Betting on Sparsity with the Lasso. Part II: More on ridge/lasso and beyond linear regression

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Recap on regularised linear regression

Basic lasso theory

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If we mainly want to do prediction, we're mostly interested in estimating β (and the noise term is not too important to estimate).

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Since Legendre anbd Gauss ($\approx$ 1805), the traditional approach to linear regression is through ordinary least squares

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In this course, we're concerned by cases where the number of features p is very large. Which leads $\mathbf{X}^T\mathbf{X}$ to be ill-conditioned or non-invertible. This renders OLS impractical.

OLS fails in high dimensions

We have $\text{rank}(\mathbf{X}^T\mathbf{X}) \leq n$, so if $p > n$, the matrix $\mathbf{X}^T\mathbf{X}$ is not invertible!
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- adding an ℓ_0 penalty to the sum of squared errors ("lasso", "basis pursuit").

Exercise: What are the advantages/drawbacks of the three methods?

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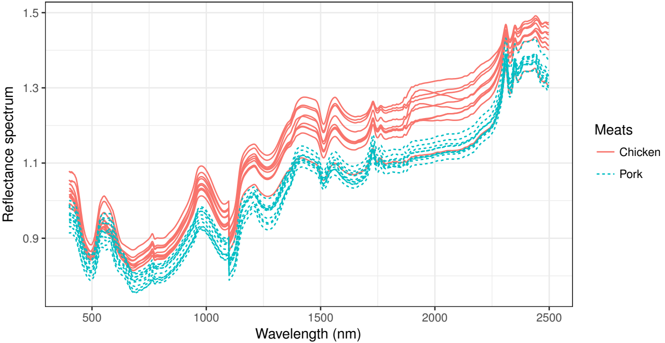
For example, when dealing with spectra, not all wavelengths are useful in general.



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$$||\boldsymbol{\beta}||_0 = \#\{\beta_j \mid \beta_j \neq 0\} = \text{number of nonzero coefficients of } \boldsymbol{\beta}.$$

We say that $\boldsymbol{\beta} \in \mathbb{R}^p$ is k-sparse when it contains only k coefficients different from zero. In other words, $\boldsymbol{\beta} \in \mathbb{R}^p$ is k-sparse when $||\boldsymbol{\beta}||_0 = k$. Of course, we need to have $k \in \{0, ..., p\}$. The sparsity pattern of $\boldsymbol{\beta}$ is the subset of $\{1, ..., p\}$ corresponding to nonzero coefficients.

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There are 2^p possible sparsity patterns. This means that, for 20 features, we'll already have more than one million patterns... Trying all of them will be impossible in "large p" cases!

Sparsity through ℓ_0 penalisation

Since we have a measure of non-sparsity (the ℓ_0 pseudonorm), we could just use that to obtain sparse solutions!

$$\hat{\boldsymbol{\beta}}_{\ell_0,\lambda} \in \mathrm{argmin}_{\boldsymbol{\beta}\in\mathbb{R}^p} ||\mathbf{Y} - \mathbf{X}\beta||_2^2 + \lambda||\boldsymbol{\beta}||_0.$$

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If we use a large enough λ, this will give us sparse solutions. However, the loss function is non-differentiable, if we wanted to solve the problem exactly, we would basically need to try all possible 2^p sparsity patterns and compute OLS on them. This is impossible when p becomes bigger than around 50...

Since we can't do ℓ_0 regularisation, what can we do?

Another way of seeing the ℓ_0 regularised problem is as an ℓ_0 constrained problem

$$\text{argmin}_{\boldsymbol{\beta}\in\mathbb{R}^p, ||\boldsymbol{\beta}||_{\mathbf{0}}\le k} ||\mathbf{Y} - \mathbf{X}\beta||_2^2.$$

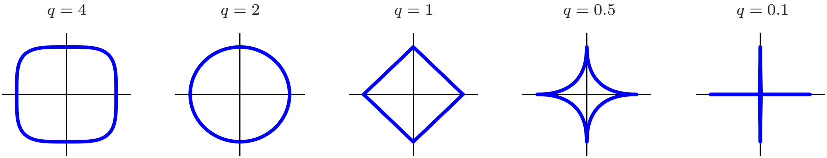
What does the ℓ_0 ball $\{\boldsymbol{\beta} \in \mathbb{R}^p,\ ||\boldsymbol{\beta}||_0 \le k\}$ look like?

