Adaptive Lasso for correlated predictors

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OUTLINE

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1. INTRODUCTION

- Assume a linear model for $\{(\boldsymbol{x}_i.Y_i) : i = 1.\cdots,n\}$:

$$\begin{aligned} Y_i &= \beta_0 + \beta_1 x_{1i} + \cdots + \beta_p x_{pi} + \varepsilon_i \\ &= \boldsymbol{x}_i^T \boldsymbol{\beta} + \varepsilon_i \qquad (i = 1,\cdots,n) \end{aligned}$$

- Assume that the predictors are centred and scaled to have mean 0 and variance 1.
  - We can estimate β_0 by $\bar{Y}$ — least squares estimator.
  - Thus we can assume that $\{Y_i\}$ are centred to have mean 0.
- In many applications, p can be much greater than n.
- In this talk, we will assume implicitly that $p < n$.

Shrinkage estimation

- **Bridge regression:** Minimize

$$\sum_{i=1}^{n}(Y_i - \boldsymbol{x}_i^T\boldsymbol{\beta})^2 + \lambda\sum_{j=1}^{p}|\beta_j|^\gamma$$

  for some $\gamma > 0$.

- Includes the Lasso (Tibshirani, 1996) and ridge regression as special cases with $\gamma = 1$ and 2 respectively.
  - For $\gamma \leq 1$, it's possible to obtain exact 0 parameter estimates.
  - Many other variations of the Lasso: elastic nets (Zou & Hastie, 2005), fused lasso (Tibshirani *et al.*, 2006) among others.
  - The Dantzig selector of Candès & Tao (2007) is similar in spirit to the Lasso.

- **Stagewise fitting:** Given $\widehat{\boldsymbol{\beta}}^{(k)}$, minimize

$$\sum_{i=1}^{n}(Y_i - \boldsymbol{x}_i^T\widehat{\boldsymbol{\beta}}^{(k)} - \boldsymbol{x}_i^T\boldsymbol{\phi})^2$$

  over $\boldsymbol{\phi}$ with all but 1 (or a small number) of its elements equal to 0. Then define

$$\widehat{\boldsymbol{\beta}}^{(k+1)} = \widehat{\boldsymbol{\beta}}^{(k)} + \epsilon\widehat{\boldsymbol{\phi}} \quad (0 < \epsilon \le 1)$$

  and repeat until "convergence".

  – This is a special case of **boosting** (Shapire, 1990).

  – Also related to LARS (Efron *et al.*, 2004), which in turn is related to the Lasso.

2. THE LASSO UNDER COLLINEARITY

- For given λ, the Lasso estimator $\widehat{\boldsymbol{\beta}}(\lambda)$ can be defined in a number of equivalent ways:

  1. $\widehat{\boldsymbol{\beta}}(\lambda)$ minimizes

  $$\sum_{i=1}^{n}(Y_i - \boldsymbol{x}_i^T\boldsymbol{\beta})^2 \quad \text{subject to } \textstyle\sum_{j=1}^{p} |\beta_j| \le t(\lambda);$$

  2. $\widehat{\boldsymbol{\beta}}(\lambda)$ minimizes

  $$\sum_{i=1}^{n}(\boldsymbol{x}_i^T\boldsymbol{\beta})^2 \quad \text{subject to} \quad \left|\sum_{i=1}^{n}(Y_i - \boldsymbol{x}_i^T\boldsymbol{\beta})x_{ij}\right| \le \lambda$$

  for $j = 1, \cdots, p$.

- The advantage of the Lasso is that it produces exact 0 estimates while $\widehat{\boldsymbol{\beta}}(\lambda)$ is a smooth function of λ.
  - This is very useful when $p \gg n$ to produce "sparse" models.
- However, when the predictors $\{\boldsymbol{x}_i\}$ are highly correlated then $\widehat{\boldsymbol{\beta}}(\lambda)$ may contain too many zeroes.
- This is not necessarily undesirable but some important effects may be missed as a result.
  - How does one interpret a "sparse" model under high collinearity?

