MATH 680 Computation Intensive Statistics

November 27, 2019

Dual Norm and Conjugate Function

1 Dual Norm

- Let ||x|| be a norm, e.g.,
 - ℓ_p norm: $||x||_p = (\sum_{i=1}^n |x_i|^p)^{1/p}$, for $p \ge 1$.
 - Trace norm: $\|X\|_{tr} = \sum_{i=1}^r \sigma_i(X)$
- **Dual norm:** for a vector x, we define its dual norm $||x||_*$ as

$$||x||_* = \max_{||z|| \le 1} z^\top x,$$

where $\|\cdot\|$ is the original norm.

We have the inequality (Cauchy-schwarz like)

$$|z^{\top}x| \le ||z|| ||x||_*.$$

This is because $||x^*|| = \max_{\|z\| \le 1} z^\top x \ge \left(\frac{z}{\|z\|}\right)^\top x$

• The dual norm of the ℓ_1 norm is the ℓ_∞ norm. Let $||z|| = \sum_{i=1}^p |z_i| = ||z||_1$ (ℓ_1 norm).

$$\max_{\sum_{i}|z_{i}| \leq 1} \sum_{i} z_{i} y_{i}$$
$$= \max_{i} |y_{i}| = ||y||_{\infty}.$$

• The dual norm of the ℓ_2 norm is the ℓ_2 norm. Since $||z||_2 \le 1$,

$$\max_{\|z\|_2 \le 1} z^\top y \le \|z\|_2 \|y\|_2 \le \|y\|_2,$$

where the "=" is taken when

$$z = \begin{cases} ||y||_2^{-1} \cdot y, & y \neq 0 \\ 0, & y = 0. \end{cases}$$

• The dual norm of the ℓ_p norm (p>1) is the ℓ_q norm (q>1) and $\frac{1}{p}+\frac{1}{q}=1$. Since

$$|a_1b_1 + \dots + a_kb_k| \le (a_1^p + \dots + a_k^p)^{1/p}(b_1^q + \dots + b_k^q)^{1/q}$$

for $\frac{1}{p} + \frac{1}{q} = 1$, p > 1, and q > 1.

- Trace norm dual: $(\|X\|_{tr})_* = \|X\|_{op} = \sigma_1(X)$.
- Dual norm of dual norm: can show that $\|x\|_{**} = \|x\|$

2 Conjugate Function

• Conjugate function: given $f: \mathbb{R}^n \to \mathbb{R}$, the function

$$f^*(y) = \max_{x} y^{\top} x - f(x)$$

is called its conjugate.

Proposition 1. f^* is always convex.

Proof. For any y_1,y_2 and $0 \le \alpha \le 1$, let $y_\alpha = \alpha y_1 + (1-\alpha)y_2$. Then,

$$f^*(y_\alpha) = \max_x y_\alpha^\top x - f(x).$$

Note that

$$y_{\alpha}^{\top}x - f(x) = \alpha \left(y_1^{\top}x - f(x)\right) + (1 - \alpha)\left(y_2^{\top}x - f(x)\right)$$

which implies that

$$f^*(y_\alpha) \le \alpha f^*(y_1) + (1 - \alpha) f^*(y_2).$$

• Fenchel's inequality: $f(x) + f^*(y) \ge y^\top x$.

- Conjugate of conjugate f^{**} satisfies $f^{**} \leq f$

Proof. We have

$$f^*(y) \ge y^\top x - f(x)$$

$$\Longrightarrow f(x) \ge y^\top x - f^*(y)$$

$$\Longrightarrow f(x) \ge \max_y y^\top x - f^*(y) = f^{**},$$

so $f \ge f^{**}$.

If f is closed (continuous) and convex, then $f^{**} = f$. Also for any x, y.

$$y \in \partial f(x) \Longleftrightarrow x \in \partial f^*(y)$$

$$\Longleftrightarrow x \in \arg\min_{z} f(z) - y^{\top}z \Longleftrightarrow x \in \arg\max_{z} y^{\top}z - f(z)$$

$$\Longleftrightarrow f(x) + f^*(y) = y^{\top}x$$

If f is strictly convex, then $\nabla f^*(y) = \arg\min_z f(z) - y^\top z$.

