# The lasso

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# Introduction

- In the last topic, we introduced penalized regression and discussed ridge regression, in which the penalty took the form of a sum of squares of the regression coefficients
- In this topic, we will instead penalize the absolute values of the regression coefficients, a seemingly simple change with widespread consequences

# The lasso

- Specifically, consider the objective function

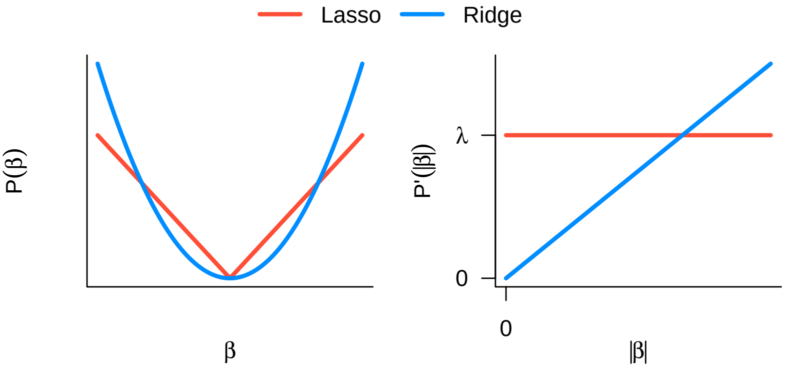
$$Q(\boldsymbol{\beta}|\mathbf{X},\mathbf{y}) = \frac{1}{2n}\|\mathbf{y}-\mathbf{X}\boldsymbol{\beta}\|_2^2 + \lambda\|\boldsymbol{\beta}\|_1,$$

  where $\|\boldsymbol{\beta}\|_1 = \sum_j |\beta_j|$ denotes the $\ell_1$ norm of the regression coefficients
- As before, estimates of $\boldsymbol{\beta}$ are obtained by minimizing the above function for a given value of $\lambda$, yielding $\widehat{\boldsymbol{\beta}}(\lambda)$
- This approach was originally proposed in the regression context by Robert Tibshirani in 1996, who called it the *least absolute shrinkage and selection operator*, or lasso

# Shrinkage, selection, and sparsity

- Its name captures the essence of what the lasso penalty accomplishes
    - *Shrinkage:* Like ridge regression, the lasso penalizes large regression coefficients and shrinks estimates towards zero
    - *Selection:* Unlike ridge regression, the lasso produces *sparse* solutions: some coefficient estimates are exactly zero, effectively removing those predictors from the model
- Sparsity has two very attractive properties
    - *Speed:* Algorithms which take advantage of sparsity can scale up very efficiently, offering considerable computational advantages
    - *Interpretability:* In models with hundreds or thousands of predictors, sparsity offers a helpful simplification of the model by allowing us to focus only on the predictors with nonzero coefficient estimates

# Ridge and lasso penalties



# Semi-differentiable functions

- One obvious challenge that comes with the lasso is that, by introducing absolute values, we are no longer dealing with differentiable functions
- For this reason, we're going to take a moment and extend some basic calculus results to the case of non-differentiable (more specifically, semi-differentiable) functions
- A function $f : \mathbb{R} \to \mathbb{R}$ is said to be *semi-differentiable* at a point $x$ if both $d_- f(x)$ and $d_+ f(x)$ exist as real numbers, where $d_- f(x)$ and $d_+ f(x)$ are the left- and right-derivatives of $f$ at $x$

# Subderivatives and subdifferentials

- Given a semi-differentiable function $f : \mathbb{R} \to \mathbb{R}$, we say that $d$ is a *subderivative* of $f$ at $x$ if $d \in [d_- f(x), d_+ f(x)]$; the set $[d_- f(x), d_+ f(x)]$ is called the *subdifferential* of $f$ at $x$, and is denoted $\partial f(x)$
- The subdifferential is a set-valued function: it may consist of a single value (if $f$ is differentiable), an interval of values, or it may be empty (if $d_- f(x) > d_+ f(x)$)
  - Subderivatives are useful for minimization problems; if we were maximizing a function, we would care about the mirror idea of superdifferentials
  - This is a somewhat looser definition of subdifferential than the one used in the convex optimization literature, but we need it in order to consider non-convex penalties later in the course

