Lecture 7

Linear Model Selection and Regularization

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Lecture Outline

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Introduction

- Despite that linear models are often questioned if they can properly characterize the systematic behavior of the variable of interest, they remain a popular choice in applications because they are easy to interpret and capable of reasonable predictions.
- On the other hand, finding a proper nonlinear model is always a challenging task; this difficulty becomes more severe when there are many potential regressors. Moreover, a specific nonlinear model may perform well for one data set, but its performance may not generalize to other data sets (or a validation set).
- If we want to confine ourselves with linear models with a large number of regressors, it is important to determine a subset of most relevant regressors using some model selection criteria or regularization methods.

Model Selection Criteria

Given the model with p potential regressors, let $\hat{u}_{p,i}$ denote the i th OLS residual and $\tilde{\sigma}_p^2 = \sum_{i=1}^n \hat{u}_{p,i}^2/n$. Then, for the model with k out of these p regressors, the C_p measure defined in p. 233 of JWHT (2021) is:

$$C_p = \frac{1}{n}\left(\mathsf{RSS}_k + 2k\tilde{\sigma}_p^2\right),$$

where $\mathsf{RSS}_k = \sum_{i=1}^n \hat{u}_{k,i}^2$, with $\hat{u}_{k,i}$ the i th OLS residual from the model with k regressors, and $\tilde{\sigma}_k^2 = \mathsf{RSS}_k/n$. Note that C_p can be written as

$$C_p = \tilde{\sigma}_p^2\left(\frac{\tilde{\sigma}_k^2}{\tilde{\sigma}_p^2} + \frac{2k}{n}\right).$$

We select the model with the smallest C_p in a collection of candidate models.

As the the factor $\tilde{\sigma}_p^2$ does not depend on k and has no impact on the selection result, C_p is equivalent to:

$$\frac{\tilde{\sigma}_k^2}{\tilde{\sigma}_p^2} + \frac{2k}{n}.$$

While $\tilde{\sigma}_k^2$ decreases when k increases, this measure is determined by the trade-off between model complexity (in terms of proportion of the number of regressors k/n) and model fitness (in terms of $\tilde{\sigma}_k^2/\tilde{\sigma}_p^2$).

Note that Mallows' original C_p is slightly different:

$$\text{Mallows' } C_p = \frac{\mathsf{RSS}_k}{\tilde{\sigma}_p^2} - n + 2k = n\left(\frac{\tilde{\sigma}_k^2}{\tilde{\sigma}_p^2} + \frac{2k}{n} - 1\right).$$

Yet, it is essentially the C_p measure discussed above.

Information Criteria

In the context of maximum likelihood, there are various information criteria for model selection. Let $L_n(\boldsymbol{\theta}_k)$ denote the log-likelihood function of n observations with k parameters $\boldsymbol{\theta}_k$ and $L_n(\tilde{\boldsymbol{\theta}}_k)$ its value based on the MLE $\tilde{\boldsymbol{\theta}}_k$. The Akaike information criterion (AIC) is:

$$\text{AIC} = -2L_n(\tilde{\boldsymbol{\theta}}_k) + 2k,$$

and the Bayesian (Schwarz) information criterion (BIC or SIC) is:

$$\text{BIC} = -2L_n(\tilde{\boldsymbol{\theta}}_k) + \ln(n)k.$$

These criteria also consider balance between model complexity and likelihood value (model fitness). We select the model with the smallest AIC/BIC from a collection of candidate models.

Recall that for the linear model $y = \boldsymbol{x}'\boldsymbol{\beta}_k + u$ with Gaussian error u,

$$L_n(\boldsymbol{\theta}_k) \propto -\frac{n}{2}\ln(\sigma^2) - \sum_{i=1}^{n} \frac{(y_i - \boldsymbol{x}_i'\boldsymbol{\beta})^2}{2\sigma^2}.$$

Plugging $\tilde{\boldsymbol{\theta}}_k = (\tilde{\boldsymbol{\beta}}_k', \tilde{\sigma}_k^2)'$ into $L_n(\boldsymbol{\theta}_k)$, where $\tilde{\sigma}_k^2 = \sum_{i=1}^{n}(y_i - \boldsymbol{x}_i'\tilde{\boldsymbol{\theta}}_k)^2/n$, we have

$$L_n(\tilde{\boldsymbol{\theta}}_k) = -\frac{n}{2}\ln(\tilde{\sigma}_k^2) - \frac{n}{n}\sum_{i=1}^{n} \frac{(y_i - \boldsymbol{x}_i'\tilde{\boldsymbol{\beta}}_k)^2}{2\tilde{\sigma}_k^2} = -\frac{n}{2}\ln(\tilde{\sigma}_k^2) - \frac{n}{2}.$$

It follows that, under normality,

$$\mathsf{AIC} = -2L_n(\tilde{\boldsymbol{\theta}}_k) + 2k = n[\ln(\tilde{\sigma}_k^2) + 1 + 2k/n].$$

Thus, model selection under normality may be based on a version of AIC: $\ln(\tilde{\sigma}_k^2) + 2k/n$. Similarly, a version of BIC is $\ln(\tilde{\sigma}_k^2) + \ln(n)k/n$.

Note that if we consider the log-likelihood function with a known σ_o^2,

$$L_n(\boldsymbol{\beta}_k) \propto -\sum_{i=1}^{n} \frac{(y_i - \boldsymbol{x}_i'\boldsymbol{\beta}_k)^2}{2\sigma_o^2},$$

and $L_n(\tilde{\boldsymbol{\beta}}_k) = -n\tilde{\sigma}_k^2/(2\sigma_o^2)$, so that

$$\text{AIC} = -2L_n(\tilde{\boldsymbol{\beta}}_k) + 2k = n\left(\frac{\tilde{\sigma}_k^2}{\sigma_o^2} + \frac{2k}{n}\right).$$

This is virtually the AIC in JWHT (2021) if σ_o^2 is replaced with $\tilde{\sigma}_p^2$.

