Modern Statistical Methods — Example Sheet 3

Lucas Riedstra

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In all of the below, assume that any design matrices X are $n \times p$ and have their columns centred and then scaled to have ℓ^2 -norm \sqrt{n} , and that any responses $Y \in \mathbb{R}^n$ are centred.

Question 1. When proving the theorems on the prediction error of the Lasso, we started with the so-called basic inequality that

$$\frac{1}{2n} \left\| X(\beta^0 - \hat{\beta}) \right\|_2^2 \leq \frac{1}{n} \varepsilon^\top X(\hat{\beta} - \beta^0) + \lambda \big\| \beta^0 \big\|_1 - \lambda \big\| \hat{\beta} \big\|_1.$$

Show that in fact we can improve this to

$$\frac{1}{n} \left\| X(\beta^0 - \hat{\beta}) \right\|_2^2 \le \frac{1}{n} \varepsilon^\top X(\hat{\beta} - \beta^0) + \lambda \left\| \beta^0 \right\|_1 - \lambda \left\| \hat{\beta} \right\|_1.$$

Proof. By the KKT conditions, we there exists $\hat{\nu} \in \mathbb{R}^p$ with $\|\hat{\nu}\|_{\infty} \leq 1$ and $\langle \hat{\nu}, \hat{\beta} \rangle = \|\beta\|_1$ such that

$$\begin{split} \frac{1}{n} X^\top (Y - X \hat{\beta}) &= \lambda \hat{\nu} \\ \frac{1}{n} X^\top (X (\beta^0 - \hat{\beta}) + \varepsilon) &= \lambda \hat{\nu} \\ \frac{1}{n} X^\top X (\beta^0 - \hat{\beta}) &= -\frac{1}{n} X^\top \varepsilon + \lambda \hat{\nu} \\ \frac{1}{n} (\beta^0 - \hat{\beta})^\top X^\top X (\beta^0 - \hat{\beta}) &= -\frac{1}{n} (\beta^0 - \hat{\beta})^\top X^\top \varepsilon + \lambda (\beta^0 - \hat{\beta})^\top \hat{\nu} \\ \frac{1}{n} \left\| X (\beta^0 - \hat{\beta}) \right\|_2^2 &= \frac{1}{n} \varepsilon^\top X (\hat{\beta} - \beta^0) + \lambda \langle \hat{\nu}, \beta^0 \rangle - \lambda \|\hat{\beta}\|_1, \end{split}$$

and now plugging in $\langle \beta^0, \hat{\nu} \rangle \leq \|\beta^0\|_1 \|\hat{\nu}\|_{\infty} \leq \|\beta^0\|_1$ yields the result.

Question 2. Under the assumptions of Theorem 23 on the prediction and estimation properties of the Lasso under a compatibility condition, show that, with probability $1 - 2p^{-(A^2/8-1)}$, we have

$$\frac{1}{n} \Big\| X(\beta^0 - \hat{\beta}) \Big\|_2^2 \leq \frac{9A^2 \log(p)}{4\varphi^2} \frac{\sigma^2 s}{n}.$$

Proof. We have

$$\begin{split} \frac{1}{\lambda n} \left\| X(\beta^0 - \hat{\beta}) \right\|_2^2 &\leq \frac{1}{2\lambda n} \left\langle \frac{2X^\top \varepsilon}{n}, (\hat{\beta} - \beta^0) \right\rangle + \left\| \beta^0 \right\|_1 - \left\| \hat{\beta} \right\|_1 \\ &\leq \frac{1}{2} \left\| \hat{\beta} - \beta^0 \right\|_1 + \left\| \beta^0 \right\|_1 - \left\| \hat{\beta} \right\|_1 \\ &= \frac{1}{2} \left(\left\| \hat{\beta}_S - \beta_S^0 \right\|_1 + \left\| \hat{\beta}_N \right\|_1 \right) + \left\| \beta_S^0 \right\|_1 - \left\| \hat{\beta}_S \right\|_1 - \left\| \hat{\beta}_N \right\|_1 \\ &= \frac{1}{2} \left\| \hat{\beta}_S - \beta_S^0 \right\|_1 + \left\| \beta_S^0 \right\|_1 - \left\| \hat{\beta}_S \right\|_1 - \frac{1}{2} \left\| \hat{\beta}_N \right\|_1 \\ &\leq \frac{3}{2} \left\| \hat{\beta}_S - \beta_S^0 \right\|_1 + \left\| \beta_S^0 \right\|_1 \\ &\leq \frac{3}{2} \left\| \hat{\beta}_S - \beta_S^0 \right\|_1, \end{split}$$