Question: Why does this happen?

Answer: Redundancy in the constraints

$$\left|\sum_{i=1}^{n}(Y_i - \boldsymbol{x}_i^T\boldsymbol{\beta})x_{ij}\right| \leq \lambda \quad \text{for } j = 1, \cdots, p$$

due to collinearity; that is, we don't have p independent constraints.

- The Dantzig selector minimizes $\sum_j |\beta_j|$ subject to similar constraints on the correlations, and thus will tend to behave similarly.

- For LS estimation ($\lambda = 0$), we have

$$\sum_{i=1}^{n} (Y_i - \boldsymbol{x}_i^T \widehat{\boldsymbol{\beta}}) \boldsymbol{x}_i^T \boldsymbol{a} = 0$$

  for any $\boldsymbol{a}$.

- Similarly, we could try to consider estimates $\widetilde{\boldsymbol{\beta}}$ such that

$$\left| \sum_{i=1}^{n} (Y_i - \boldsymbol{x}_i^T \widetilde{\boldsymbol{\beta}}) \boldsymbol{x}_i^T \boldsymbol{a}_\ell \right| \leq \lambda$$

  for some set of vectors (projections) $\{\boldsymbol{a}_\ell : \ell \in \mathcal{L}\}$.

- If the set $\mathcal{L}$ is finite, we can incorporate predictors $\{\boldsymbol{a}_\ell^T \boldsymbol{x}\}$ into the Lasso.

Example: Principal components regression ($|\mathcal{L}| = p$) where $\boldsymbol{a}_1, \cdots, \boldsymbol{a}_p$ are the eigenvectors of

$$C = \sum_{i=1}^{n} \boldsymbol{x}_i \boldsymbol{x}_i^T.$$

However ...

- Projections obtain via PC are based solely on information in the design.
- Moreover, they need not be particular easy to interpret.
- More generally, there's no problem in taking $|\mathcal{L}| \gg p$.

3. PROJECTION PURSUIT WITH THE LASSO

- For collinear predictors, it's often desirable to consider projections of the original predictors.
- Given predictors $x_1, \cdots, x_p$ and projections $\{\boldsymbol{a}_\ell : \ell \in \mathcal{L}\}$, we want to identify "interesting" (data-driven) projections $\boldsymbol{a}_{\ell_1}, \cdots, \boldsymbol{a}_{\ell_p}$ and define new predictors $\boldsymbol{a}_{\ell_1}^T \boldsymbol{x}, \cdots, \boldsymbol{a}_{\ell_p}^T \boldsymbol{x}$.
- We can take $\mathcal{L}$ to be very large – but the projections we consider should be easily interpretable.
  - Coordinate projections (i.e. original predictors).
  - Sums and differences of two or more predictors.

Question: How do we do this?

Answer: Two possibilities:

- Use the Lasso on the projections.
  - But we need to worry about the choice of λ.
  - The "active" projections will depend on λ.
- Look at the Lasso solution as $\lambda \downarrow 0$.
  - This identifies a set of p projections.
  - These projections can be used in the Lasso.

Question: What happens to the Lasso solution as $\lambda \to 0$?

- Suppose that $\widehat{\boldsymbol{\beta}}(\lambda)$ minimizes

  $$\sum_{i=1}^{n}(Y_i - \boldsymbol{x}_i^T \boldsymbol{\beta})^2 + \lambda \sum_{j=1}^{p} |\beta_j|$$

  and that

  $$C = \sum_{i=1}^{n} \boldsymbol{x}_i \boldsymbol{x}_i^T$$

  is singular.