Note: BIC involves a higher penalty on model complexity than does AIC when $\ln(n) > 2$, i.e., $n > 7$. Hence, BIC usually results in a simpler model.

Model Selection Criteria or Cross Validation?

In model selection procedures, a model with the "best" performance may be determined by some model selection criteria (C_p, AIC, or BIC) or by cross validation. As discussed in the previous lecture, cross validation is computationally very demanding, especially when p and/or n are large, but it (unlike C_p, AIC and BIC) requires less assumptions on the true model and data. JWHT (2021) suggest that, when computation is no longer a concern,

> *"cross-validation is a very attractive approach for selecting from among a number of models under consideration" (p. 235).*

Best Subset Selection

Suppose there are p potential regressors. Let $\mathcal{M}_k$ denote the linear model with the constant term and k (out of p) regressors and $\mathcal{M}_0$ denote the model with the constant term only. Best Subset Selection is a procedure that selects regressors among all possible combinations of p regressors; there are 2^p such combinations.

Best Subset Selection Procedure

1. For $k = 1$, fit all $\binom{p}{k}$ $\mathcal{M}_k$ linear models; the model with the highest R^2 is denoted as $\mathcal{M}_1^*$.
2. For $k = 2, 3, \ldots, p$, repeat the procedure above and find $\mathcal{M}_2^*, \ldots, \mathcal{M}_p^*$.
3. Among $\mathcal{M}_0$, $\mathcal{M}_1^*, \ldots, \mathcal{M}_p^*$, select the one with the smallest $\bar{R}^2$, C_p, AIC, BIC, or Cross Validation error.

- Best subset selection is computationally costly because it has to search among a very large number of candidate models. For $p = 10$, there are about 1,000 candidate models; when $p = 20$, the number of candidate models grows over a million. This approach becomes practically infeasible when p is large, say, $p > 40$.
- Another drawback: It is more likely to find an over-fitting model (the number of regressors is more than needed) when searching in a large space of models. An over-fitting model tends to perform well on training data but very poorly on test data.
- In practice, it is desirable to have a computationally more efficient alternative that searches in a much smaller space of models.

Forward Stepwise Selection

Forward Stepwise Selection starts from the simplest model (with the constant term only) and at each step adds one regressor that generates the largest additional improvement to model fitness from the previous step. Compared with Best Subset Selection, this approach admits a much smaller space of candidate models and is computationally more feasible.

Forward Stepwise Selection Procesure

1. For $k = 0$, fit all $p - k$ models that add one regressor to $\mathcal{M}_0$; the model with the highest R^2 is denoted as $\mathcal{M}_1^*$.
2. For $k = 1, 2, \ldots, p - 1$, fit all $p - k$ models that add one regressor to $\mathcal{M}_k^*$; the one with the highest R^2 is denoted as $\mathcal{M}_{k+1}^*$.
3. Among $\mathcal{M}_0$, $\mathcal{M}_1^*, \ldots, \mathcal{M}_p^*$, select the one with the smallest $\bar{R}^2$, C_p, AIC, BIC, or Cross Validation error.

- Forward Stepwise Selection fits only $1 + p(p+1)/2$ models and is computationally more efficient than Best Subset Selection when p is large. For example, when $p = 30$, Best Subset Selection searches among $1,073,741,842$ models, while Forward Stepwise Selection fits only 466 models.
- Note that Forward Stepwise Selection is computationally simpler but need not find the best possible model even with infinitely many data. For instance, it may be the case that the best possible one-variable model contains x_1 and the best possible two-variable model contains x_2 and x_3. In this case, Forward Stepwise Selection would never find the best two-variable model, because the selected model in the second step must contain x_1.

Backward Stepwise Selection

Backward Stepwise Selection starts from the most complex model with p regressors and at each step removes the regressor that makes the least contribution to model fitness from the previous step. Similar to Forward Stepwise Selection, this procedure searches among $1 + p(p+1)/2$ models.

Backward Stepwise Selection Procedure

1. For $k = p$, fit all k models that take out one regressor from $\mathcal{M}_p$; the model with the highest R^2 is denoted as $\mathcal{M}^*_{p-1}$.
2. For $k = p-1, \ldots, 2$, fit all k models that take out one regressor from $\mathcal{M}^*_k$; the one with the highest R^2 is denoted as $\mathcal{M}^*_{k-1}$.
3. Among $\mathcal{M}_p$, $\mathcal{M}^*_{p-1}, \ldots, \mathcal{M}^*_1$, $\mathcal{M}_0$, select the one with the smallest $\bar{R}^2$, C_p, AIC, BIC, or Cross Validation error.

Example: Taiwan Criminal Data (Subset Selection)

We consider Taiwan's criminal and employment data from March 2001 through July 2018. These monthly data are taken from Department of Statistics, Ministry of Interior of Taiwan.

- `Theft`: This is the variable of interest y, which is the monthly theft incidents occurred in Taiwan.
- `Clearance`: Clearance rate of criminal cases, which is calculated by:

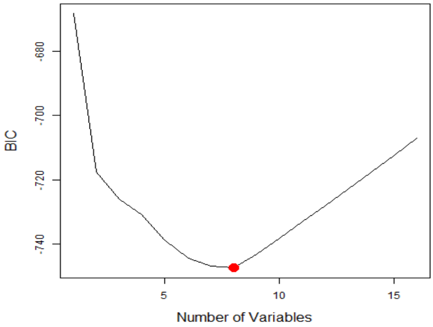
  $$100 \times \frac{\text{(Monthly clearance cases)}}{\text{(Total criminal cases in the same month)}}.$$

  Note that this variable may be larger than 100.

