

STA 35C: Statistical Data Science III

Lecture 16: Linear Model Selection – Regularization Methods

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Announcements

Homework 5 is posted

- Please review the problems early and ask questions as needed.
- Submit a single PDF on time and follow the submission instructions.

Office hours today

- Instructor office hours: 3:30–4:30 PM, MSB 4220.
- You are welcome to bring any questions about Homework 5 or recent lecture material.

Agenda

- **Last time:** Model selection via subset selection
 - Best subset selection: identify relevant predictors among many
 - Stepwise selection: A computationally cheaper greedy alternative
- **Today:** Regularization as an alternative to subset selection
 - Overview: what regularization is & why it can help
 - Two main examples in linear regression
 - Ridge regression
 - The lasso (least absolute shrinkage and selection operator)

Recap: Subset selection

Best subset selection:

- Exhaustively search all 2^p subsets
- Pick the best model for each size k , then choose among them (via R_{adj}^2 or CV)
- Feasible only for smaller p (high computational cost)

Forward stepwise selection:

- Greedy approach: add one predictor at a time
- Complexity: $\mathcal{O}(p^2)$ instead of 2^p
- May miss the global optimum if local decisions are suboptimal

Backward stepwise selection:

- Greedy approach: remove one predictor at a time
- Similar pros/cons as forward stepwise

Recap: Subset selection – Comparison of search paths

An illustrative example with $p = 4$:

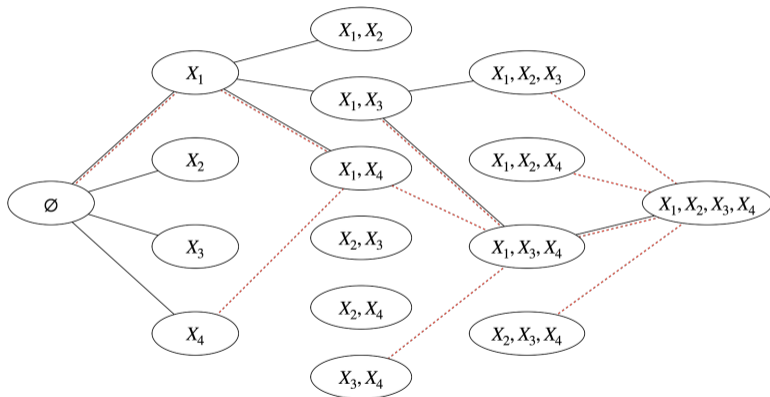


Figure: Illustration of forward stepwise (**black solid path**; successively adding $X_1 \rightarrow X_4 \rightarrow X_3 \rightarrow X_2$) and backward stepwise (**red dashed path**; removing $X_2 \rightarrow X_3 \rightarrow X_4 \rightarrow X_1$). Best subset selection checks all 2^p possibilities; all three can yield different outcomes.

Recap: Subset selection – Summary

- **Summary:**

- **Goal:** identify a relevant subset of predictors
- **Procedure:** evaluate subsets (all or partial), then pick best via R_{adj}^2 , CV, etc.
- BSS is exhaustive but expensive; stepwise is faster
- Typically refit the final chosen “best” subset with least squares

- **Advantages:**

- Direct variable selection: some $\beta_j = 0$ (excluded)
- Straightforward implementation and intuitive interpretation

- **Disadvantages:**

- Even stepwise can be costly if p is very large
- Instability: small changes in the data can alter the chosen “best” subset

⇒ **Regularization** controls model complexity continuously by shrinking coefficients, often giving more stable or sparser estimates without searching over all subsets

Regularization: What and why?

Recall least squares: find parameters $\hat{\beta}_0, \dots, \hat{\beta}_p$ that minimize

$$\text{RSS} = \sum_{i=1}^n (y_i - \hat{y}_i)^2 \quad \text{where} \quad \hat{y}_i = \hat{\beta}_0 + \hat{\beta}_1 x_{i1} + \dots + \hat{\beta}_{ip} x_{ip}$$

- **Challenges:**

- If p is large, predictors are highly correlated, or the data are noisy, least squares estimates can have high variance
- This can lead to overfitting, unstable coefficients, or no unique least-squares solution when $p > n$

- **Idea:** *modify* the objective by **adding a penalty on β_j 's to stabilize fitting**

- Balance data fidelity vs. “simplicity” (by favoring smaller β_j)
- This approach is called *regularization* (or *shrinkage*)

We will learn two prominent regularization techniques for linear regression:

- **Ridge regression** (ℓ_2 penalty)
- **Lasso** (ℓ_1 penalty)

Ridge regression: 1) Formulation

Ridge regression: Find $\hat{\beta}_0, \dots, \hat{\beta}_p$ that minimize

$$\underbrace{\sum_{i=1}^n \left(y_i - \beta_0 - \sum_{j=1}^p \beta_j x_{ij} \right)^2}_{\text{RSS}} + \lambda \underbrace{\sum_{j=1}^p \beta_j^2}_{\text{penalty}}$$

- $\lambda \geq 0$ is a tuning parameter
- Each λ yields a different set of coefficient estimates $\hat{\beta}_\lambda^R$

Remarks:

- No penalty on β_0 (the intercept)
- As $\lambda \rightarrow 0$, ridge regression \rightarrow standard least squares
- As λ grows, $\beta_{1:p} = (\beta_1, \dots, \beta_p)$ shrinks toward 0
 - Reduces variance of $\beta_{1:p}$ but increases bias

Ridge regression: 2) Effects of scaling

The least squares coefficients are *scale equivariant*:

- Multiplying X_j by constant c scales $\hat{\beta}_j$ by $1/c$
- Regardless of scaling, $X_j \hat{\beta}_j$ remains the same, not affecting other coefficients

Ridge regression is *not* scale-equivariant:

- Rescaling one predictor can affect others through the penalty term
- Hence, $X_j \hat{\beta}_{j,\lambda}^R$ depends on both λ *and* predictor scaling

Therefore, we usually *standardize predictors* before ridge:

$$\tilde{x}_{ij} = \frac{x_{ij}}{s_{ij}} \quad \text{where} \quad s_{ij}^2 = \frac{1}{n} \sum_{i=1}^n (x_{ij} - \bar{x}_j)^2 \quad \text{and} \quad \bar{x}_j = \frac{1}{n} \sum_{i=1}^n x_{ij}$$

Ridge regression: 3) Credit dataset example

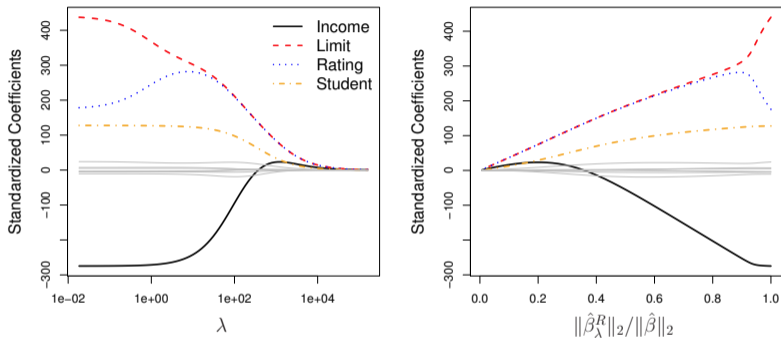


Figure: Standardized ridge coefficients for **Credit**, plotted vs. λ and $\|\hat{\beta}_\lambda^R\|_2 / \|\hat{\beta}\|_2$ [JWHT21, Figure 6.4]. (Note: $\|v\|_2 = \sqrt{v_1^2 + \dots + v_p^2}$.)

- As λ increases, all β_j shrink toward 0 (none exactly zero though)
- If variables are correlated, ridge shrinks them together in a “group” manner

Ridge regression: 4) Advantages over least squares

Ridge's advantage rooted in **Bias-variance tradeoff**:

- $\lambda = 0$: no bias but high variance
- Larger λ : more bias but lower variance

When ridge can be most helpful:

- If least squares has high variance (e.g. $p \approx n$ or predictors are collinear)
- If data are noisy and β_j can fluctuate a lot
- For $\lambda > 0$, ridge still works even if $p > n$, producing a unique solution

Computational advantages of ridge:

- No need for 2^p model fits (as in best subset); for any λ , ridge requires only a single fit
- Indeed, we can compute solutions for all λ at near the same cost as one OLS fit

