Sparse Modeling: Best Subset and the Lasso

Statistical Learning

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References

– Tibshirani, Wasserman (2017). Sparsity, the Lasso, and Friends. Lecture notes on Statistical Machine Learning

Three norms: ℓ_0, ℓ_1 and ℓ_2

- Let's consider three canonical choices: the ℓ_0, ℓ_1 and ℓ_2 norms:

$$\|\beta\|_0 = \sum_{j=1}^{p} \mathbb{1}\{\beta_j \neq 0\}, \quad \|\beta\|_1 = \sum_{j=1}^{p} |\beta_j|, \quad \|\beta\|_2 = \sqrt{\sum_{j=1}^{p} \beta_j^2}$$

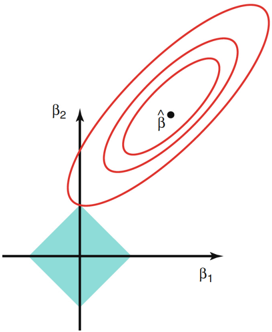
- ℓ_0 is not a proper norm: it does not satisfy positive homogeneity, i.e. $\|a\beta\|_0 \neq |a|\|\beta\|_0$ for $a \in \mathbb{R}$

Constrained form

$$\min_{\beta \in \mathbb{R}^p} \|y - X\beta\|_2^2 \text{ subject to } \|\beta\|_0 \leq c \qquad \text{Best Subset Selection}$$

$$\min_{\beta \in \mathbb{R}^p} \|y - X\beta\|_2^2 \text{ subject to } \|\beta\|_1 \leq c \qquad \text{Lasso Regression}$$

$$\min_{\beta \in \mathbb{R}^p} \|y - X\beta\|_2^2 \text{ subject to } \|\beta\|_2^2 \leq c \qquad \text{Ridge Regression}$$



The “classic” illustration comparing lasso and ridge constraints.
From Chapter 3 of ESL

Sparsity

- *Signal sparsity* is the assumption that only a small number of predictors have an effect, i.e. have $\beta_j \neq 0$
- In this case we would like our estimator $\hat{\beta}$ to be sparse, meaning that $\hat{\beta}_j = 0$ for many components $j \in \{1, \ldots, p\}$
- Sparse estimators are desirable because perform variable selection and improve interpretability of the result
- The best subset selection and the lasso estimators are sparse, the ridge estimator is not sparse

Penalized form

$$\min_{\beta \in \mathbb{R}^p} \frac{1}{2}\|y - X\beta\|_2^2 + \lambda\|\beta\|_0 \qquad \text{Best Subset Selection}$$

$$\min_{\beta \in \mathbb{R}^p} \frac{1}{2}\|y - X\beta\|_2^2 + \lambda\|\beta\|_1 \qquad \text{Lasso Regression}$$

$$\min_{\beta \in \mathbb{R}^p} \frac{1}{2}\|y - X\beta\|_2^2 + \lambda\|\beta\|_2^2 \qquad \text{Ridge Regression}$$

- Suppose that $y \sim N(\mu, 1)$
- ℓ_0 penalty

$$\min_{\mu} \frac{1}{2}(y-\mu)^2 + \lambda \mathbb{1}\{\mu \neq 0\}, \qquad \hat{\mu} = H_{\sqrt{2\lambda}}(y)$$

  where $H_a(y) = y\mathbb{1}\{|y| > a\}$ is the hard-thresholding operator
- ℓ_1 penalty

