Duality, Gradient-free, in Application

Axel Böhm

January 23, 2022

1. Duality
2. Derivative free
3. methods in practice

Duality

Establishes some relation between two classes of objects.

Definition ("Legendre transform" or "Fenchel conjugate")

Given a function $f : \mathbb{R}^d \to \mathbb{R} \cup \{+\infty\}$, we define its **conjugate** $f^* : \mathbb{R}^d \to \mathbb{R} \cup \{+\infty\}$ by

$$f^*(y) = \sup_x \{\langle y, x \rangle - f(x)\}$$

Convex conjugate

$$f^*(y) = \sup_x \{\langle y, x\rangle - f(x)\}$$

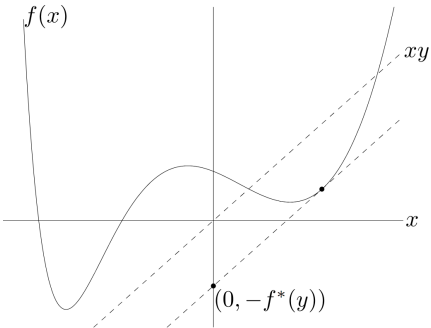

Figure: maximum gap between linear function $x \mapsto \langle y, x\rangle$ and f

Properties

- f^* is always convex. point-wise max of affine function
- Fenchel's inequality:

$$f(x) + f^*(y) \geq \langle x, y \rangle.$$

- Hence the biconjugate $f^{**} := (f^*)^*$ satisfies $f^{**} \leq f$.
- If f is convex an lsc. then $f^{**} = f$.
- etc.

Examples

◇ Norm: If $f(x) = \|x\|$, then

$$f^*(y) = \mathbb{1}(\|y\|_* \leq 1),$$

i.e. the indicator of the dual norm ball. Recall the definition of the dual norm:

$$\|y\|_* := \max_{\|x\| \leq 1} \{\langle y, x \rangle\}.$$

In particular: $\|\cdot\|_1 \leftrightarrow \|\cdot\|_\infty$

More examples

Generalized linear models: $\min_{x \in \mathbb{R}^d} f(Ax) + g(x).$

Two approaches to reformulate:

$$\min_x \underbrace{\max_y \langle y, Ax \rangle - f^*(y)}_{=f(Ax)} + g(x).$$

Switch min and max

$$\min_x \max_y -f^*(y) + \langle y, Ax \rangle + g(x).$$

Change sign to go from max to min

$$\min_x -f^*(y) - \min_y \underbrace{-\langle y, Ax \rangle - g(x)}_{=g^*(-A^T y)}.$$

Generalized linear models continued

Or reformulate

$$\min_{x \in \mathbb{R}^d} f(Ax) + g(x)$$

as

$$\min_{x \in \mathbb{R}^d, w \in \mathbb{R}^m} f(w) + g(x) \quad \text{s.t.} w = Ax$$

Use Lagrange function

$$\mathcal{L}(x, w, u) := f(w) + g(x)\langle u, w - Ax\rangle,$$

then the dual function is given by

$$\varphi(u) = \min_{x \in \mathbb{R}^d, w \in \mathbb{R}^m} \mathcal{L}(x, w, u).$$

Dual problem

$$\max_{u \in \mathbb{R}^m} [\varphi(u) = -f^*(-u) - g^*(A^T u)].$$

Example: Lasso

ℓ_1 regularized regression

$$\min_{x \in \mathbb{R}^d} \frac{1}{2}\|Ax - b\|^2 + \lambda \|x\|_1$$

fits this template with

$$f(w) = \frac{1}{2}\|w - b\|^2 \quad \text{and} \quad g(x) = \lambda \|x\|_1$$

Computation gives

$$f^*(u) = \frac{1}{2}\|b\|^2 - \frac{1}{2}\|b - u\|^2 \quad \text{and} \quad g^*(v) = \mathbb{1}(\|v/\lambda\|_\infty \leq 1).$$

Dual of Lasso

We had

$$f^*(u) = \frac{1}{2}\|b\|^2 - \frac{1}{2}\|b-u\|^2 \quad \text{and} \quad g^*(v) = \mathbb{1}(\|v/\lambda\|_\infty \leq 1).$$

So the dual is

$$\begin{aligned} &\max_{u \in \mathbb{R}^m} -f^*(-u) - g^*(A^T u) \\ \Leftrightarrow &\min_{u \in \mathbb{R}^m} \|b+u\|^2 \quad \text{s.t.} \quad \|A^T u\|_\infty \leq \lambda \end{aligned}$$

Similarly, for least squares, ridge/logistic regression, SVM, etc.

But why?