# Example: $|x|$

For the most part in this course, you don't really need to know much about subdifferentials and subgradients (the multidimensional version of subdifferentials), but you should be familiar with the subdifferential for $f(x) = |x|$:

$$\partial\,|x| = \begin{cases} -1 & \text{if } x < 0 \\ [-1, 1] & \text{if } x = 0 \\ 1 & \text{if } x > 0 \end{cases}$$

# Optimization

- The essential results of optimization can be extended to semi-differentiable functions
- **Theorem:** If $f$ is a semi-differentiable function and $x_0$ is a local minimum of $f$, then $0 \in \partial f(x_0)$
- As with regular calculus, the converse is not true in general

# Computation rules

- As with regular differentiation, the following basic rules apply
- **Theorem:** Suppose $f$ is semi-differentiable, $a$, $b$ are constants, and $g$ is differentiable. Then
  - $\partial\{af(x)+b\} = a\partial f(x)$
  - $\partial\{f(x)+g(x)\} = \partial f(x) + g'(x)$
- The notions extend to higher-order derivatives as well; a function $f:\mathbb{R}\to\mathbb{R}$ is said to be *second-order semi-differentiable* at a point $x$ if both $d_-^2 f(x)$ and $d_+^2 f(x)$ exist as real numbers
- The second-order subdifferential is denoted $\partial^2 f(x) = [d_-^2 f(x), d_+^2 f(x)]$

# Convexity

- As in the differentiable case, a convex function can be characterized in terms of its subdifferential
- **Theorem:** Suppose $f$ is semi-differentiable on $(a, b)$. Then $f$ is convex on $(a, b)$ if and only if $\partial f$ is increasing on $(a, b)$.
- **Theorem:** Suppose $f$ is second-order semi-differentiable on $(a, b)$. Then $f$ is convex on $(a, b)$ if and only if $\partial^2 f(x) \geq 0 \, \forall x \in (a, b)$.

# Multidimensional results

- The previous results can be extended (although we'll gloss over the details) to multidimensional functions by replacing left- and right-derivatives with directional derivatives
- A function $f : \mathbb{R}^n \to \mathbb{R}$ is said to be *semi-differentiable* if the directional derivative $d_u f(x)$ exists in all directions $u$
- **Theorem:** If $f$ is a semi-differentiable function and $x_0$ is a local minimum of $f$, then $d_u f(x_0) \geq 0 \, \forall u$
- **Theorem:** Suppose $f$ is a semi-differentiable function. Then $f$ is convex over a set $\mathcal{S}$ if and only if $d_u^2 f(x) \geq 0$ for all $x \in \mathcal{S}$ and in all directions $u$

# Score functions and penalized score functions

- In classical statistical theory, the derivative of the log-likelihood function is called the *score function*, and maximum likelihood estimators are found by setting this derivative equal to zero, thus yielding the *likelihood equations* (or *score equations*):

  $$0 = \frac{\partial}{\partial\theta} L(\theta),$$

  where $L$ denotes the log-likelihood.
- Extending this idea to penalized likelihoods involves taking the derivatives of objective functions of the form $Q(\theta) = L(\theta) + P(\theta)$, yielding the *penalized score function*