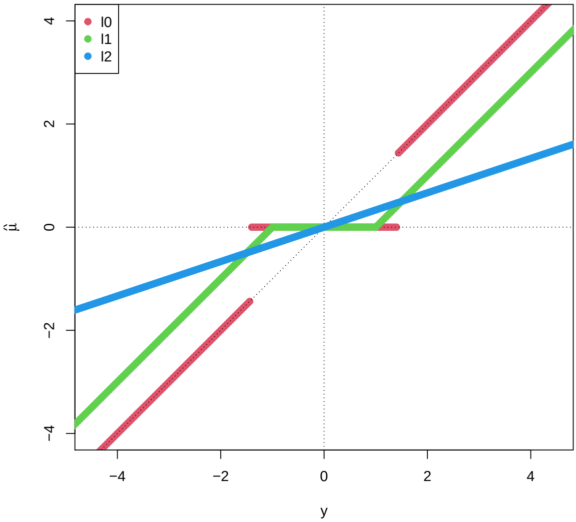
$$\min_{\mu} \frac{1}{2}(y-\mu)^2 + \lambda|\mu|, \qquad \hat{\mu} = S_\lambda(y)$$

  where

$$S_a(y) = \begin{cases} y-a & \text{if } y > a \\ 0 & \text{if } -a \leq y \leq a \\ y+a & \text{if } y > a \end{cases}$$

  is the soft-thresholding operator
- ℓ_2 penalty

$$\min_{\mu} \frac{1}{2}(y-\mu)^2 + \lambda\mu^2, \qquad \hat{\mu} = \big(\frac{1}{1+2\lambda}\big)y$$



$$\lambda = 1$$

Hard and soft thresholding

- ℓ_0 penalty creates a zone of sparsity but it is discontinuous (hard thresholding)
- ℓ_1 penalty creates a zone of sparsity but it is continuous (soft thresholding)
- ℓ_2 penalty creates a nice smooth estimator but it is never sparse

Orthogonal case

- Suppose $X^t X = I_p$
- OLS estimator

$$\hat{\beta}_j = X^t y$$

- BSS estimator

$$\hat{\beta}_j = H_{\sqrt{2\lambda}}(X^t y)$$

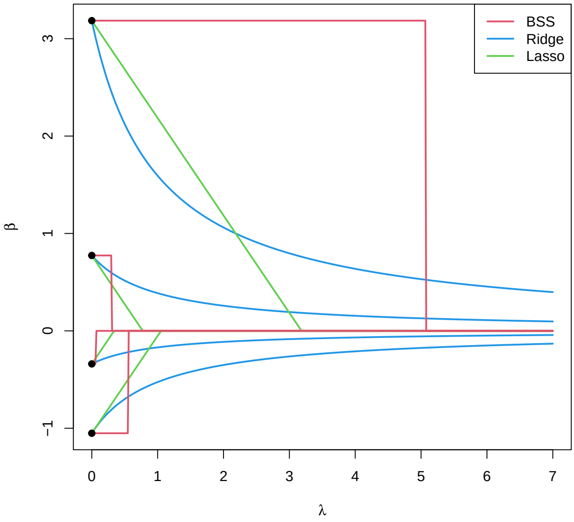
- Lasso estimator

$$\hat{\beta} = S_\lambda(X^t y)$$

- Ridge estimator

$$\hat{\beta} = (\frac{1}{1 + 2\lambda})X^t y$$

where $H_a(\cdot)$, $S_a(\cdot)$ are the componentwise hard- and soft-thresholding operators



Solution paths of ℓ_0, ℓ_1 and ℓ_2 penalties as a function of λ

Convexity

- Consider using the norm $\|\beta\|_q = (\sum_{j=1}^q |\beta_j|^q)^{1/q}$ as a penalty. Sparsity requires $q \leq 1$ and convexity requires $q \geq 1$. The only norm that gives sparsity and convexity is $q = 1$
- The lasso and ridge regression are *convex optimization problems*, best subset selection is not
- The ridge regression optimization problem is always *strictly convex* for $\lambda > 0$
- The best subset selection optimization problem is N-P-complete because of its combinatorial complexity (there are 2^p subsets), the worst kind of non convex problem