and note that from \star we conclude $\|\hat{\beta}_N\|_1 \leq 3\|\hat{\beta}_S - \beta_S^0\|_1$, and therefore $\hat{\beta} - \beta^0$ can be plugged into the compatibility constant. We find

$$\frac{1}{n} \Big\| X(\beta^0 - \hat{\beta}) \Big\|_2^2 \leq \frac{3\lambda\sqrt{s}}{2\varphi\sqrt{n}} \Big\| X(\beta^0 - \hat{\beta}) \Big\|_2 \implies \frac{1}{\sqrt{n}} \Big\| X(\beta^0 - \hat{\beta}) \Big\|_2 \leq \frac{3\lambda\sqrt{s}}{2\varphi},$$

and squaring both sides gives

$$\frac{1}{n} \Big\| X(\beta^0 - \hat{\beta}) \Big\|_2^2 \leq \frac{9\lambda^2 s}{4\varphi^2}$$

Question 3. Let $Y = X\beta^0 + \varepsilon - \varepsilon \mathbf{1}$ and let $S = \{k \mid \beta^0 \neq 0\}$, $N \coloneqq \{1, \dots, p\} \setminus S$. Without loss of generality assume $S = \{1, \dots, |S|\}$. Assume that X has full column rank and let $\Omega = \{\|X^{\top}\varepsilon\|_{\infty}/n \leq \lambda_0\}$. Show that, when $\lambda > \lambda_0$, if the following two conditions hold

$$\sup_{\|\tau\|_{\infty} \le 1} \|X_N^{\top} X_S (X_S^{\top} X_S)^{-1} \tau\|_{\infty} < \frac{\lambda - \lambda_0}{\lambda + \lambda_0}$$
$$(\lambda + \lambda_0) \left\| \left\{ (\frac{1}{n} X_S^{\top} X_S)^{-1} \right\}_k \right\|_1 < |\beta_k^0| \qquad \qquad for \ k \in S,$$

then on Ω the (unique) Lasso solution satisfies $\operatorname{sgn}(\hat{\beta}_{\lambda}^{L}) = \operatorname{sgn}(\beta^{0})$.

Proof. Following the proof of theorem 22 in the lecture notes, the KKT conditions become

$$\frac{1}{n} \begin{pmatrix} X_S^\top X_S & X_S^\top X_N \\ X_N^\top X_S & X_N^\top X_N \end{pmatrix} \begin{pmatrix} \beta_S^0 - \hat{\beta}_S \\ -\hat{\beta}_N \end{pmatrix} + \frac{1}{n} \begin{pmatrix} X_S^\top \\ X_N^\top \end{pmatrix} \varepsilon = \lambda \begin{pmatrix} \hat{\nu}_S \\ \hat{\nu}_N \end{pmatrix}.$$

We first prove there exists a Lasso solution $(\hat{\beta}_S, 0)$ which satisfies the KKT conditions. Solving the top equation block for $\hat{\beta}_S$ gives

$$\hat{\beta}_S = \beta_S^0 - \left(\frac{1}{n} X_S^\top X_S\right)^{-1} \left(\lambda \operatorname{sgn}(\beta_S^0) - \frac{1}{n} X_S^\top \varepsilon\right). \tag{1}$$