- Recession: A dummy variable, 1 for recession period.
- Time: Linear time trend.
- Unemploy_ppl: Number of unemployed persons in 1,000.
- Workforce: Number of workforce persons in 1,000.
- Job_partici: Job participation rate.
- Drug_lag1: Drug-related criminal cases in the previous month.
- Violence_lag1: Violence-related criminal cases in the previous month.

The other variables include: Non_workforce, Clearance_lag1, Clearance_lag2, Recession_lag1, Recession_lag2, Unemploy_rate, Drug_lag2, Violence_lag2. Note that we have a variable of interest, Theft, and 16 regressors in the data set.

We apply 3 model selection procedures to this sample. While Best Subset Selection and Backward Stepwise Selection both select a 8-variable model, Forward Stepwise Selection finds a 9-variable model. Below is the plot of the BIC values of the models found by Best Subset Selection.



- In this example, the models selected by Best Subset Selection and Backward Stepwise Selection are identical with the following variables: `Recession`, `Time`, `Clearance_lag1`, `Unemploy_rate`, `Job_partici`, `Workforce`, `Non_workforce`, `Violence_lag1`.
- Compared with the model selected above, the 9-variable model selected by Forward Stepwise Selection has 7 variables in common. Yet, it replaces `Unemploy_rate` with `Unemploy_ppl` and includes an additional variable Drug_lag2. Note that Forward Stepwise Selection identifies `Unemploy_ppl` in the 5 th round, which is not selected by other methods.

Selection results:

```
> Best Subset Selection: Select 8 Variables
(Intercept)      Recession     Time         Clearance_lag1
-1.677e+06       -6.218e+02    1.489e+02    -5.053e+01
Unemploy_rate    Job_partici   Workforce
-6.149e+02       3.461e+04     -9.286e+01
Non_workforce    Violence_lag1
8.704e+01        4.557e+00
> Forward Stepwise Selection: Select 9 Variables
(Intercept)      Recession     Time         Clearance_lag1
-1.618e+06       -6.3766e+02   1.442e+02    -5.10e+01
Unemploy_ppl     Job_partici   Workforce
-5.559e+00       3.346e+04     -8.988e+01
Non_workforce    Drug_lag2     Violence_lag1
8.385e+01        8.260e-02     4.476e+00
```

Shrinkage Methods

- Instead of searching among a large collection of candidate models to find the best subset of regressors, shrinkage methods regularize the coefficient estimates in the model with p regressors by "forcing" some of them to shrink towards zero or to be exactly zero. This is done by imposing a constraint on parameters when minimizing the sum of squared errors.
- This approach finds more influential regressors (coefficients away from zero) and significantly reduces the variance of coefficient estimates.
- There are two major shrinkage methods: ridge regression and LASSO (Least Absolute Shrinkage and Selection Operator), which are based on different parameter constraints.

Ridge Regression

The ridge regression considers the following minimization problem:

$$\min_{\boldsymbol{\beta}} \sum_{i=1}^{n} \left(y_i - \beta_0 - \sum_{j=1}^{p} \beta_j x_{ij} \right)^2 \quad \text{subject to} \quad \sum_{j=1}^{p} \beta_j^2 \leq s,$$

where s is a "budget" for all coefficients but the intercept β_0. This is equivalent to minimizing the constrained objective function:

$$\min_{\boldsymbol{\beta}} \sum_{i=1}^{n} \left(y_i - \beta_0 - \sum_{j=1}^{p} \beta_j x_{ij} \right)^2 + \lambda \sum_{j=1}^{p} \beta_j^2,$$

where λ is the tuning parameter. The solution is the ridge estimator, denoted as $\hat{\boldsymbol{\beta}}^R(\lambda)$.

- The ridge estimates find a balance between the sum of squared errors and the shrinkage penalty $\lambda \sum_{j=1}^{p} \beta_j^2$ (the "size" of coefficients in term of ℓ_2-norm). The shrinkage penalty plays the role of "shrinking" coefficients towards zero. As a result, less influential estimates would be close to zero, yet they cannot be exactly zero. Clearly, the ridge estimates become the OLS estimates when $\lambda = 0$.
- The ridge estimates are not scale equivariant, i.e., they will not be scaled by $1/c$ when a regressor is multiplied by a constant c. To circumvent this scaling problem, we apply ridge estimation to regression with standardized regressors:

$$\frac{x_{ij}}{\sqrt{\frac{1}{n}\sum_{i=1}^{n}(x_{ij}-\bar{x}_j)^2}}, \quad j = 1, \ldots, p,$$

where $\bar{x}_j = \sum_{i=1}^{n} x_{ij}/n$.

- While the OLS estimator is unbiased, the ridge estimator is biased in general, because the shrinkage penalty tends to push the coefficients away from the unbiased (OLS) estimates.
- When λ approaches infinity, the shrinkage penalty is so large that all coefficients would have to be arbitrarily small.
- In practice, we usually consider a grid of λ values and compute the associated ridge estimates $\hat{\beta}_j^R(\lambda)$. The optimal λ can be found by minimizing cross validation errors across different λ values.