# Penalized likelihood equations

- For ridge regression, the penalized likelihood is everywhere differentiable, and the extension to penalized score equations is straightforward
- For the lasso, and for the other penalties we will consider in this class, the penalized likelihood is not differentiable – specifically, not differentiable at zero – and subdifferentials are needed to characterize them
- Letting $\partial Q(\theta)$ denote the subdifferential of $Q$, the *penalized likelihood equations* (or *penalized score equations*) are:

$$0 \in \partial Q(\theta).$$

# KKT conditions

- In the optimization literature, the resulting equations are known as the Karush-Kuhn-Tucker (KKT) conditions
- For convex optimization problems such as the lasso, the KKT conditions are both necessary and sufficient to characterize the solution
- A rigorous proof of this claim in multiple dimensions would involve some of the details we glossed over, but applying the idea is straightforward: to solve for $\widehat{\boldsymbol{\beta}}$, we simply replace the derivative with the subderivative and the likelihood with the penalized likelihood

# KKT conditions for the lasso

- **Result:** $\widehat{\boldsymbol{\beta}}$ minimizes the lasso objective function if and only if it satisfies the KKT conditions

$$\begin{aligned} &\frac{1}{n}\mathbf{x}_j^T(\mathbf{y} - \mathbf{X}\widehat{\boldsymbol{\beta}}) = \lambda \text{sign}(\widehat{\beta}_j) && \widehat{\beta}_j \neq 0 \\ &\frac{1}{n}|\mathbf{x}_j^T(\mathbf{y} - \mathbf{X}\widehat{\boldsymbol{\beta}})| \leq \lambda && \widehat{\beta}_j = 0 \end{aligned}$$

- In other words, the correlation between a predictor and the residuals, $\mathbf{x}_j^T(\mathbf{y} - \mathbf{X}\widehat{\boldsymbol{\beta}})/n$, must exceed a certain minimum threshold $\lambda$ before it is included in the model
- When this correlation is below $\lambda$, $\widehat{\beta}_j = 0$

# Remarks

- If we set

$$\lambda = \lambda_{\max} \equiv \max_{1 \le j \le p} |\mathbf{x}_j^T \mathbf{y}|/n,$$

  then $\widehat{\boldsymbol{\beta}} = 0$ satisfies the KKT conditions
- That is, for any $\lambda \ge \lambda_{\max}$, we have $\widehat{\boldsymbol{\beta}}(\lambda) = 0$
- On the other hand, if we set $\lambda = 0$, the KKT conditions are simply the normal equations for OLS, $\mathbf{X}^T(\mathbf{y} - \mathbf{X}\widehat{\boldsymbol{\beta}}) = 0$
- Thus, the coefficient path for the lasso starts at $\lambda_{\max}$ and continues until $\lambda = 0$ if $\mathbf{X}$ is full rank; otherwise the solution will fail to be unique for $\lambda$ values below some point $\lambda_{\min}$

# Lasso and uniqueness

- To elaborate, note that the lasso objective function is convex, but not strictly convex if $\mathbf{X}^T\mathbf{X}$ is not full rank
- For example, suppose $n = 2$ and $p = 2$, with $(y_1, x_{11}, x_{12}) = (1, 1, 1)$ and and $(y_2, x_{21}, x_{22}) = (-1, -1, -1)$
- Then the solutions are

$$
\begin{aligned}
(\widehat{\beta}_1, \widehat{\beta}_2) =& (0, 0) \text{ if } \lambda \geq 1, \\
(\widehat{\beta}_1, \widehat{\beta}_2) \in& \{(\beta_1, \beta_2) : \beta_1 + \beta_2 = 1 - \lambda, \beta_1 \geq 0, \beta_2 \geq 0\} \\
& \qquad \text{if } 0 \leq \lambda < 1
\end{aligned}
$$