Best Subset Selection

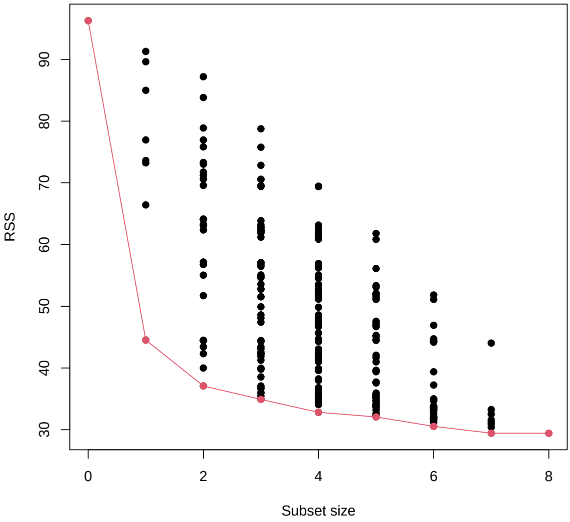
BSS algorithm

A natural approach is to consider all possible regression models each involving regressing the response on a different set of predictors

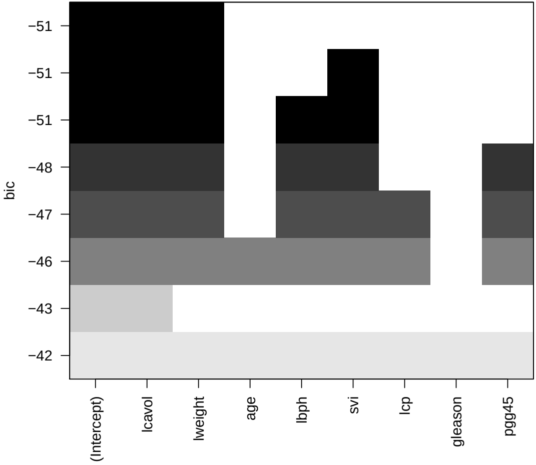
- Set B_0 as the null model (intercept only)
- For $k = 1, \ldots, p$
  1. Fit all $\binom{p}{k}$ models that contain exactly k predictors
  2. Pick the best among these $\binom{p}{k}$ models, and call it B_k, where best is defined having the smallest residual sum of squares
- Select a single best model from among $B_0, B_1, \ldots, B_p$ (e.g. using Cp, BIC, Cross-Validation, validation set, etc.)

`prostate`

	lcavol	lweight	age	lbph	svi	lcp	gleason	pgg45	RSS
B_1	*								44.53
B_2	*	*							37.09
B_3	*	*			*				34.91
B_4	*	*		*	*				32.81
B_5	*	*		*	*			*	32.07
B_6	*	*		*	*	*		*	30.54
B_7	*	*	*	*	*	*		*	29.44
B_8	*	*	*	*	*	*	*	*	29.43



All possible subset models for the prostate cancer example



BIC Best Subset = B_2

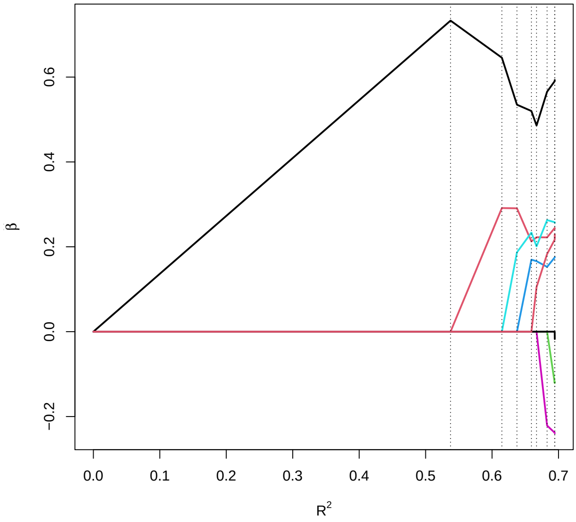
Computational bottleneck

- Furnival and Wilson (1974) and Hofmann et al. (2006) solve with $p \approx 30$ by using branch and bound algorithms. Implemented in the R packages `leaps` and `lmSubsets`
- Bertsimas et al. (2016) solve with $p \approx 100$ by using a mixed integer quadratic program along with the gurobi solver. Implemented in the R package `bestsubset`