To prove that $\operatorname{sgn}(\beta_S^0) = \operatorname{sgn}(\hat{\beta}_S)$ holds, note that for $k \in S$ we have

$$\begin{split} \left| \left\{ \left(\frac{1}{n} X_S^\top X_S \right)^{-1} \left(\lambda \operatorname{sgn}(\beta_S^0) - \frac{1}{n} X_S^\top \varepsilon \right) \right\}_k \right| &= \left| \left(\frac{1}{n} X_S^\top X_S \right)_k^{-1} \left(\lambda \operatorname{sgn}(\beta_S^0) - \frac{1}{n} X_S^\top \varepsilon \right) \right| \\ &\leq \left\| \left(\frac{1}{n} X_S^\top X_S \right)_k^{-1} \right\|_1 \left\| \lambda \operatorname{sgn}(\beta_S^0) - \frac{1}{n} X_S^\top \varepsilon \right\|_{\infty} \\ &< \frac{\left| \beta_k^0 \right|}{\lambda + \lambda_0} \cdot (\lambda + \lambda_0) = \left| \beta_k^0 \right|, \end{split}$$

since $\left\|\frac{1}{n}X_S^{\top}\varepsilon\right\|_{\infty} \leq \left\|\frac{1}{n}X^{\top}\varepsilon\right\|_{\infty} \leq \lambda_0$. Plugging this result into eq. (1) shows that $\operatorname{sgn}(\hat{\beta}_S) = \operatorname{sgn}(\beta_S^0)$. We must show that with this choice of $\hat{\beta}$, the bottom block is satisfied, i.e.,

$$\lambda \ge \left\| \frac{1}{n} X_N^\top X_S(\beta_S^0 - \hat{\beta}_S) + \frac{1}{n} X_N^\top \varepsilon \right\|_{\infty} = \left\| X_N^\top X_S(X_S^\top X_S)^{-1} \left(\lambda \operatorname{sgn}(\beta_S^0) - \frac{1}{n} X_S^\top \varepsilon \right) + \frac{1}{n} X_N^\top \varepsilon \right\|_{\infty} = (*).$$

Note that

$$\left\| \lambda \operatorname{sgn}(\beta_S^0) - \frac{1}{n} X_S^\top \varepsilon \right\|_{\infty} \le \lambda + \lambda_0,$$

and plugging that into the previous equation yields

$$(*) \le (\lambda + \lambda_0) \cdot \sup_{\|\tau\|_{\infty} \le 1} \|X_N^\top X_S (X_S^\top X_S)^{-1} \tau\|_{\infty} + \lambda_0 \le \lambda - \lambda_0 + \lambda_0 = \lambda,$$

which concludes the proof.

Question 4. Find the KKT conditions for the group Lasso.

Proof. Recall the objective function in group Lasso is the convex function

$$\frac{1}{2n} \|Y - X\beta\|_2^2 + \lambda \sum_{j=1}^q m_j \|\beta_{G_j}\|_2.$$

Note that the subdifferential of the 2-norm is given by

$$\partial \|x\|_2 = \begin{cases} \{x/\|x\|_2\}, & x \neq 0, \\ \{v : \|v\|_2 \leq 1\}, & x = 0. \end{cases}$$

Furthermore, note that the subdifferential of $\frac{1}{2n}\|Y - X\beta\|_2^2$ is $\left\{-\frac{1}{n}X^\top(Y - X\beta)\right\}$. We therefore find that 0 lies in the subdifferential if and only if, for $j = 1, \ldots, q$, we have

$$\begin{cases} \left(\frac{1}{n}X^{\top}(Y - X\beta)\right)_{G_j} = \lambda m_j \beta_{G_j} / \|\beta_{G_j}\|_2, & \text{if } \beta_{G_j} \neq 0, \\ \left\| \left(\frac{1}{n}X^{\top}(Y - X\beta)\right)_{G_j} \right\|_2 \leq \lambda m_j, & \text{if } \beta_{G_j} = 0. \end{cases}$$