Proof. We can easily see that

$$y \in \partial f(x)$$

$$\iff 0 \in \partial (f(x) - y^{\top} x)$$

$$\iff x \in \arg\min_{z} f(z) - y^{\top} z$$

$$\iff x \in \arg\max_{z} y^{\top} z - f(z)$$

$$\iff y^{\top} x - f(x) = \max_{z} (y^{\top} z - f(z)) = f^{*}(y)$$

Now we just need to prove $y^{\top}x - f^*(y) = f(x) \Longleftrightarrow x \in \partial f^*(y)$. Since

$$y^{\top}x - f^{*}(y) = f(x)$$

$$\iff y^{\top}x - f^{*}(y) = \max_{z} z^{\top}x - f^{*}(z) \qquad (f = f^{**})$$

$$\iff y \in \arg\max_{z} z^{\top}x - f^{*}(z)$$

$$\iff y \in \arg\min_{z} f^{*}(z) - z^{\top}x$$

$$\iff 0 \in \partial (f^{*}(y) - y^{\top}x)$$

$$\iff x \in \partial f^{*}(y)$$

• If $f(u,v) = f_1(u) + f_2(v)$, then $(u \in \mathbb{R}^n, v \in \mathbb{R}^m)$,

$$f^*(w,z) = f_1^*(w) + f_2^*(z)$$

• Example: $f(x) = \frac{1}{2}x^{\mathsf{T}}Qx, \ Q \succ 0.$

$$f^{*}(y) = \max_{x} y^{\top} x - \frac{1}{2} x^{\top} Q x$$

$$= -\min_{x} \frac{1}{2} x^{\top} Q x - y^{\top} x \qquad (taking \ x = Q^{-1} y)$$

$$= -\min_{x} \frac{1}{2} (Q^{-1} y)^{\top} Q (Q^{-1} y) - y^{\top} Q^{-1} y$$

$$= \frac{1}{2} y^{\top} Q^{-1} y.$$

• Fenchel's inequality gives

$$f(x) + f^*(y) \ge x^\top y \Longrightarrow \frac{1}{2} x^\top Q x + \frac{1}{2} y^\top Q^{-1} y \ge x^\top y$$

• Conjugate of indicator function: if $f(x) = I_c(x)$, then its conjugate is

$$f^*(y) = I_C^*(y) = \max_{x \in C} y^{\top} x$$

Since $f^*(y) = \max_x y^\top x - I_C(x) = \max_{x \in C} y^\top x$.

• Conjugate of norm: If f(x) = ||x|| (any norm), then its conjugate is

$$f^*(y) = \begin{cases} 0 & \|y\|_* \le 1 \\ +\infty & \|y\|_* > 1 \end{cases}$$

or can be written as

$$f^*(y) = I_{\{z: ||z||_* < 1\}}(y)$$

Proof. recall the definition of dual norm

$$||y||_* = \max_{||x|| \le 1} x^{\top} y$$

to evaluate

$$f^*(y) = \max_{x} y^{\top} x - \|x\|$$

we distinguish two cases

– If $||y||_* \le 1$, then by definition of dual norm

$$y^{\top} x \le ||x|| ||y||_* \le ||x|| \qquad \forall x$$

and equality holds if x = 0; Therefore $f^*(y) = \max_x y^\top x - ||x|| = 0$.

– If $||y||_* > 1$, by the definition of dual norm $||y||_* = \max_{||x|| \le 1} x^\top y > 1$, there exists an x with $||x|| \le 1$, $x^\top y > 1$, then

$$f^*(y) \ge y^\top (tx) - ||tx|| = t(y^\top x - ||x||) \xrightarrow{t \to \infty} \infty$$

3 Conjugates and Dual Problem

Conjugates appear frequently in derivation of dual problems, via

$$f^*(u) = \max_{x} u^{\top} x - f(x)$$
$$= -\min_{x} f(x) - u^{\top} x$$

Therefore

$$-f^*(u) = \min_{x} f(x) - u^{\top} x$$

in minimization of the Lagrangian.

E.g. consider

$$\min_{x} f(x) + g(x)$$
 $\iff \min_{x} f(x) + g(z)$ subject to $x = z$

Lagrange dual function is

$$g(u) = \min f(x) + g(z) + u^{\top}(z - x) = -f^{*}(u) - g^{*}(-u)$$

Hence the dual problem is

$$\max_{u} -f^*(u) - g^*(-u)$$

4 Lasso Dual (through duality)

The Lasso primal is

$$\min_{\beta} \frac{1}{2} ||y - X\beta||_2^2 + \lambda ||\beta||_1.$$

Introduce $z = X\beta$, and the dual variable u

$$\min \frac{1}{2} ||y - z||^2 + \lambda ||\beta||_1$$

s.t. $X\beta - z = 0$.