Forward Stepwise Selection

Greedy forward algorithm, sub-optimal but feasible alternative to BSS and applicable when $p > n$

- Set S_0 as the null model (intercept only)
- For $k = 0, \dots, \min(n-1, p-1)$:
    1. Consider all $p - k$ models that augment the predictors in S_k with one additional predictor
    2. Choose the best among these $p - k$ models and call it S_{k+1}, where best is defined having the smallest RSS
- Select a single best model from among $S_0, S_1, S_2, \dots$ (e.g. using Cp, BIC, Cross-Validation, validation set, etc.)



Forward Stepwise solution path as a function of training R^2

The Lasso

- The name "lasso" was also introduced as an acronym for *Least Absolute Selection and Shrinkage Operator* (Tibshirani, 1996)
- The lasso finds the solution $(\hat{\alpha}, \hat{\beta})$ to the optimization problem

$$\min_{\beta \in \mathbb{R}^p} \frac{1}{2n} \|y - 1\alpha - X\beta\|_2^2 + \lambda \|\beta\|_1$$

- Typically, we first standardize the predictors X so that each column is centered $((1/n)\sum_{i=1}^{n} x_{ij} = 0)$ and has unit variance $((1/n)\sum_{i=1}^{n} x_{ij}^2 = 0)$
- Without standardization, the lasso solutions would depend on the units (e.g., feet versus meters) used to measure the predictors. On the other hand, we typically would not standardize if the features were measured in the same units
- For convenience, we also assume that the outcome values y_i have been centered $((1/n)\sum_{i=1}^{n} y_i = 0)$. Centering is convenient, since we can omit the intercept term α in the lasso optimization, and given the solution $\hat{\beta}$

$$\hat{\alpha} = \bar{y} - \sum_{j=1}^{p} \bar{x}_j \hat{\beta}_j$$

- Lagrange form

$$\frac{1}{2n} \min_{\beta \in \mathbb{R}^p} \|y - X\beta\|_2^2 + \lambda \|\beta\|_1$$

- Intercept term omitted (center / scale y and the columns of X)
- The solution satisfies the subgradient / Karush-Kuhn-Tuker conditions

$$\frac{1}{n} X^t (y - X\hat{\beta}) = \lambda s$$

where $s \in \partial \|\beta\|_1$, a subgradient of the ℓ_1 norm evaluated at $\hat{\beta}$

- The solution satisfies

$$-\frac{1}{n}\langle X_j, y - X\hat{\beta}\rangle + \lambda s_j = 0 \quad j = 1, \ldots, p$$

where

$$s_j \in \begin{cases} 1 & \text{if } \hat{\beta}_j > 0 \\ [\text{-1,1}\ ] & \text{if } \hat{\beta}_j = 0 \\ -1 & \text{if } \hat{\beta}_j < 0 \end{cases}$$

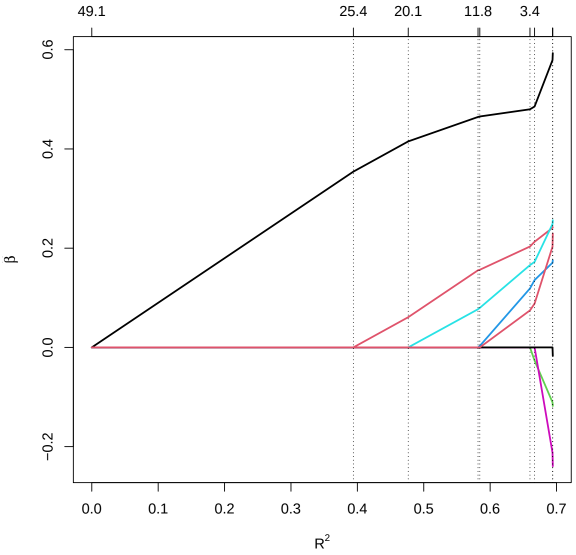
- Each of the variables in the model (with nonzero coefficient) has the same covariance with the residuals (in absolute value), i.e.