- Define

  $$\mathcal{D} = \left\{ \boldsymbol{\phi} : \sum_{i=1}^{n}(Y_i - \boldsymbol{x}_i^T \boldsymbol{\phi})^2 = \min_{\beta} \sum_{i=1}^{n}(Y_i - \boldsymbol{x}_i^T \boldsymbol{\beta})^2 \right\}.$$

Proposition: For the Lasso estimate $\boldsymbol{\beta}(\lambda)$, we have

$$\lim_{\lambda \downarrow 0} \widehat{\boldsymbol{\beta}}(\lambda) = \operatorname{argmin} \left\{ \sum_{j=1}^{p} |\phi_j| : \boldsymbol{\phi} \in \mathcal{D} \right\}.$$

"Proof". Assume (for simplicity) that the minimum RSS is 0. Then $\widehat{\boldsymbol{\beta}}(\lambda)$ minimizes

$$Z_\lambda(\boldsymbol{\beta}) = \frac{1}{\lambda} \sum_{i=1}^{n} (Y_i - \boldsymbol{x}_i^T \boldsymbol{\beta})^2 + \sum_{j=1}^{p} |\beta_j|.$$

As $\lambda \downarrow 0$, the first term of Z_λ blows up for $\boldsymbol{\beta} \notin \mathcal{D}$ and is exactly 0 for $\boldsymbol{\beta} \in \mathcal{D}$. The conclusion follows using convexity of Z_λ.

Corollary: The Dantzig selector estimator has the same limit as $\lambda \downarrow 0$.

- In our problem, define $t_{i\ell}$ to be a scaled version of $\boldsymbol{a}_\ell^T \boldsymbol{x}_i$.
- The model now becomes

$$\begin{aligned} Y_i &= \sum_{\ell \in \mathcal{L}} \phi_\ell t_{i\ell} + \varepsilon_i \\ &= \boldsymbol{t}_i^T \boldsymbol{\phi} + \varepsilon_i \quad (i = 1, \cdots, n) \end{aligned}$$

- We estimate $\boldsymbol{\phi}$ by minimizing

$$\sum_{\ell \in \mathcal{L}} |\phi_\ell| \quad \text{subject to} \quad \sum_{i=1}^{n} (Y_i - \boldsymbol{t}_i^T \boldsymbol{\phi}) \boldsymbol{t}_i = \boldsymbol{0}.$$

- This can be solved using linear programming methods.
  – Software for the Lasso tends to be unstable as $\lambda \downarrow 0$.

Asymptotics:

- Assume $p < r = |\mathcal{L}|$ are fixed and $n \to \infty$.
- Define matrices

$$
\begin{aligned}
C &= \lim_{n\to\infty} \frac{1}{n} \sum_{i=1}^{n} \boldsymbol{x}_i \boldsymbol{x}_i^T \\
D &= \lim_{n\to\infty} \frac{1}{n} \sum_{i=1}^{n} \boldsymbol{t}_i \boldsymbol{t}_i^T
\end{aligned}
$$