- Duality gap gives a certificate of current optimization quality

$$\begin{aligned} f(A\bar{x}) + g(\bar{x}) &\geq \min_{x \in \mathbb{R}^d} f(Ax) + g(x) \\ &\geq \max_{u \in \mathbb{R}^m} -f^*(-u) - g^*(A^T u) \\ &\geq -f^*(-\bar{u}) - g^*(A^T \bar{u}) \end{aligned}$$

- Stopping criterion
- Dual problem is sometimes easier to solve

Zero-order Optimization
$\Leftrightarrow$ Derivative-Free
$\Leftrightarrow$ Blackbox

Look, no gradients!

Can we solve $\min_{x \in \mathbb{R}^d} f(x)$ without access to gradients?

Algorithm Random search

1: **for** $k = 1, 2, \ldots$ **do**
2: **for** pick a random direction $d_k \in \mathbb{R}^d$ **do**
3: $\gamma_k := \arg\min_{\gamma \in \mathbb{R}} f(x_k + \gamma d_k)$
4: $x_{k+1} := x_k + \gamma_k d_k$

Convergence rate for derivative-free random search

Converges same as gradient descent - up to a slow-down factor d.
Proof.

$$f(x_k + \gamma d_k) \leq f(x_k) + \gamma \langle d_k, \nabla f(x_k) \rangle + \frac{\gamma^2 L}{2} \|d_k\|^2$$

Minimizing the upper bound (RHS), there exists a step $\bar{\gamma}$ for which

$$f(x_k + \bar{\gamma} d_k) \leq f(x_k) - \frac{1}{L} \left\langle \frac{d_k}{\|d_k\|^2}, \nabla f(x_k) \right\rangle.$$

So our (exact line-search) step can only be better

$$f(x_k + \gamma_k d_k) \leq f(x_k + \bar{\gamma} d_k)$$

Taking expectation and using $\mathbb{E}_r \langle r, g \rangle^2 = 1/d \|g\|^2$ for $r \sim$ sphere, gives

$$\mathbb{E}[f(x_k + \gamma_k d_k)] \leq E[f(x_k)] - \frac{1}{Ld} \mathbb{E}\left[\|\nabla f(x_k)\|^2\right].$$

Convergence rate for derivative-free random search

Same as what we obtained for gradient descent,
now with an extra factor of d. d can be huge!!!

Similarly for other function classes

- For convex functions, we get a rate of $\mathcal{O}(\frac{dL}{\epsilon})$.
- For μ-strongly convex functions, we get a rate of $\mathcal{O}(d\kappa \log(1/\epsilon))$.

Always d times the complexity of gradient descent on the function class.

But assumed differentiability. Can also approximate the gradient.

Applications for derivative-free random search

Applications

- competitive method for reinforcement learning
- No need to store a gradient
- hyperparameter optimization, and other difficult e.g. discrete optimization problems, black-box, noisy

Reinforcement learning

$$s_{k+1} = f(s_k, a_k, e_k),$$

where s_k is the state of the system, a_k is the control action, and e_t is some random noise. We assume existence of f, but it is unknown.

We search for a "policy"

$$a_k := \pi(a_1, \ldots, a_{k-1}, s_0, \ldots, s_k)$$

Goal: Maximize reward

$$\max_{a_k} \mathbb{E}_{e_k} \left[\sum_{k=1}^{N} R_k(s_k, a_k) \right]$$
$$\text{s.t.} s_{k+1} = f(s_k, a_k, e_k)$$

Adaptive & other SGD methods

Adagrad

An adaptive variant of SGD

Algorithm Adagrad

1: **for** $k = 1, \ldots$ **do**
2: pick stochastic gradient g_k
3: $[G_k]_i = \sum_{l=}^{k} ([g_k]_i)^2, \quad \forall i$
4: $[x_{k+1}]_i = [x_k]_i - \frac{\gamma}{\sqrt{[G_k]_i}} [g_k]_i, \quad \forall i$

- chooses an adaptive, coordinate-wise learning rate
- strong performance in practice
- many variants: Adadelta, Adam, RMSprop

Adam

A momentum variant of Adagrad

Algorithm Adam

1: **for** $k = 1, \ldots$ **do**
2: pick stochastic gradient g_k
3: $m_k = \beta_1 m_{k-1} + (1-\beta_1) g_k$ `momentum`
4: $[v_k]_i = \beta_2 [v_{k-1}]_i + (1-\beta_2)([g_k]_i)^2$ `2nd-order statistics`
5: $[x_{k+1}]_i = [x_k]_i - \frac{\gamma}{\sqrt{[v_k]_i}} [m_k]_i, \quad \forall i$

- forgetting of old weights
- momentum (see lecture on acceleration)
- strong performance for certain DL problems

SignSGD

Only use the sign (one bit) of each gradient entry:
Yields a communication efficient variant of SGD.

Algorithm SignSGD

1: **for** $k = 1, \ldots$ **do**
2: pick stochastic gradient g_k
3: $[x_{k+1}]_i = [x_k]_i - \gamma_k \operatorname{sign}([m_k]_i), \quad \forall i$

(possible rescaling of γ_k by $\|g_k\|_1$)

- combats communication bottleneck for distributed training
- convergence issues