$$\frac{1}{n}|\langle X_j, y - X\hat{\beta}\rangle| = \lambda$$

- For all variables with zero coefficient

$$\frac{1}{n}|\langle X_j, y - X\hat{\beta}\rangle| \leq \lambda$$

- The coefficient profiles for the lasso are continuous and piecewise linear over the range of λ, with knots occurring whenever the *active set* changes, or the sign of the coefficients changes



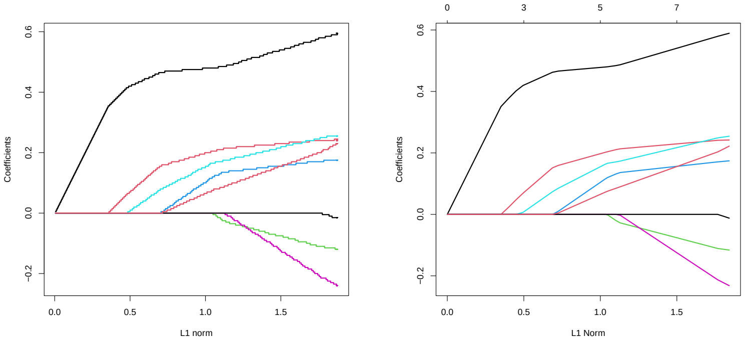
Lasso solution path as a function of training R^2

Boosting with componentwise linear least squares

- Response and predictors are standardized to have mean zero and unit norm
- Initialize $\hat{\beta}^{(0)} = 0$
- For $b = 1, \ldots, B$
  - compute the residuals $r = y - X\hat{\beta}^{(b-1)}$
  - find the predictor X_j most correlated with the residuals r
  - update $\hat{\beta}^{(b-1)}$ to $\hat{\beta}^{(b)}$ with

$$\hat{\beta}_j^{(b)} = \hat{\beta}_j^{(b-1)} + \epsilon \cdot s_j$$

    where s_j is the sign of the correlation
- This is known as *forward stagewise regression* and converges to the least squares solution when $n > p$
- Forward stagewise regression with infinitesimally small step-sizes, i.e. $\epsilon \to 0$, produces a set of solutions which is approximately equivalent to the set of Lasso solutions



Left: forward stagewise regression with $\epsilon = 0.005$; Right: lasso

Degrees of freedom

- Let $A(\lambda) = \{j \in \{1, \ldots, p\} : \beta_j(\lambda) \neq 0\}$ denotes the active set
- The degrees of freedom of the Lasso are the