Simulations: Ridge Regression

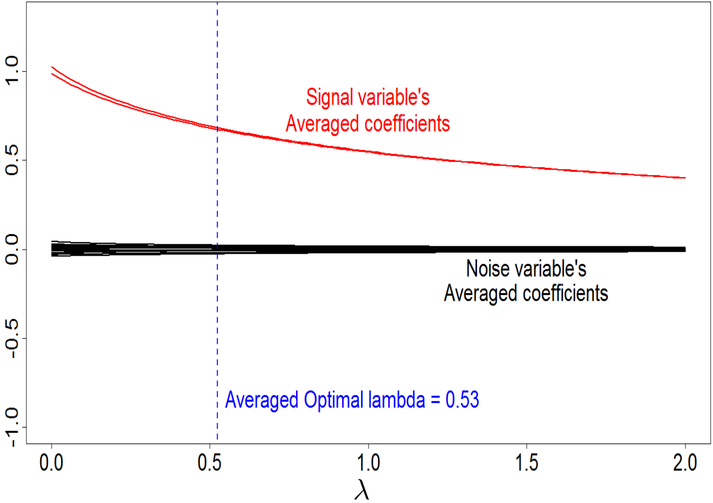
We conduct simulations to assess the performance of the ridge regression estimates. The data generating processes (DGPs) are

$$\text{DGP 1}: \; y_i = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \epsilon_i, \quad \beta_0 = 2, \; \beta_1 = \beta_2 = 1,$$

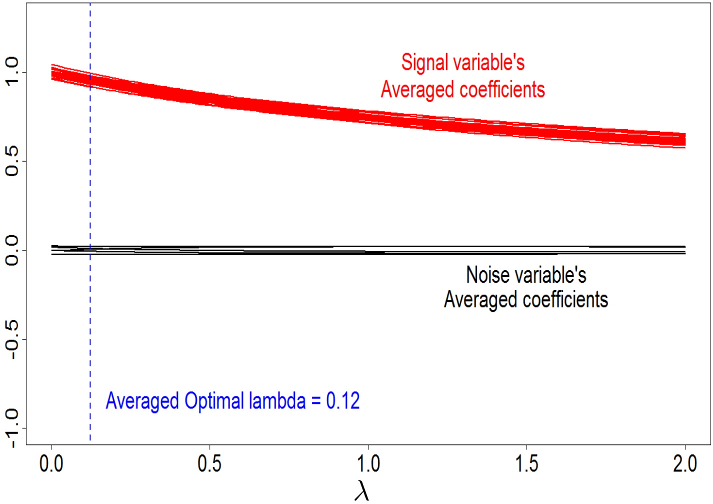
$$\text{DGP 2}: \; y_i = \beta_0 + \sum_{j=1}^{20} \beta_j x_{ij} + \epsilon_i, \quad \beta_0 = 2, \; \beta_1 = \cdots = \beta_{20} = 1,$$

where all x_{ij} and ϵ_i are i.i.d. $\mathcal{N}(0,1)$, and the sample size is $n = 55$. For each DGP, we estimate two models with 25 and 50 regressors, including the "signal" variables in the DGP and other "noise" variables (generated as i.i.d. $\mathcal{N}(0,1)$). We consider 100 λ values in $[0,2]$, with the optimal λ determined by 10-fold CV. All the lines in the following figures are the ridge estimates averaged over 100 replications.

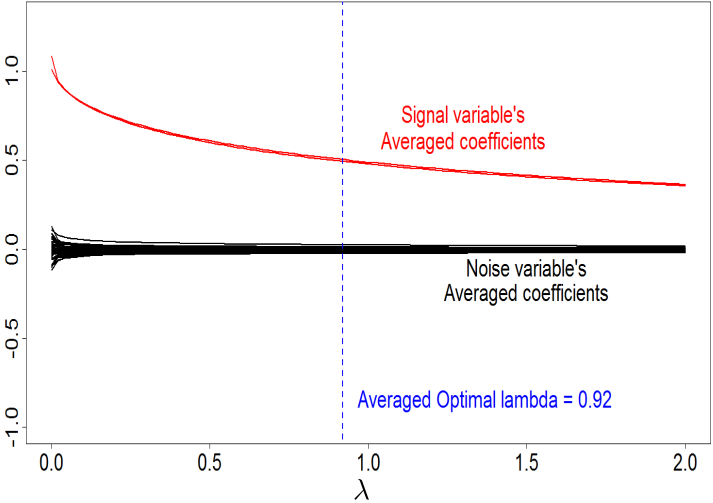
DGP 1: 2 signal variables; ridge regression with 25 regressors.



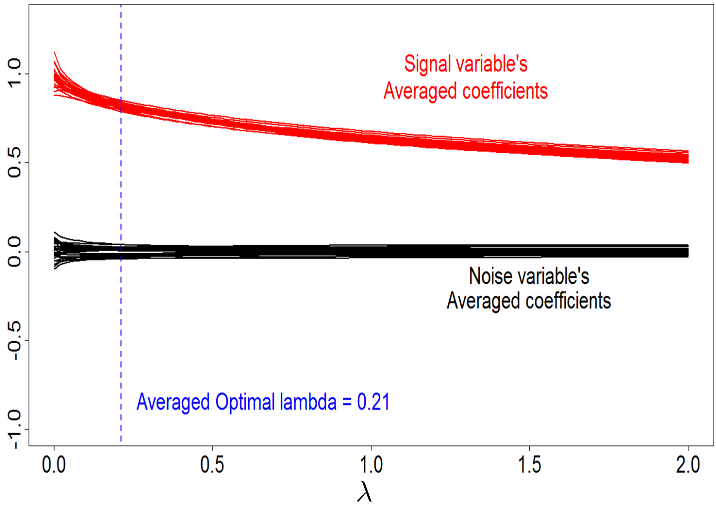
DGP 2: 20 signal variables; ridge regression with 25 regressors.



DGP 1: 2 signal variables; ridge regression with 50 regressors.



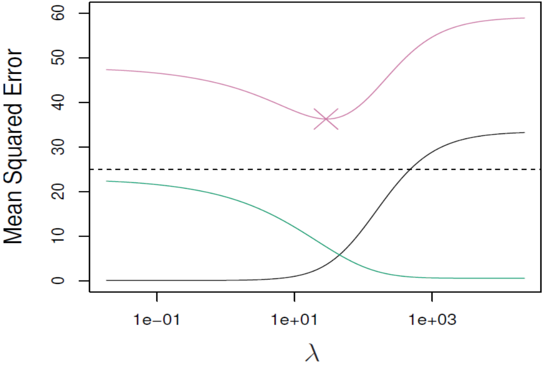
DGP 2: 20 signal variables; ridge regression with 50 regressors.