# Special case: Orthonormal design

- As with ridge regression, it is instructive to consider the special case where the design matrix $\mathbf{X}$ is orthonormal: $n^{-1}\mathbf{X}^T\mathbf{X} = \mathbf{I}$
- **Result:** In the orthonormal case, the lasso estimate is

$$\widehat{\beta}_j(\lambda) = \begin{cases} z_j - \lambda, & \text{if } z_j > \lambda, \\ 0, & \text{if } |z_j| \le \lambda, \\ z_j + \lambda, & \text{if } z_j < -\lambda \end{cases},$$

where $z_j = \mathbf{x}_j^T\mathbf{y}/n$ is the OLS solution

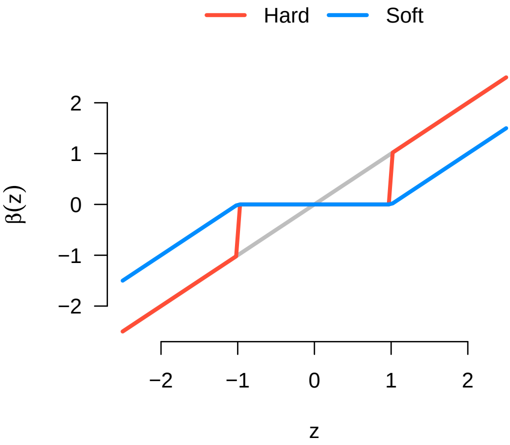
# Soft thresholding

- The result on the previous slide can be written more compactly as

$$\widehat{\beta}_j(\lambda) = S(z_j|\lambda),$$

  where the function $S(\cdot|\lambda)$ is known as the *soft thresholding operator*
- This was originally proposed by Donoho and Johnstone in 1994 for soft thresholding of wavelets coefficients in the context of nonparametric regression
- By comparison, the "hard" thresholding operator is $H(z, \lambda) = zI\{|z| > \lambda\}$, where $I(S)$ is the indicator function for set $S$

# Soft and hard thresholding operators



# Probability that $\widehat{\beta}_j = 0$

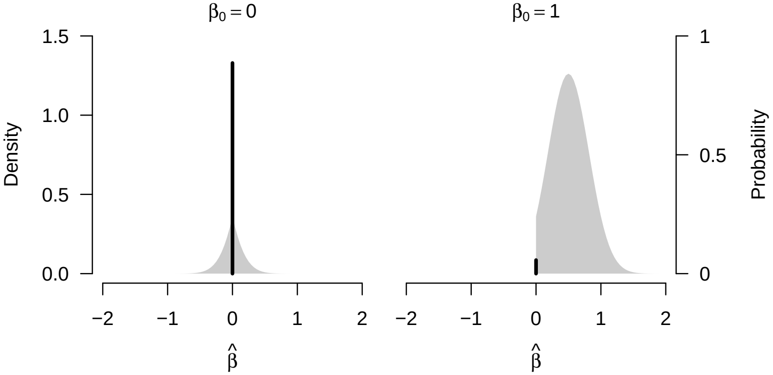
- With soft thresholding, it is clear that the lasso has a positive probability of yielding an estimate of exactly 0 – in other words, of producing a sparse solution
- Specifically, the probability of dropping $\mathbf{x}_j$ from the model is $\mathbb{P}(|z_j| \leq \lambda)$
- Under the assumption that $\epsilon_i \overset{\perp\!\!\!\perp}{\sim} \mathrm{N}(0, \sigma^2)$, we have $z_j \sim \mathrm{N}(\beta, \sigma^2/n)$ and

$$\mathbb{P}(\widehat{\beta}_j(\lambda) = 0) = \Phi\left(\frac{\lambda - \beta}{\sigma/\sqrt{n}}\right) - \Phi\left(\frac{-\lambda - \beta}{\sigma/\sqrt{n}}\right),$$

where $\Phi$ is the Gaussian CDF

# Sampling distribution

For $\sigma = 1$, $n = 10$, and $\lambda = 1/2$:



# Remarks

- This sampling distribution is very different from that of a classical MLE:
  - The distribution is mixed: a portion is continuously distributed, but there is also a point mass at zero
  - The continuous portion is not normally distributed
  - The distribution is asymmetric (unless $\beta = 0$)
  - The distribution is not centered at the true value of $\beta$
- These facts create a number of challenges for carrying out inference using the lasso; we will be putting this issue aside for now, but will return to it later in the course