$$\mathrm{df}(\lambda) = |A(\lambda)|$$

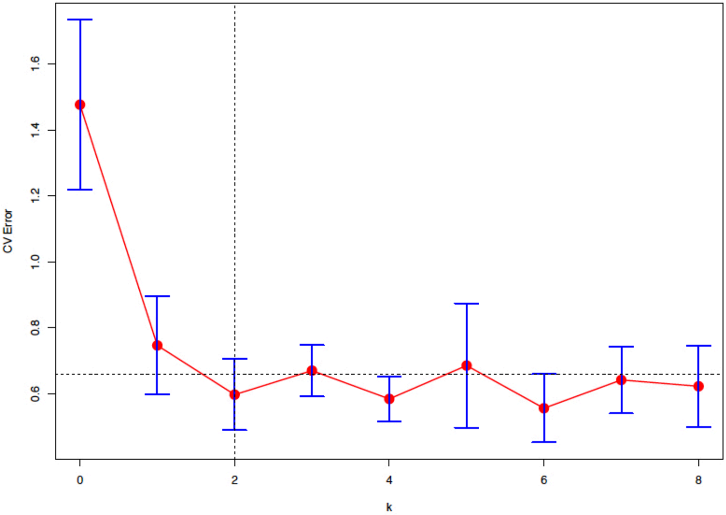
  i.e. the size of the active set

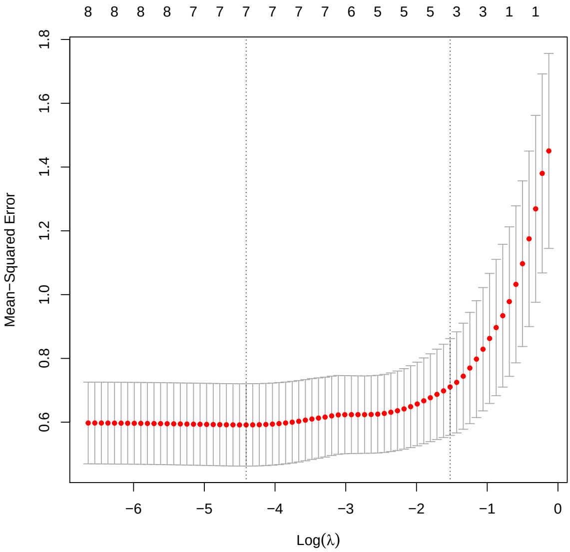
Cross-validation

- `lambda.min`: λ that minimize the cross-validation error
- `lambda.1se`: largest value of lambda such that error is within 1 standard error of the minimum (*one standard error rule*). To compute cross-validation ”standard errors”

$$\mathrm{se} = \frac{1}{\sqrt{K}}\mathrm{sd}(\mathrm{Err}^{-1}, \ldots, \mathrm{Err}^{-K})$$

where Err^{-k} denotes the error incurred in predicting the observations in the k hold-out fold, $k = 1, \ldots, K$.


CV Error
1.6
1.4
1.2
1.0
0.8
0.6
0
2
4
6
8
k



$$\lambda_{\min} = 0.012 \text{ (7 nonzero)}, \lambda_{1se} = 0.21 \text{ (3 nonzero)}$$

Bayesian interpretation

- A Bayesian viewpoint assumes that β has a double-exponential (Laplace) prior distribution with mean zero and scale parameter a function of λ
$$(1/2\tau)\exp(-\|\beta\|_1/\tau)$$
with $\tau = 1/\lambda$
- It follows that the posterior mode for β is the lasso solution
- However, the lasso solution is not the posterior mean and, in fact, the posterior mean does not yield a sparse coefficient vector

Extensions of the lasso

Group Lasso

- Suppose we have a partition $G_1, \ldots, G_q$ of $\{1, \ldots, p\}$
- The group Lasso penalty (Yuan and Lin, 2006) is given by

$$\lambda \sum_{k=1}^{q} m_k \|\beta_{G_k}\|_2$$

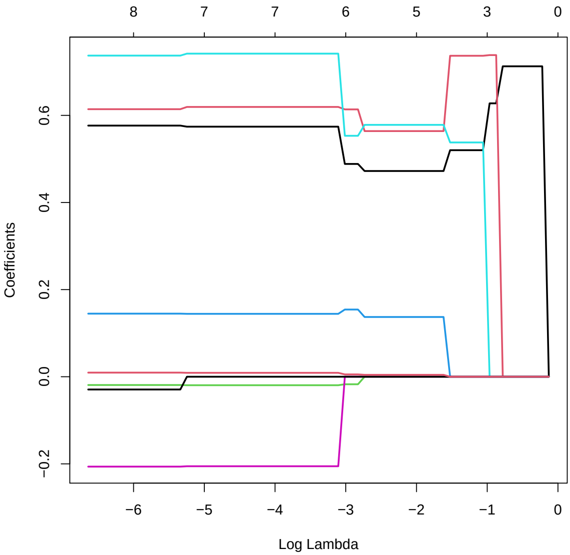
  The multipliers $m_k > 0$ serve to balance cases where the groups are of very different sizes; typically we choose $m_k = \sqrt{|G_k|}$
- This penalty encourages either an entire group G to have $\hat{\beta}_G = 0$ or $\hat{\beta}_j \neq 0$ for all $j \in G$
- Such a property is useful when groups occur through coding for categorical predictors or when expanding predictors using basis functions.