Question 5. (a) Show that

$$\max_{\vartheta: \left\|X^{\top}\vartheta\right\|_{\infty} \leq \lambda} G(\vartheta) = \frac{1}{2n} \left\|Y - X\hat{\beta}_{\lambda}^{L}\right\|_{2}^{2} + \lambda \left\|\hat{\beta}_{\lambda}^{L}\right\|_{1},$$

where

$$G(\vartheta) = \frac{1}{2n} \|Y\|_2^2 - \frac{1}{2n} \|Y - n\vartheta\|_2^2.$$

Show that the unique ϑ maximising G is $\vartheta^* = (Y - X \hat{\beta}_{\lambda}^L)/n$.

Hint: Treat the Lasso optimisation problem as minimising $\|Y - z\|_2^2/(2n) + \lambda \|\beta\|_1$ subject to $z - X\beta = 0$ over $(\beta, z) \in \mathbb{R}^p \times \mathbb{R}^n$ and consider the Lagrangian.

(b) Let $\tilde{\vartheta}$ be such that $\|X^{\top}\tilde{\vartheta}\|_{\infty} \leq \lambda$. Explain why if

$$\max_{\vartheta: G(\vartheta) \geq G(\tilde{\vartheta})} \left| X_k^\top \vartheta \right| < \lambda,$$

then we know that $\hat{\beta}_{\lambda,k}^L = 0$. By considering $\tilde{\vartheta} = Y\lambda/(n\lambda_{\max})$, show that $\hat{\beta}_{\lambda,k}^L = 0$ if

$$\frac{1}{n} |X_k^\top Y| < \lambda - \frac{\|Y\|_2}{\sqrt{n}} \frac{\lambda_{\max} - \lambda}{\lambda_{\max}}.$$

Proof. (a) As in the hint, we write the Lasso objective problem as

$$\min_{\substack{(\beta,z) \in \mathbb{R}^p \times \mathbb{R}^n \\ z - X \beta = 0}} \frac{1}{2n} \|Y - z\|_2^2 + \lambda \|\beta\|_1.$$

The Lagrangian is now

$$L(z, \beta, \vartheta) = \frac{1}{2n} \|Y - z\|_{2}^{2} + \lambda \|\beta\|_{1} + \vartheta^{\top}(z - X\beta),$$

and the dual function is given by

$$\tilde{f}(\vartheta) = \inf_{(\beta,z) \in \mathbb{R}^p \times \mathbb{R}^n} L(z,\beta,\vartheta) = \inf_{\beta \in \mathbb{R}^p} \left(\lambda \|\beta\|_1 - \vartheta^\top X \beta \right) + \inf_{z \in \mathbb{R}^n} \left(\frac{1}{2n} \|Y - z\|_2^2 + \vartheta^\top z \right).$$

For the first term: note that $\vartheta^\top X \beta \leq \|X^\top \vartheta\|_{\infty} \|\beta\|_1$, with equality for β suitably chosen. Therefore, the first term has infimum $-\infty$ if $\|X^\top \vartheta\|_{\infty} > \lambda$, and otherwise has infimum 0 when setting $\beta = 0$.

The second term has z-gradient $-\frac{1}{n}(Y-z)+\vartheta$, and equating that to 0 gives $z=Y-n\vartheta$. Plugging this into the second term gives

$$\begin{split} \frac{1}{2n}\|n\vartheta\|_2^2 + \vartheta^\top Y - n\vartheta^\top \vartheta &= \vartheta^\top Y - \frac{n}{2}\vartheta^\top \vartheta \\ 0 &= \vartheta^\top Y - \frac{n}{2}\vartheta^\top \vartheta + \frac{1}{2n}Y^\top Y - \frac{1}{2n}Y^\top Y \\ &= \frac{1}{2n}Y^\top Y - \frac{1}{2n}(Y - n\vartheta)^\top (Y - n\vartheta) \\ &= \frac{1}{2n}\|Y\|_2^2 - \frac{1}{2n}\|Y - n\vartheta\|_2^2 = G(\vartheta). \end{split}$$