Then we have Lagrangian

$$L(\beta, z, u) = \frac{1}{2} ||y - z||^2 + \lambda ||\beta||_1 + u^{\top} (X\beta - z)$$

and Lagrange dual function

$$\begin{split} g(u) &= \min_{\beta, z} L(\beta, z, u) \\ &= \min_{\beta} \left\{ \lambda \|\beta\|_1 - (X^\top u)^\top \beta \right\} + \min_{z} \left\{ \frac{1}{2} \|y - z\|_2^2 + u^\top z \right\} \\ &= -\lambda \max_{\beta} \left(\frac{(X^\top u)^\top}{\lambda} \beta - \|\beta\|_1 \right) + \frac{1}{2} \|y\|_2^2 - \frac{1}{2} \|y - u\|_2^2 \\ &= -\lambda I_{\{z: \|z\|_{\infty} \le 1\}} \left(\frac{X^\top u}{\lambda} \right) + \frac{1}{2} \|y\|_2^2 - \frac{1}{2} \|y - u\|_2^2 \end{split}$$

Thus the dual problem is

$$\max_{u} - \frac{1}{2} \|y - u\|_{2}^{2} - \lambda I_{\{z: \|z\|_{\infty} \le 1\}} \left(\frac{X^{\top} u}{\lambda} \right)$$

which is equivalent to

$$\max_u -\frac{1}{2}\|y-u\|_2^2$$
 subject to
$$\|\frac{X^\top u}{\lambda}\|_\infty \leq 1$$

which is equivalent to

$$\min_{u} \|y - u\|_2^2$$
 subject to
$$\|X^\top u\|_{\infty} \le \lambda$$

Note that the problem now becomes solving $u \in \mathbb{R}^n$ instead of solving $\beta \in \mathbb{R}^p$. Suppose now we have solve the dual problem and the solution is u^* . Then β^*, z^* must minimize $L(\beta, z, u^*)$

$$\nabla_z L(\beta, z, u^*) = 0 \iff z^* = y - u^* \iff X\beta^* = y - u^*$$

Therefore

$$||X^{\top}u^*||_{\infty} \leq \lambda \Longrightarrow ||X^{\top}(y - X\beta^*)||_{\infty} \leq \lambda \text{ (fitted residual)}$$

and

$$\beta^* = \arg\max_{\beta} \left\{ \frac{(X^{\top}u^{\star})^{\top}}{\lambda} \beta - \|\beta\|_1 \right\}.$$

5 Lasso Dual (through KKT)

Recall the definition of polyhedron. A set $C \subseteq \mathbb{R}^n$ is called a convex Polyhedron if C is the intersection of many half-spaces:

$$C=\cap_{i=1}^k\{x\in\mathbb{R}^n:a_i^\top x\leq b_i\}$$
 Where $a_1,\dots,a_k\in\mathbb{R}^n$ and $b_1,\dots,b_k\in\mathbb{R}$

The aim of this section is to show that the LASSO problem can be formulated as a projection onto a polyhedron. Before we delve into the details of the derivation, we state a couple of preliminary results that will be used in later proofs:

- A polyhedron is a closed and convex set.
- For any closed and convex set $C \subseteq \mathbb{R}^n$ and point $x \in \mathbb{R}^n$, there is a unique point $u \in C$ minimizing

 $\|x-u\|_2$. This point is a projection of x onto set C, which we denote by $\Pi_C(x)$.

In the linear regression setting, with response variable $y \in \mathbb{R}^n$ and design matrix $X \in \mathbb{R}^{n \times p}$, if we regress Y on X using the LASSO, the optimal model parameters $X\hat{\beta}$ can be written as:

$$X\hat{\beta} = y - \Pi_C(y) = (I - \Pi_C)(y),$$

where C is a polyhedron

Proof. Given $y \in \mathbb{R}^n$.