Relaxed Lasso

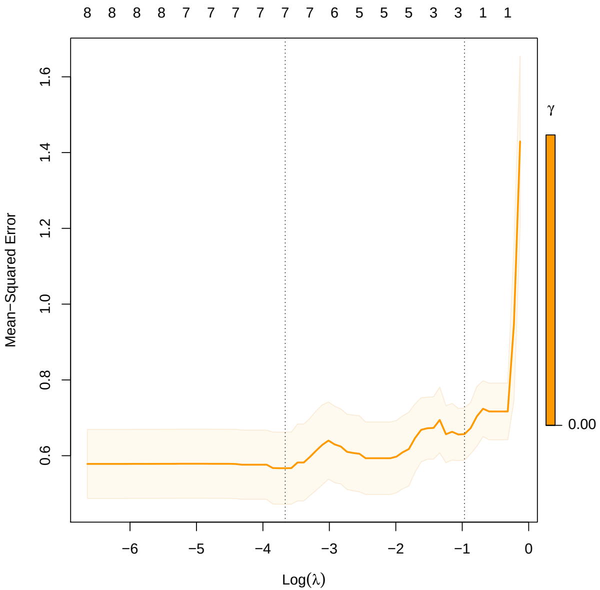
- Originally proposed by Meinshausen (2006). We present a simplified version.
- Suppose $\hat{\beta}_\lambda$ is the lasso solution at λ and let $\hat{A}$ be the active set of indices with nonzero coefficients in $\hat{\beta}_\lambda$
- Let $\hat{\beta}^{\text{LS}}$ be the coeffcients in the least squares fit, using only the variables in $\hat{A}$. Let $\hat{\beta}^{\text{LS}}_\lambda$ be the full-sized version of this coeffcient vector, padded with zeros. $\hat{\beta}^{\text{LS}}_\lambda$ debiases the lasso, while maintaining its sparsity.
- Define the Relaxed Lasso

$$\hat{\beta}^{\text{RELAX}}_\lambda = \gamma\hat{\beta}_\lambda + (1-\gamma)\hat{\beta}^{\text{LS}}_\lambda$$

with $\gamma \in [0, 1]$ is an additional tuning parameter which can be selected by cross-validation



$$\gamma = 0$$



8 8 8 8 7 7 7 7 7 7 6 5 5 5 3 3 1 1
Mean−Squared Error
0.6
0.8
1.0
1.2
1.4
1.6
−6 −5 −4 −3 −2 −1 0
Log(λ)
γ
0.00

$$\gamma = 0$$

Elastic Net

- Define the objective function f for some $\lambda > 0$ and $\alpha \in [0, 1]$ as

$$f(\beta; \lambda, \alpha) = \frac{1}{2n} \|y - X\beta\|_2^2 + \lambda \left((1 - \alpha) \frac{1}{2} \|\beta\|_2^2 + \alpha \|\beta\|_1 \right)$$

  and the corresponding *elastic net* estimator as

$$\hat{\beta}_{\lambda,\alpha} = \arg\min_{\beta} f(\beta; \lambda, \alpha)$$

- Setting α to 1 yields the Lasso regression and setting it to 0 the ridge regression.
- Adding a small ℓ_2-penalty preserves the variable selection and convexity properties of the ℓ_1-penaltized regression, while reducing the variance of the model when X contains sets of highly correlated variables.