Therefore, the dual function is given by

$$\tilde{f}(\vartheta) = \begin{cases} -\infty & \text{if } \|X^{\top}\vartheta\| > \lambda, \\ G(\vartheta) & \text{if } \|X^{\top}\vartheta\| \leq \lambda. \end{cases}$$

The optimal value of the dual problem is therefore

$$d^* = \max_{\vartheta \in \mathbb{R}^n} \tilde{f}(\vartheta) = \max_{\vartheta : \|X^\top \vartheta\|_{L^*} \le \lambda} G(\vartheta),$$

which equals the optimal value of the primal problem. This proves the first claim.

By the KKT conditions we have $\|X^{\top}\vartheta\|_{\infty} = \frac{1}{n} \|X^{\top}(Y - X\hat{\beta})\|_{\infty} \leq \lambda$, and plugging in ϑ^* in G gives

$$\begin{split} G(\vartheta^*) &= \frac{1}{2n} \bigg(\|Y\|_2^2 - \left\|X\hat{\beta}\right\|_2^2 \bigg) = \frac{1}{2n} \bigg(\left\|Y - X\hat{\beta}\right\|_2^2 + 2Y^\top X\hat{\beta} - 2\left\|X\hat{\beta}\right\|_2^2 \bigg) \\ &= \frac{1}{2n} \left\|Y - X\hat{\beta}\right\|_2^2 + \hat{\beta}^\top \bigg\{ \frac{1}{n} X^\top (Y - X\hat{\beta}) \bigg\} \\ &\stackrel{\star}{=} \frac{1}{2n} \left\|Y - X\hat{\beta}\right\|_2^2 + \lambda \|\beta\|_1, \end{split}$$

where \star follows from the KKT conditions. This shows that ϑ^* maximises G over the objective set. TODO: Uniqueness of ϑ^* ?

(b) Clearly

$$\max_{\vartheta:G(\vartheta)>G(\tilde{\vartheta})}\left|X_k^\top\vartheta\right|<\lambda\implies\left|X_k^\top\vartheta^*\right|<\lambda.$$

We compute

$$X_k^{\top} \vartheta^* = (X^{\top} \vartheta^*)_k = \left(\frac{1}{n} X^{\top} (Y - X \hat{\beta})\right)_k = \lambda \hat{\nu}_k,$$

where $\hat{\nu}$ is from the KKT conditions, and we know that $\hat{\beta}_{\lambda,k}^L \neq 0 \implies |\hat{\nu}_k| = 1$. However, we have

$$\lambda > |X_k^\top \vartheta^*| = \lambda |\hat{\nu}_k| \implies |\hat{\nu}_k| < 1 \implies \hat{\beta}_{\lambda,k}^L = 0.$$

Now let $\tilde{\vartheta} = Y\lambda/(n\lambda_{\max})$. It is easily checked that $\|X^{\top}\vartheta\|_{\infty} = \lambda$. Now, clearly we have

$$G(\vartheta) \geq G(\tilde{\vartheta}) \implies \|Y - n\vartheta\|_2^2 \leq \|Y - n\tilde{\vartheta}\|_2^2 = \left(1 - \frac{\lambda}{\lambda_{\max}}\right)^2 \|Y\|_2^2 = \left(\frac{\lambda_{\max} - \lambda}{\lambda_{\max}}\right)^2 \|Y\|_2^2.$$