Summary of Simulation Results

- The larger the λ, the closer the ridge estimates $\hat{\beta}_j^R(\lambda)$ to 0.
- Regression with 25 regressors
  - DGP 1: Optimal $\lambda^* = 0.53$, $\bar{\hat{\beta}}_1^R(\lambda^*) = 0.6739$ and $\bar{\hat{\beta}}_2^R(\lambda^*) = 0.6834$.
  - DGP 2: Optimal $\lambda^* = 0.12$, the average ridge estimates at λ^* for the signal variables range from 0.9191 to 0.9947.
- Regression with 50 regressors
  - DGP 1: Optimal $\lambda^* = 0.92$, $\bar{\hat{\beta}}_1^R(\lambda^*) = 0.5067$ and $\bar{\hat{\beta}}_2^R(\lambda^*) = 0.4962$.
  - DGP 2: Optimal $\lambda^* = 0.21$, the average ridge estimates at λ^* for the signal variables range from 0.7844 to 0.8475.
- The ridge estimates perform well when the number of signal variables is large relative to the number of variables included in the model. The ridge estimates have large biases when the number of signal variables is relatively small.

The bias-variance trade-off: The graph below, taken from JWHT (2021), shows the *squared bias* (black), *variance* (green), and the *testing MSE* (purple) for a ridge regression with different λ. The cross indicates the λ value that yields the smallest MSE.



Source: Figure 6.5 of JWHT (2021)

LASSO

The ridge regression does not possess the ability of variable (model) selection because all p regressors are included in the final model. This may not be a problem for prediction accuracy, but it may affect model interpretability, especially when p is large. Instead, the LASSO considers the following minimization problem:

$$\min_{\boldsymbol{\beta}} \sum_{i=1}^{n} \left(y_i - \beta_0 - \sum_{j=1}^{p} \beta_j x_{ij} \right)^2 \quad \text{subject to} \quad \sum_{j=1}^{p} |\beta_j| \le s.$$

Note that the "budget" s is imposed on the absolute values of the coefficients (except the intercept term).

The LASSO problem is equivalent to minimizing:

$$\sum_{i=1}^{n}\left(y_i-\beta_0-\sum_{j=1}^{p}\beta_j x_{ij}\right)^2+\lambda\sum_{j=1}^{p}|\beta_j|,$$

where every regressor x_j is standardized. The LASSO estimates, $\hat{\beta}_j^L(\lambda)$, find a balance between the sum of squared errors and the shrinkage penalty $\lambda\sum_{j=1}^{p}|\beta_j|$ (the "size" of the coefficients in terms of ℓ_1-norm).

- The LASSO estimates become the OLS estimates when $\lambda=0$, and they are zero when $\lambda\to\infty$. In practice, we may also apply cross validation to determine the optimal λ from a grid of λ values.
- LASSO is capable of variable selection because the LASSO penalty has the effect of "forcing" the estimates $\hat{\beta}_j^L(\lambda)$ to be exactly zero when λ is sufficiently large. See also discussion below.

Simulations: LASSO

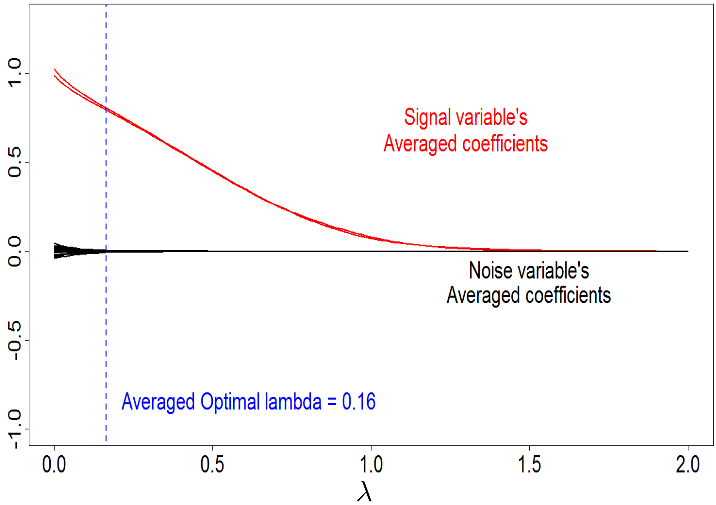
We conduct simulations to assess the performance of the LASSO estimates. The DGPs are as in the previous simulations:

$$\text{DGP 1}: \; y_i = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \epsilon_i, \quad \beta_0 = 2, \; \beta_1 = \beta_2 = 1,$$

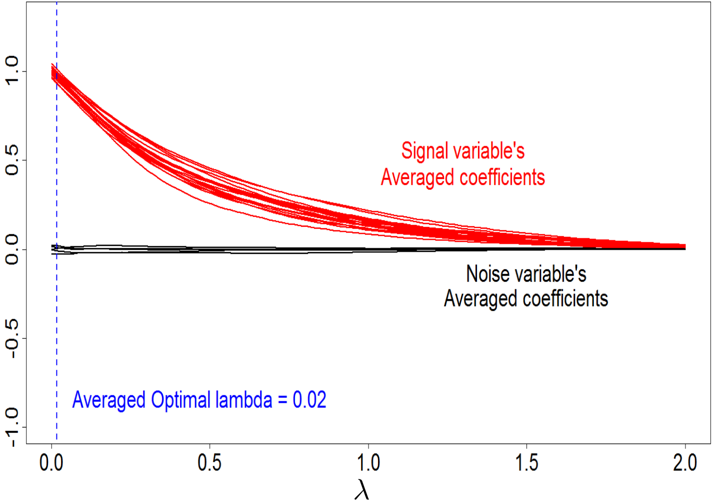
$$\text{DGP 2}: \; y_i = \beta_0 + \sum_{j=1}^{20} \beta_j x_{ij} + \epsilon_i, \quad \beta_0 = 2, \; \beta_1 = \cdots = \beta_{20} = 1,$$

where all x_{ij} and ϵ_i are i.i.d. $\mathcal{N}(0,1)$, and the sample size is $n = 55$. For each DGP, we estimate two models with 25 and 50 regressors, including the "signal" variables in the DGP and other "noise" variables (generated as i.i.d. $\mathcal{N}(0,1)$). We consider 100 λ values in $[0,2]$, with the optimal λ determined by 10-fold CV. All the lines in the following figures are the LASSO estimates averaged over 100 replications.

