variable y often plays the role of an auxiliary variable.
- Here the penalty is an additional modification to stabilize and accelerate convergence. It is not necessary to make ρ very large.