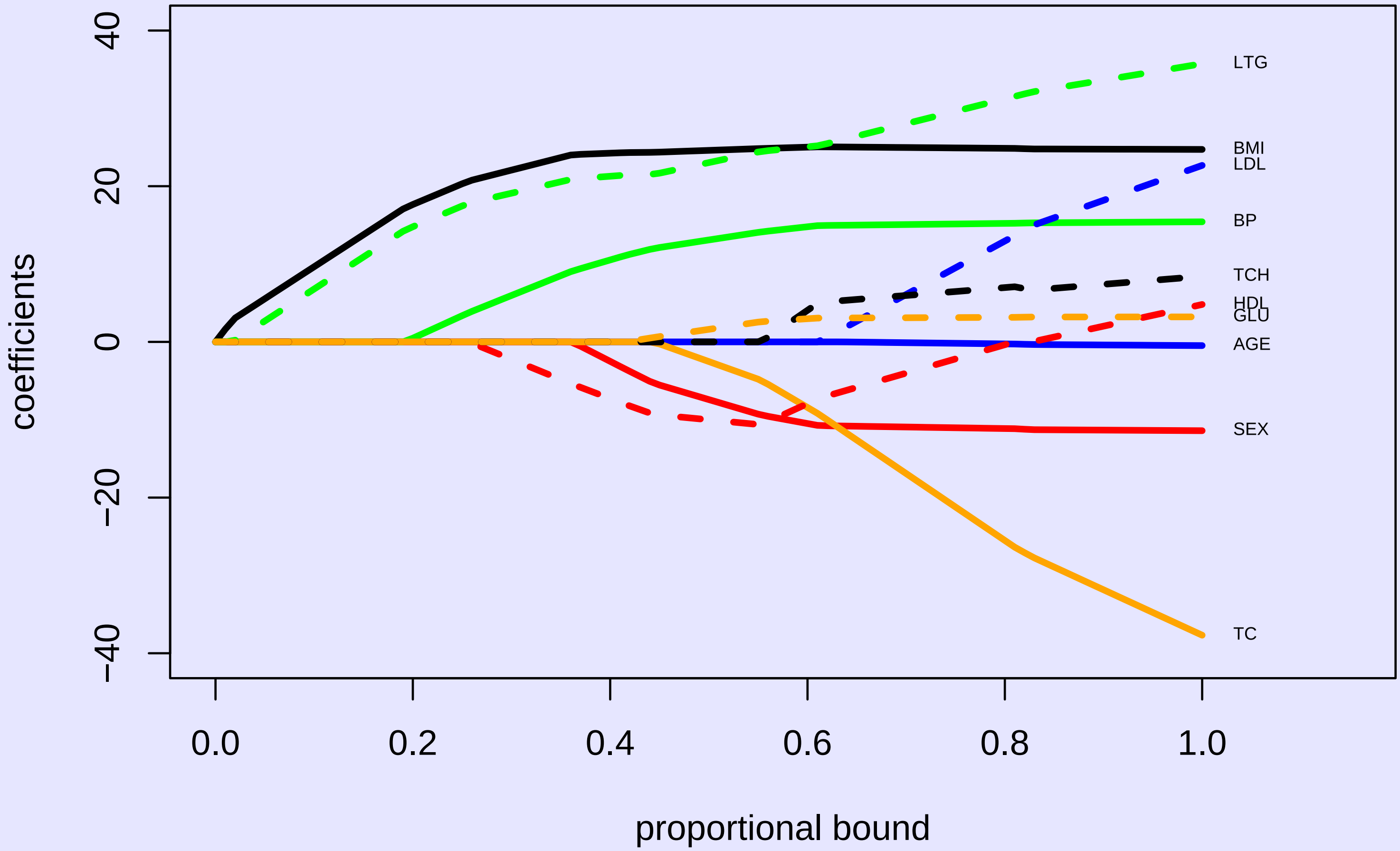
  where C is non-singular and D singular with rank p.

- Then $\widehat{\boldsymbol{\phi}}_n \xrightarrow{p}$ some $\boldsymbol{\phi}_0$.
- We also have $\sqrt{n}(\widehat{\boldsymbol{\phi}}_n - \boldsymbol{\phi}_0) \xrightarrow{d} \boldsymbol{V}$ where the distribution of $\boldsymbol{V}$ is concentrated on the orthogonal complement of the null space of D.

4. EXAMPLE

Diabetes data (Efron *et al.*, 2004)