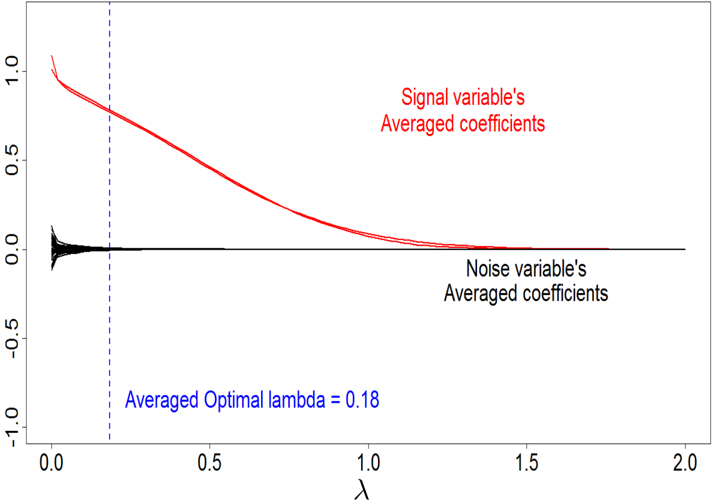
DGP 1: 2 signal variables; LASSO with 25 regressors.



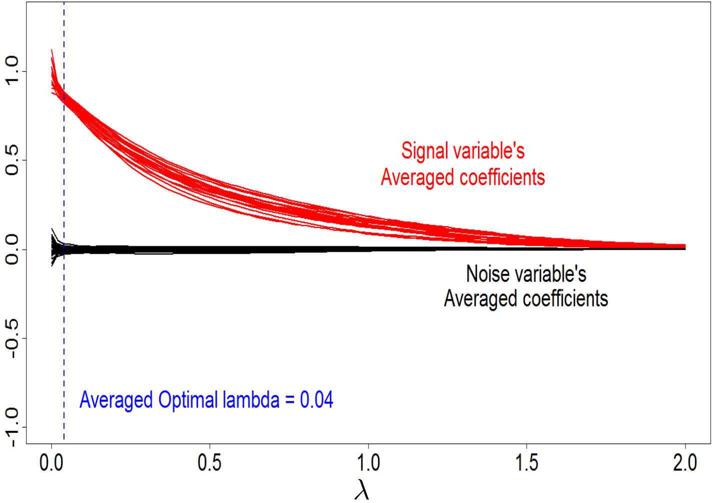
DGP 2: 20 signal variables; LASSO with 25 regressors.



DGP 1: 2 signal variables; LASSO with 50 regressors.



DGP 2: 20 signal variables; LASSO with 50 regressors.



Summary of Simulation Results

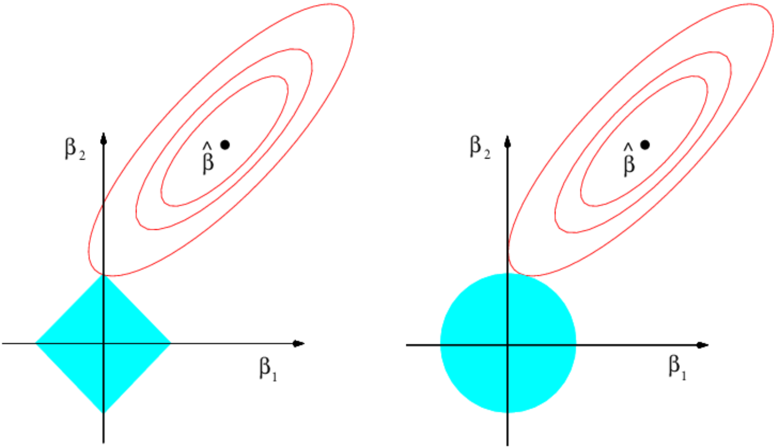
- The LASSO estimates $\hat{\beta}_j^L(\lambda)$ become 0 quickly as λ increases.
- Model with 25 regressors
  - DGP 1: Optimal $\lambda^* = 0.16$, $\bar{\hat{\beta}}_1^L(\lambda^*) = 0.7969$ and $\bar{\hat{\beta}}_2^L(\lambda^*) = 0.8082$.
  - DGP 2: Optimal $\lambda^* = 0.02$, the average ridge estimates at λ^* for the signal variables range from 0.9262 to 1.0077.
- Model with 50 regressors
  - DGP 1: Optimal $\lambda^* = 0.18$, $\bar{\hat{\beta}}_1^L(\lambda^*) = 0.7850$ and $\bar{\hat{\beta}}_2^L(\lambda^*) = 0.7729$.
  - DGP 2: Optimal $\lambda^* = 0.04$, the average ridge estimates at λ^* for the signal variables range from 0.8207 to 0.8834.
- Compared with the ridge estimates, the LASSO estimates tend to have a smaller bias when the number of signal variables is small. The LASSO also performs very well when there are many signal variables.

LASSO vs. Ridge Regression

To see how the LASSO differs from the ridge regression, consider the case of $p = 2$. Note that the budget set for the ridge regression is the circle: $\beta_1^2 + \beta_2^2 \leq s$, and that for the LASSO is the diamond: $|\beta_1| + |\beta_2| \leq s$; see the graph in the next page.