We find that for $G(\vartheta) \geq G(\tilde{\vartheta})$ we have

$$\begin{split} \left| X_k^\top \vartheta \right| &= \frac{1}{n} \middle| X_k^\top (n\vartheta) \middle| = \frac{1}{n} \middle| X_k^\top (n\vartheta - Y + Y) \middle| \\ &\leq \frac{1}{n} \middle| X_k^\top (Y - n\vartheta) \middle| + \frac{1}{n} \middle| X_k^\top Y \middle| \\ &< \frac{1}{n} || X_k ||_2 || Y - n\vartheta ||_2 + \lambda - \frac{|| Y ||_2}{\sqrt{n}} \frac{\lambda_{\max} - \lambda}{\lambda_{\max}} \\ &\leq \frac{1}{\sqrt{n}} \frac{\lambda_{\max} - \lambda}{\lambda_{\max}} || Y ||_2 + \lambda - \frac{|| Y ||_2}{\sqrt{n}} \frac{\lambda_{\max} - \lambda}{\lambda_{\max}} = \lambda, \end{split}$$

and from the previous observation we conclude $\hat{\beta}_{\lambda,k}^L = 0$ (note that we used $||X_k||_2 = \sqrt{n}$).

Question 6. Consider the Lasso and let $\hat{E}_{\lambda} := \left\{ k : \frac{1}{n} \left| X_k^{\top} (Y - X \hat{\beta}_{\lambda}^L) \right| = \lambda \right\}$ be the equicorrelation set at λ . Suppose that $\operatorname{rank}(X_{\hat{E}_{\lambda}}) = \left| \hat{E}_{\lambda} \right|$ for all $\lambda > 0$, so the Lasso solution is unique for all $\lambda > 0$. Let $\hat{\beta}_{\lambda_1}^L$ and $\hat{\beta}_{\lambda_2}^L$ be two Lasso solutions at different values of the regularisation parameter. Suppose that $\operatorname{sgn}(\hat{\beta}_{\lambda_1}^L) = \operatorname{sgn}(\hat{\beta}_{\lambda_2}^L)$. Show that then for all $t \in [0, 1]$,

$$t\hat{\beta}_{\lambda_1}^L + (1-t)\hat{\beta}_{\lambda_2}^L = \hat{\beta}_{t\lambda_1 + (1-t)\lambda_2}^L.$$

Conclude that the solution path $\lambda \mapsto \hat{\beta}_{\lambda}^{L}$ is piecewise linear with a finite number of knots (points λ where the solution path is not linear at λ) and these occur when the sign of the Lasso solution changes.

Proof. Write $\hat{\beta}_i = \hat{\beta}_{\lambda_i}^L \ \gamma = t \hat{\beta}_1 + (1-t)\hat{\beta}^2$, then we have

$$\frac{1}{n}X^{\top}(Y - X\gamma) = t\frac{1}{n}X^{\top}(Y - X\hat{\beta}_1) + (1 - t)\frac{1}{n}X^{\top}(Y - X\hat{\beta}_2)$$
$$= t\lambda_1\hat{\nu}_1 + (1 - t)\lambda_2\hat{\nu}_2.$$

Note that $\hat{\nu}_1$ and $\hat{\nu}_2$ agree on \hat{E}_{λ} , and on the other points we clearly have $\|\hat{\nu}\|_{\infty} \leq 1$, so we conclude

$$\frac{1}{n}X^{\top}(Y - X\gamma) = (t\lambda_1 + (1 - t)\lambda_2)\hat{\nu},$$

where $(\hat{\nu})_S = \operatorname{sgn}(\gamma)_S$ and $\|\hat{\nu}\|_{\infty} \leq 1$. This shows that γ is a Lasso solution.

It follows that the solution path is piecewise linear with knots whenever the sign of the Lasso solution changes. Since the Lasso solution is 0 for λ large enough, there can only be finitely many sign changes, which concludes the proof. (TODO: elaborate on last step)

Question 7. The elastic net estimator in the linear model minimises

$$\frac{1}{2n} \|Y - X\beta\|_2^2 + \lambda \left(\alpha \|\beta\|_1 + (1 - \alpha) \|\beta\|_2^2 / 2\right)$$

over $\beta \in \mathbb{R}^p$, where $\alpha \in [0,1]$ is fixed.