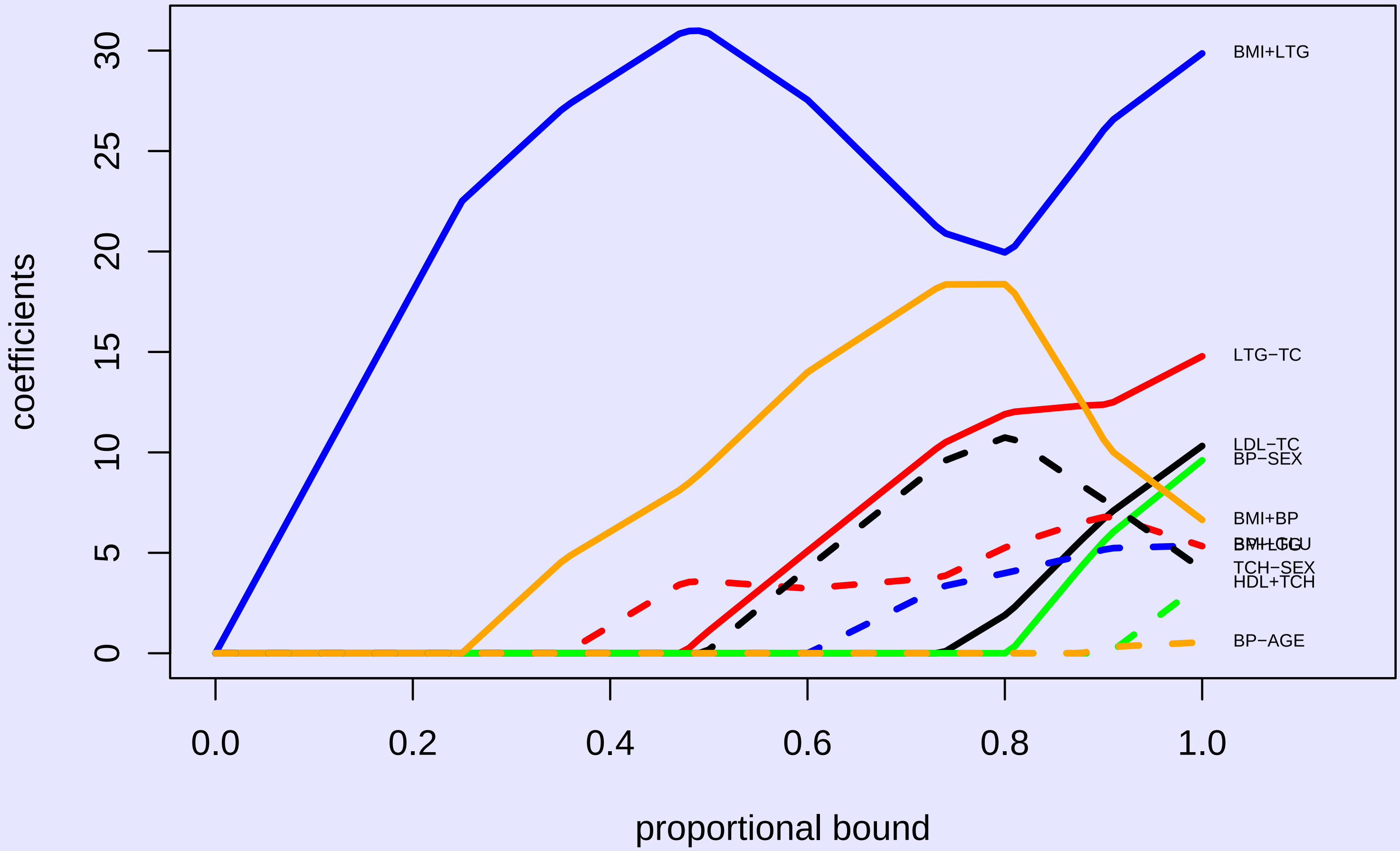
- Response: measure of disease progression.
- Predictors: age, sex, BMI, blood pressure, and 6 blood serum measurements (TC, LDL, HDL, TCH, LTG, GLU).
  - Some predictors are quite highly correlated.
- Analysis indicates that the most important variables are LTG, BMI, BP, TC, and sex.
- Look at coordinate-wise projections as well as pairwise sums and differences (100 projections in total).