- Optimization with a smooth budget sets often leads to interior solutions, while optimization with a budget sets with non-differentiable points often yields corner solutions.
- If s is so large that the OLS estimates fall within the budget set, $\sum_{j=1}^{p} \beta_j^2 \leq s$ and $\sum_{j=1}^{p} |\beta_j| \leq s$ are not binding, and the ridge regression and the LASSO would yield the OLS solutions.

In the graphs below, the red solid lines are the contours of the sum of squared errors, and the light blue regions are the budget sets.



Source: Figure 6.7 of JWHT (2021)

A Special Case

Consider now the special case that $\boldsymbol{y} = \boldsymbol{X}\boldsymbol{\beta} + \boldsymbol{\epsilon}$, with $\boldsymbol{X} = \boldsymbol{I}_p$ (so that $n = p$). In this case, the OLS estimates minimize:

$$\sum_{j=1}^{p} \left(y_j - \beta_j\right)^2,$$

and hence $\hat{\beta}_j = y_j$. The ridge regression and LASSO estimates minimize:

$$\begin{aligned}\text{ridge: } & \sum_{j=1}^{p} \left(y_j - \beta_j\right)^2 + \lambda \sum_{j=1}^{p} \beta_j^2, \\ \text{LASSO: } & \sum_{j=1}^{p} \left(y_j - \beta_j\right)^2 + \lambda \sum_{j=1}^{p} |\beta_j|.\end{aligned}$$

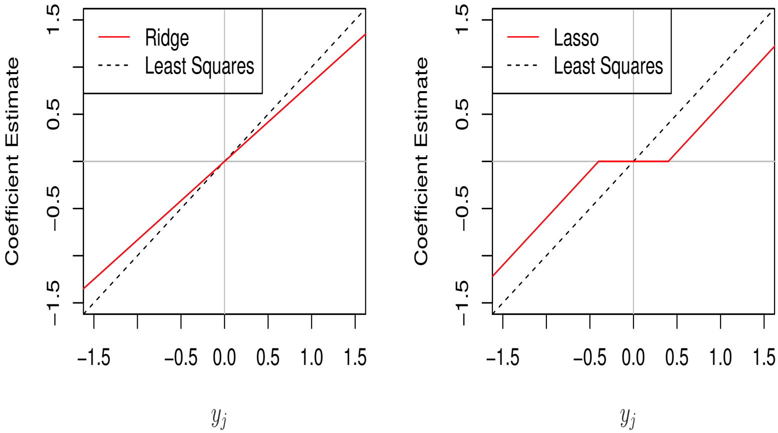
It is easy to verify that the ridge regression estimates are:

$$\hat{\beta}_j^R(\lambda) = y_j/(1+\lambda),$$

and the LASSO estimates are:

$$\hat{\beta}_j^L(\lambda) = \begin{cases} y_j - \lambda/2, & \text{if } y_j > \lambda/2, \\ y_j + \lambda/2, & \text{if } y_j < -\lambda/2, \\ 0, & \text{if } |y_j| \le \lambda/2. \end{cases}$$

Thus, the ridge regression shrinks each OLS coefficient towards zero by the same proportion $1/(1+\lambda)$. Clearly, the ridge estimates approach zero when λ increases, but they will not be exactly zero. On the other hand, the LASSO shrinks the OLS coefficients by a given amount $\lambda/2$; the larger the λ values, the more the estimates shrink. See Figure 6.10 of JWHT (2021).



Source: Figure 6.10 of JWHT (2013)

LASSO vs. Best Subset Selection

Note that the Best Subset Selection problem can be written as:

$$\min_{\boldsymbol{\beta}} \sum_{i=1}^{n} \left(y_i - \beta_0 - \sum_{j=1}^{p} \beta_j x_{ij} \right)^2 \quad \text{subject to} \quad \sum_{j=1}^{p} \mathbf{1}(\beta_j \neq 0) \leq s,$$

where $\mathbf{1}(\cdot)$ denotes the indicator function. In other words, this problem finds parameter estimates to minimize the sum of squared errors, subject to the constraint that no more than s coefficients can be selected. As we learned earlier, this minimization problem is computationally prohibited when p is large. Hence, we may view both the ridge regression and LASSO as two computationally feasible alternatives to Best Subset Selection.

LASSO vs. OLS

To further examine the difference between the LASSO and OLS estimates, we conduct simulations with the DGPs considered earlier:

$$\text{DGP 1}: \; y_i = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \epsilon_i, \quad \beta_0 = 2, \; \beta_1 = \beta_2 = 1,$$

$$\text{DGP 2}: \; y_i = \beta_0 + \sum_{j=1}^{20} \beta_j x_{ij} + \epsilon_i, \quad \beta_0 = 2, \; \beta_1 = \cdots = \beta_{20} = 1,$$

and the sample size is $n = 55$; another 55 observations are also generated and reserved as the testing sample. We estimate two models with 25 and 50 regressors, including the "signal" variables in the DGP and other "noise" variables. The optimal λ is chosen from 100 λ values in $[0, 2]$ using 10-fold CV. The number of replications is $10,000$.

- In the following tables, we consider three methods: OLS, LASSO, and LASSO-OLS, where for LASSO-OLS we first select the variables by the LASSO and then apply OLS with the LASSO-selected variables as regressors.
- To illustrate, we report only the results of the coefficient of the first signal variable $\hat{\beta}_1$ and those of the coefficient of the first noise variable $\hat{\beta}_3$ (for DGP 1) or $\hat{\beta}_{21}$ (for DGP 2). Their bias, variance, and MSE are the averages over $10,000$ replications.
- The model testing MSEs are the averages over $10,000$ testing samples.