The ℓ_q pseudonorms

One neat way of gaining insight on the ℓ_0 ball is to see it as a limit of ℓ_q balls. For all $q > 0$, let us define

$$||\boldsymbol{\beta}||_q = \left(\sum_{j=1}^{p} {\beta_j}^q \right)^{1/q} .$$

Note that this measure is not a proper norm unless $q \geq 1$. The ℓ_0 case corresponds to $q \to 0$. Here are various ℓ_q balls (figure from Hastie, Tibshirani & Wainwright, 2015).



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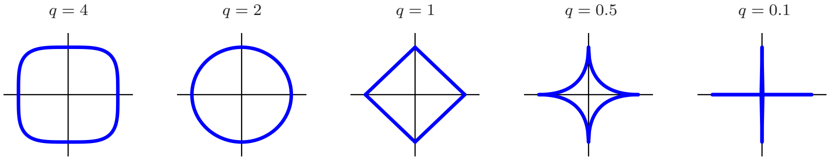
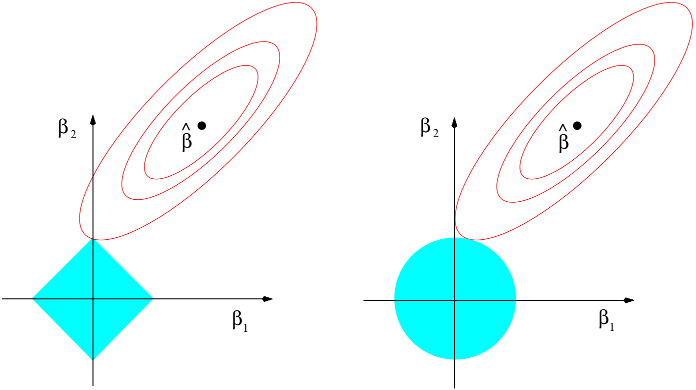


Key idea of the lasso: replace the discrete, non-differentiable, non-convex ℓ_0 ball by a more regular object, like an ℓ_q ball.

From ridge to lasso

We already studied the ℓ_2 case, it's just ridge! But ridge does not give sparsity.... To get sparsity, we need sharp edges on the ball (figure from Hastie, Tibshirani & Wainwright, 2015).



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The only convex ℓ_q ball is the ℓ_1 ball, which justifies the choice of $q = 1$. This leads to the lasso estimate

$$\hat{\boldsymbol{\beta}}_{\text{lasso},\lambda} \in \text{argmin}_{\boldsymbol{\beta} \in \mathbb{R}^p} ||\mathbf{Y} - \mathbf{X}\boldsymbol{\beta}||_2^2 + \lambda ||\boldsymbol{\beta}||_1.$$

Recap on regularised linear regression

Basic lasso theory

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There are many goals one could have in mind. Here are a few examples, on the fundamental side...

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- predictive performance: does the lasso solution give better predictions than other (linear) predictions?

An important question is whether or not one has to make asymptotic assumptions (i.e. n, p, or both go to infinity) in order to have theoretical results. Non-asymptotic results are usually more realistic and useful, but they are harder to derive and sometimes uglier/more cryptic. All these results can be useful to know under which assumptions the lasso "works", and when it is relevant to practically use it.

What does it mean to do lasso theory?

... and on a more practical side...

- optimisation: is the lasso solution unique? what are the guarantees that we will find it in reasonable time?
- degrees of freedom: can we derive AIC/BIC-type criteria for the lasso?
- properties of $\hat{\beta}_{\text{lasso}}$: are we sure that some coefficients will be zero? how many of them?
- can we use theoretical insight to improve the lasso, or design faster algorithms for it?