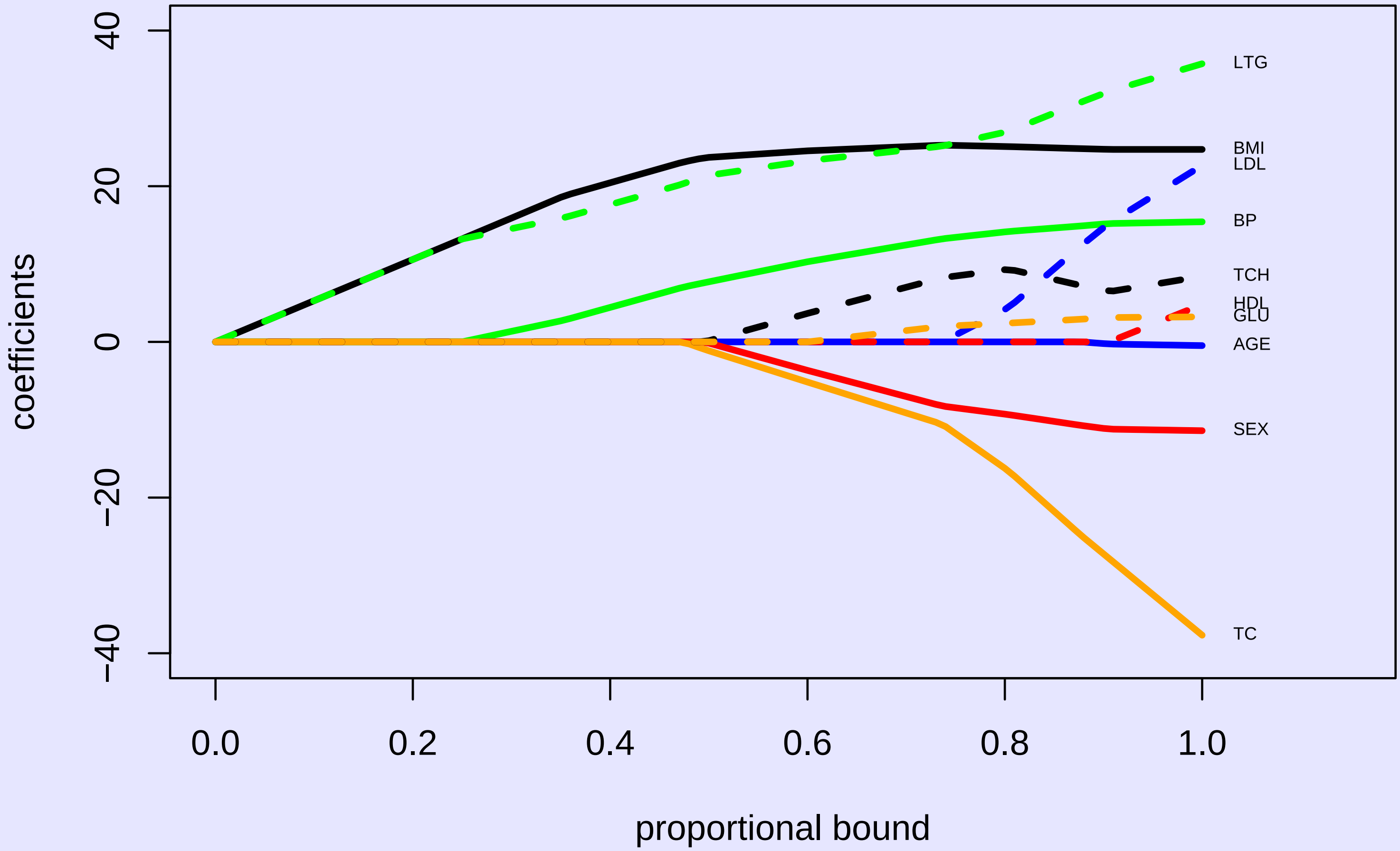
Lasso plot for original predictors.

Results: Estimated projections

Projections	Estimates
BMI + LTG	29.86
LTG − TC	14.79
LDL − TC	10.32
BP − SEX	9.61
BMI + BP	6.64
BMI + GLU	5.36
BP + LTG	5.33
TCH − SEX	4.18
HDL + TCH	3.48
BP − AGE	0.55



Lasso plot for the 10 identified projections.



Lasso trajectories for original predictors using the projections.