- 1. Suppose X has two columns X_j and X_k that are identical and $\alpha < 1$. Explain why the minimising β^* above is unique and has $\beta_k^* = \beta_j^*$.
- 2. Let $\hat{\beta}^{(0)}, \hat{\beta}^{(1)}, \ldots$ be the solutions from iterations of a coordinate descent procedure to minimise the elastic net objective. For a fixed variable index k, let $A = \{1, \ldots, k-1\}, B = \{k+1, \ldots, p\}$. Show that for $m \ge 1$,

$$\hat{\beta}_{k}^{(m)} = \frac{S_{\lambda\alpha} \left(n^{-1} X_{k}^{\top} (Y - X_{A} \hat{\beta}_{A}^{(m)} - X_{B} \hat{\beta}_{B}^{(m-1)}) \right)}{1 + \lambda (1 - \alpha)},$$

where $S_t(u) = \operatorname{sgn}(u)(|u| - t)_+$ is the soft-thresholding operator.

Proof. 1. The minimiser β^* is unique because the objective function is strictly convex: since $\alpha < 1$, the term $(1 - \alpha) \|\beta\|_2^2 / 2$ is strictly convex, and therefore the sum with another convex function is also convex.

If $\beta_k^* \neq \beta_j^*$, then it is easily seen that replacing both β_k^* and β_j^* by $\frac{1}{2}(\beta_k^* + \beta_j^*)$ gives a smaller objective value (the term $||Y - X\beta||_2^2$ stays the same and the other two terms will be less by convexity) which contradicts the fact that β^* is a minimiser.

2. For simplicity, let $\beta_A := \hat{\beta}_A^{(m)}$ and $\beta_B := \hat{\beta}_B^{(m-1)}$, so our goal is to find

$$\underset{\beta_k \in \mathbb{R}}{\arg \min} g(\beta_k) \quad \text{where } g(\beta_k) = f(\beta_A, \beta_k, \beta_B).$$

Note that for some $h(\beta_A, \beta_B)$ we can write

$$g(\beta_k) = \frac{1}{2n} \|Y - (X_A \beta_A + X_B \beta_B + X_k \beta_k)\|_2^2 + \lambda \alpha |\beta_k| + \frac{\lambda (1 - \alpha)}{2} \beta_k^2 + h(\beta_A, \beta_B),$$

and therefore the subdifferential of g in β_k becomes, using $X_k^{\top} X_k = ||X_k||_2^2 = n$,

$$\partial g(\beta_k) = -\frac{1}{n} X^{\top} (Y - X_A \beta_A - X_B \beta_B - X_k \beta_k) + \lambda \alpha \hat{\nu} + \lambda (1 - \alpha) \beta_k$$
$$= -\frac{1}{n} X^{\top} (Y - X_A \beta_A - X_B \beta_B) + \lambda \alpha \hat{\nu} + (1 + \lambda (1 - \alpha)) \beta_k,$$

where $\hat{\nu} = \operatorname{sgn}(\beta_k)$ if $\beta_k \neq 0$ and else $\hat{\nu} \in [-1, 1]$. Rewriting gives

$$0 \in \partial g(\beta_k) \iff \beta_k = \frac{\frac{1}{n} X^{\top} (Y - X_A \beta_A - X_B \beta_B) - \lambda \alpha \hat{\nu}}{1 + \lambda (1 - \alpha)}.$$
 (2)

We can distinguish three cases:

- (a) If $\frac{1}{n}X^{\top}(Y X_A\beta_A X_B\beta_B) > \lambda\alpha$, we can set $\hat{\nu} = 1$ in eq. (2) (and indeed β_k will be strictly positive).
- (b) If $\frac{1}{n}X^{\top}(Y X_A\beta_A X_B\beta_B) < -\lambda\alpha$, we can set $\hat{\nu} = -1$ in eq. (2) (and indeed β_k will be strictly negative).
- (c) If $\left|\frac{1}{n}X^{\top}(Y X_A\beta_A X_B\beta_B)\right| \leq \lambda \alpha$, we can choose $\hat{\nu} \in [-1, 1]$ such that the expression in eq. (2) becomes 0, and therefore we can choose $\beta_k = 0$.