$$\theta = \Pi_C(y)$$

onto a closed convex set $C \subseteq \mathbb{R}^n$ can be characterised as the unique point satisfying

$$\langle y - \theta, \theta - u \rangle \ge 0, \ \forall u \in C.$$
 (1)

where $\langle \cdot, \cdot \rangle$ denotes the inner product. Based on this, if we define

$$\theta = y - X\hat{\beta}(y),$$

or equivalently:

$$X\hat{\beta} = y - \theta$$

can be regarded as a function of y, We want to show that the inequality 1 holds for all $u \in C$, where C is defined as

$$C := \bigcap_{j=1}^{p} \left(\left\{ u \in \mathbb{R}^n \colon X_j^\top u \le \lambda \right\} \cap \left\{ u \in \mathbb{R}^n \colon X_j^\top u \ge -\lambda \right\} \right),$$

which is equivalent to

$$\left\{ u \in \mathbb{R}^n \colon \left\| X^\top u \right\|_{\infty} \le \lambda \right\}.$$

To show this, we can see that

$$\begin{split} \langle y - \theta, \theta - u \rangle &= \langle X \hat{\beta}, y - X \hat{\beta} - u \rangle \\ &= \langle X \hat{\beta}, y - X \hat{\beta} \rangle - \langle X^\top u, \hat{\beta} \rangle. \end{split}$$

From the KKT conditions for LASSO, we know that the optimization problem

$$\min_{\beta} g(\beta) + h(\beta) = \min_{\beta} \underbrace{\frac{1}{2} \|y - X\beta\|_{2}^{2}}_{q(\beta)} + \underbrace{\lambda \|\beta\|_{1}}_{h(\beta)}$$

satisfies the stationarity condition, which can be stated as:

$$\begin{split} 0 &\in \partial \left(g(\hat{\beta}) + h(\hat{\beta}) \right) \\ &= \nabla g(\hat{\beta}) + \partial h(\hat{\beta}) \\ &= -X^{\top} \left(y - X \hat{\beta} \right) + \lambda \partial \left\| \hat{\beta} \right\|_{1}. \end{split}$$

Thus

$$X^{\top} \left(y - X \hat{\beta} \right) = \lambda \gamma, \tag{2}$$

where

$$\gamma_j = \left(\partial \left\| \hat{\beta} \right\|_1 \right)_j = \left\{ \begin{array}{ll} \operatorname{sgn} \left(\hat{\beta}_j \right) & \text{if } \hat{\beta}_j \neq 0 \\ [-1,1] & \text{if } \hat{\beta}_j = 0 \end{array} \right..$$

Taking the inner product with $\hat{\beta}$ on both sides of 2, we always have

$$\langle X \hat{\beta}, y - X \hat{\beta} \rangle = \lambda \left\| \hat{\beta} \right\|_1 = \max_{\|w\|_{\infty} \le \lambda} w^{\top} \hat{\beta}.$$

The RHS holds since $\beta_j\gamma_j=\begin{cases} 0 & \hat{\beta_j}=0\\ |\hat{\beta_j}| & \text{otherwise} \end{cases}$. Therefore,

$$\langle y - \theta, \theta - u \rangle = \max_{\|X^{\top}u\|_{\infty} \le \lambda} \langle X^{\top}u, \hat{\beta} \rangle - \langle X^{\top}u, \hat{\beta} \rangle \ge 0 \ \forall u \in C,$$

which implies that θ is indeed a projection of y onto C,

$$\theta = y - X\hat{\beta}(y) = \Pi_C(y).$$

6 Screening

Let f be differentiable and strictly convex, let $X \in \mathbb{R}^{n \times p}$, $\lambda > 0$. Consider

$$\min_{\beta} \frac{1}{2} \|y - X\beta\|_2^2 + \lambda \|\beta\|_1$$

The KKT conditions are

$$\begin{cases} X_j^T(y-X\beta^*) = \lambda \cdot \operatorname{sgn}(\beta_j^*) & \beta_j^* \neq 0 \\ |X_j^T(y-X\beta^*)| \leq \lambda & \beta_j^* = 0 \end{cases}$$

which implies that

$$|X_j^T(y - X\beta^*)| < \lambda \quad \Longrightarrow \quad \beta_j^* = 0 \tag{3}$$

Suppose that the dual solution is u^{\star} . Then β^{\star}, z^{\star} must minimize $L(\beta, z, u^{\star})$

$$\nabla_z L(\beta, z, u^*) = 0$$

$$\iff \nabla_z \left\{ \frac{1}{2} \|y - z\|_2^2 + u^\top z \right\} = 0$$

$$\iff -(y - z^*) + u^* = 0$$

$$\iff y - X\beta^* = u^*$$

Replace $y - X\beta^*$ using u^* in (3) we get

$$|X_j^T u^*| < \lambda \implies \beta_j^* = 0.$$

This is when u^* is in the interior of the slab defined by the feature X_j , therefore