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One of the first important papers that started it was *Asymptotics for lasso-type estimators*, by Knight & Fu (*Annals of Statistics*, 2000). Then, many prominent researchers form stats/proba/optim communities tackled the issues of the previous slides, even including "famous outsiders" like Terence Tao (Candès & Tao, *Annals of Statistics*, 2007).

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A good overview of these results is provided in Chapter 11 of Hastie, Tibshirani & Wainwright (2015).

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We will state without proof a few interesting (and much harder to prove) results. Some more fundamental, some more practical.

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1. Discuss this assumption. In particular, is it compatible with $p > n$?
2. Write down the OLS estimate $\hat{\boldsymbol{\beta}}_{\text{OLS}}$ in this orthogonal case.
3. Show that the lasso problem is equivalent to a problem of the form

$$\max_{\boldsymbol{\beta} \in \mathbb{R}^p} \sum_{j=1}^{p} f_j(\beta_j),$$

where the f_js are simple (piecewise polynomial) functions. 4. Find the explicit form of $\hat{\boldsymbol{\beta}}_{\text{lasso}}$. *Possible hint: you may start by assuming that all coefficients of* $\hat{\boldsymbol{\beta}}_{\text{OLS}}$ *are positive.*

Tibshirani's simple theorem

Theorem (Tibshirani, 1996). If $\mathbf{X}^T\mathbf{X} = \mathbf{I}_p$, then

$$\hat{\boldsymbol{\beta}}_{\text{lasso},\lambda} = \text{sign}(\hat{\boldsymbol{\beta}}_{\text{OLS}})(|\hat{\boldsymbol{\beta}}_{\text{OLS}}| - \lambda)^+,$$

where $x^+ = \max(x, 0) = \text{ReLU}(x)$.

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The function $S : x \mapsto \text{sign}(x)(|x| - \lambda)^+$ is called the soft-thresholding operator, and is present a lot in sparse contexts.

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A few more complex results

There are a lot of result that show that, under some (unfortunately strong) assumtions on $\mathbf{X}$, we can have consistency of $\hat{\boldsymbol{\beta}}_{\text{lasso},\lambda}$ or of its support when both n and p are large but the model is assumed to be truly sparse. See chapter 11 of of Hastie, Tibshirani & Wainwright (2015) for more on this.

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There are also results that pretty much do not need any assumption. One of these is the one we will see in the next slide, that in particular does not assume that the "true model" is linear.

An "assumption-free" result

We just assume that $\mathbf{x}$ and y are two random variables, and that all features are bounded by some constant C. We do not assume that $x \mapsto \mathbb{E}[y|x]$ is linear.

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Note that computing $R(\boldsymbol{\beta})$ is impossible because we only have a finite data set. Let us consider

$$\boldsymbol{\beta}^* \in \mathrm{argmin}_{||\boldsymbol{\beta}||_1 \leq L} R(\boldsymbol{\beta}).$$

The parameter $\boldsymbol{\beta}^*$ does not correspond to a "true model", but is the best sparse linear predictor that we could have computed with an infinite data set.
Theorem.[2] The lasso does almost as good as $\boldsymbol{\beta}^*$:

$$R(\hat{\boldsymbol{\beta}}_{\mathrm{lasso},L}) \leq R(\boldsymbol{\beta}^*) + \sqrt{\frac{8C^2L^4}{n}\log\left(\frac{2p^2}{\delta}\right)}.$$

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Let's recap: lasso theory

- convex problem, with very fast possible optimisation
- $\hat{\boldsymbol{\beta}}_{\text{lasso},\lambda}$ is sparse (the larger the λ, the sparser)
- $\hat{\boldsymbol{\beta}}_{\text{lasso},\lambda}$ will contain at most $\min(n, p)$ nonzero coefficients