It is easily checked that these three cases can be combined into the formula

$$\beta_k = \frac{S_{\lambda\alpha}(\frac{1}{n}X^{\top}(Y - X_A\beta_A - X_B\beta_B))}{1 + \lambda(1 - \alpha)}.$$

Question 8. Assume X is an $n \times d$ matrix with i.i.d. rows with $N(\mu, \Sigma)$ distribution and $\|\Sigma\|_{\text{op}} = \sigma^2$. Prove a deviation bound similar to theorem 28 for the maximum likelihood estimator $\hat{\Sigma} = \frac{1}{n} \sum_{i=1}^{n} (x_i - \bar{X})(x_i - \bar{X})^{\top}$. The bound should hold for $\delta > d$.

Question 9. Let $X \in \mathbb{R}^{n \times p}$ (n > p) be a centred data matrix with (thin) $SVD \ X = UDV^{\top}$. Let the first principal component be $u^{(1)} = D_{11}U_1$, and the first loading vector be $v^{(1)} = V_1$. We may define the kth principal component $u^{(k)}$ and loading vector $v^{(k)}$ for k > 1 inductively as follows:

$$v^{(k)} \coloneqq \mathop{\arg\max}_{\substack{\|v\|_2 = 1, \\ Xv \perp \left\{u^{(1)}, \dots, u^{(k-1)}\right\}}} \|Xv\|_2, \qquad u^{(k)} \coloneqq Xv^{(k)}.$$

Suppose that D_{11}, \ldots, D_{pp} are all distinct. Show that $v^{(k)} = V_k$ and $u^{(k)} = D_{kk}U_k$ (up to an arbitrary sign).

Proof. We can write $X = UDV^{\top} = \sum_{i=1}^{p} D_{ii}U_{i}V_{i}^{\top}$. Now, expand any $v \in S^{p-1}$ in the basis defined by the columns of V, so $v = \sum_{i=1}^{p} \alpha_{p}V_{p}$ (we have $\sum_{i} \alpha_{i}^{2} = 1$). Then we have

$$Xv = \sum_{i=1}^{p} \sum_{j=1}^{p} D_{ii} \alpha_j U_i V_i^{\top} V_j = \sum_{i=1}^{p} \alpha_i D_{ii} U_i, \quad \|Xv\|_2^2 = \sum_{i=1}^{p} \alpha_i^2 D_{ii}^2.$$

Now, it is clear that

$$Xv \perp \left\{ u^{(1)}, \dots, u^{(k-1)} \right\} \iff Xv \perp \left\{ U_1, \dots, U_{k-1} \right\} \iff \alpha_1, \dots, \alpha_{k-1} = 0.$$

Subject to the constraint $\alpha_1, \ldots, \alpha_{k-1} = 0$ and $\sum_i \alpha_i^2 = 1$, it is clear that we can maximise $||Xv||_2^2$ by choosing $\alpha_k = \pm 1$ and $\alpha_{k+1}, \ldots, \alpha_p = 0$, and then we obtain $v^{(k)} = \pm V_k$ and $u^{(k)} = XV_k = \pm D_{kk}U_k$.

Question 10. Suppose we wish to obtain the principal components of the (not necessarily centred) matrix $\Phi \in \mathbb{R}^{n \times d}$. Explain how we can recover the principal components given only $K = \Phi \Phi^{\top}$.

Proof. If Φ were centred, we could simply compute the eigenvectors U_1, \ldots, U_p of K with nonzero eigenvalues $\lambda_1, \ldots, \lambda_p$, and the principal components would be $\sqrt{\lambda_1}U_1, \ldots, \sqrt{\lambda_p}U_p$.