DGP 1; $p = 25$		OLS	LASSO	LASSO-OLS
$\hat{\beta}_1$	Bias	0.0011	-0.1845	-0.0281
	Variance	0.0367	0.0262	0.0255
	MSE	0.0367	0.0603	0.0263
$\hat{\beta}_3$	Bias	0.0019	-0.0005	-0.0001
	Vriance	0.0353	0.0032	0.0117
	MSE	0.0353	0.0032	0.0117
Model Testing MSE		1.9323	1.2187	1.3539
DGP 1; $p = 50$				
$\hat{\beta}_1$	Bias	-0.0060	-0.2269	-0.0609
	Variance	0.3432	0.0281	0.0282
	MSE	0.3432	0.0796	0.0319
$\hat{\beta}_3$	Bias	-0.0004	0	0.0005
	Variance	0.3335	0.0020	0.0081
	MSE	0.3335	0.0020	0.0081
Model Testing MSE		18.1495	1.2812	1.4951

Summary of Simulation Results: DGP 1

- Bias-variance trade-off for $\hat{\beta}_1$ (coefficient of the first signal variable): Compared with OLS, the LASSO estimates have much larger biases, smaller variances, and smaller MSEs. When $p = 50$, OLS leads to a very large variance, but the LASSO estimate has a stable variance.
- $\hat{\beta}_3$ (coefficient of the first noise variable): Compared with OLS, the LASSO estimates have little bias, smaller variances, and smaller MSEs. Thus, there is no bias-variance trade-off for this coefficient.
- LASSO-OLS yields smaller MSE for $\hat{\beta}_1$ than do OLS and LASSO, but it yields larger MSE for $\hat{\beta}_3$ than does LASSO.
- For both models, the LASSO yields the smallest testing MSEs, and OLS yields the largest testing MSEs. The advantage of LASSO is very significant when $p = 50$.

DGP 2; $p = 25$		OLS	LASSO	LASSO-OLS
$\hat{\beta}_1$	Bias	0.0011	-0.0292	-0.0001
	Variance	0.0367	0.0372	0.0365
	MSE	0.0367	0.0381	0.0365
$\hat{\beta}_{21}$	Bias	0.0002	0.0004	0.0005
	Vriance	0.0348	0.0279	0.0340
	MSE	0.0348	0.0279	0.0340
Model Testing MSE		1.9203	1.9301	1.9234
DGP 2; $p = 50$				
$\hat{\beta}_1$	Bias	-0.0060	-0.1411	-0.0636
	Variance	0.3433	0.0742	0.0888
	MSE	0.3433	0.0942	0.0928
$\hat{\beta}_{21}$	Bias	-0.0054	-0.0003	-0.0016
	Variance	0.3245	0.0309	0.0612
	MSE	0.3245	0.0309	0.0612
Model Testing MSE		18.0081	3.7543	4.5389

Summary of Simulation Results: DGP 2

- $\hat{\beta}_1$: We observe bias-variance trade-off for the LASSO estimate when $p = 50$ but no such trade-off when $p = 25$.
- $\hat{\beta}_{21}$ (the coefficient of the first noise variable): Compared with OLS, the LASSO estimate has a smaller bias, smaller variance and smaller MSE when $p = 50$, i.e., no bias-variance trade-off. For $p = 25$, the LASSO has slightly larger bias but smaller variance and MSE.
- When $p = 50$, the LASSO yields the smallest testing MSE, but OLS has very large testing MSE. When $p = 25$, the LASSO yields slightly larger testing MSE than does OLS.
- The LASSO has clear advantages when the number of regressors is much larger than the number of signal variables. Note that bias-variance trade-off does not always exist.

Example: Taiwan Criminal Data (Shrinkage Methods)

We apply the ridge regression and LASSO to Taiwan's criminal data. Recall that the variable of interest is Theft and that there are 16 independent variables. We report the ridge estimates at $\lambda^* = 0.5005$ and the LASSO estimates at $\lambda^* = 51.2512$. Note that the ridge estimates ought to be close to the OLS estimates because λ^* is very small.

The LASSO selects 10 out of 16 regressors, among them 5 are the same as those selected by Best Subset Selection (Recession, Clearance_lag1, Workforce, Non_workforce, Violence_lag1) and one is the same as that selected by Forward Stepwise Selection (Unemploy_ppl). In addition, the LASSO selects Clearance_lag2, Recession_lag1, Drug_lag2, and Violence_lag2.

Ridge Regression Estimates

Clearance	Recession	Time	Clearance_lag1
$7.118042e+00$	$-7.165727e+02$	$5.900018e+01$	$-4.455641e+01$
Clearance_lag2	Recession_lag1	Recession_lag2	Unemploy_ppl
$-1.562688e+01$	$-1.703746e+02$	$-3.224905e+01$	$4.666036e+01$
Unemploy_rate	Job_partici	Workforce	Non_workforce
$-5.629722e+03$	$3.285448e+03$	$-1.716189e+01$	$-6.595184e+00$
Drug_lag1	Drug_lag2	Violence_lag1	Violence_lag2
$-1.984927e-02$	$1.873150e-01$	$4.773189e+00$	$9.504042e-01$
(Intercept)			
$6.047442e+04$			

LASSO Estimates

Clearance	Recession	Time	Clearance_lag1
$7.118042e+00$	$-7.240257e+02$	0	$-4.061501e+01$
Clearance_lag2	Recession_lag1	Recession_lag2	Unemploy_ppl
$-5.711850e+00$	$-1.766387e+02$	0	$-6.140723e+00$
Unemploy_rate	Job_partici	Workforce	Non_workforce
0	0	$-2.628722e+00$	$-1.454844e+01$
Drug_lag1	Drug_lag2	Violence_lag1	Violence_lag2
0	$9.107362e-02$	$4.992001e+00$	$1.338615e+00$
(Intercept)			
$1.612056e+05$			

References and Acknowledgement

References

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