Ridge regression: 5) Visualization of bias-variance tradeoff

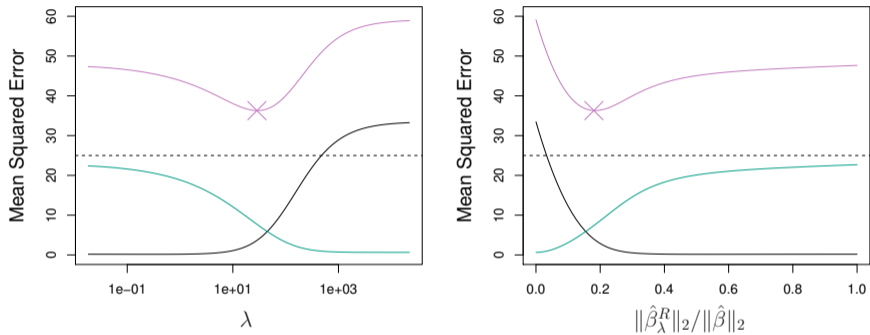


Figure: Bias-variance tradeoff in ridge for a simulated data set ($p = 45$, $n = 50$). Shown are squared bias (black), variance (green), and test MSE (purple) vs. λ [JWHT21, Figure 6.5].

- At $\lambda = 0$, there is no bias but high variance
- Increasing λ *significantly* reduces variance at the cost of *slightly* higher bias
- Eventually, added bias overtakes the benefit of reduced variance

Ridge regression: 6) Example with a toy dataset (R script)

- **Problem setup:**
 - $n = 5, p = 2$
 - Ridge vs. least squares (at $\lambda = 1$)
- **Goal:** See how ridge regression shrinks coefficients $\hat{\beta}$ compared to standard least squares

```
# Toy data: 5 obs, 2 predictors, no intercept
df <- data.frame(
  x1 = c(1,2,3,4,5),
  x2 = c(2,1,3,1,2),
  y = c(2,2.5,6,4,6.5)
)
```

```
# OLS fit (no intercept => '-1')
ols_fit <- lm(y ~ x1 + x2 - 1, data = df)
cat("OLS Coeffs:\n", coef(ols_fit), "\n")

# If needed: install.packages("glmnet")
library(glmnet)

# Prepare X,y for glmnet
X <- as.matrix(df[,c("x1","x2")])
y <- df$y

# Ridge fit with lambda=1
ridge_fit <- glmnet(
  X, y, alpha=0, lambda=1,
  intercept=TRUE, standardize=TRUE
)
cat("Ridge Coeffs (lambda=1):\n", as.matrix(
  coef(ridge_fit)), "\n")
```

Ridge regression: 7) Selecting λ

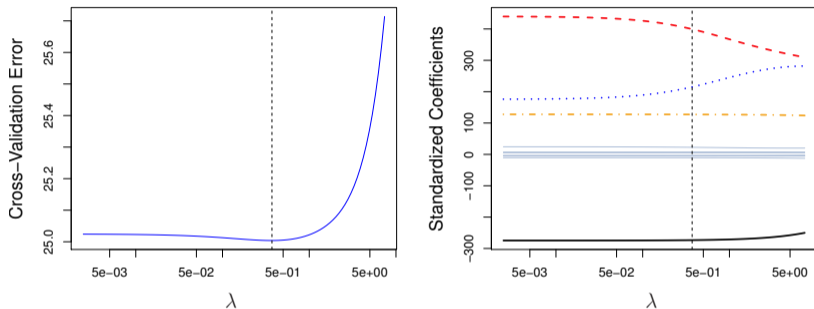


Figure: **Left:** CV errors for ridge regression on the **Credit** dataset with various values of λ . **Right:** Ridge regression coefficient estimates. The vertical dashed lines indicate the λ selected by CV [JWHT21, Figure 6.12].

- Here, the chosen λ is relatively small, meaning minimal shrinkage relative to least square
- The error curve's dip is not very pronounced, suggesting a broad range of λ values yield similar performance

Pop-up quiz: Ridge regression

Which statement below is **false** about ridge regression?

(*Hint: Think carefully. Which one might not always hold?*)

- A) It often lowers variance compared to least squares, at the cost of higher bias.
- B) All ridge coefficients are strictly smaller in magnitude than the least squares estimates for each predictor.
- C) The tuning parameter λ strongly influences ridge performance, often chosen via cross-validation.
- D) Ridge tends to shrink correlated predictors together.

Answer: B.

Brief explanation:

- While ridge regression shrinks the overall magnitude of the coefficient vector, it does *not* guarantee every individual coefficient is always smaller than its least squares counterpart.
- In some cases, ridge can redistribute weights among correlated predictors, causing some estimates to exceed their OLS magnitudes even though the sum of squares $\|\beta\|_2^2$ is reduced.

Ridge regression: 8) Summary

- **Ridge regression formulation:**
 - Add a penalty term $\sum_{j=1}^p \beta_j^2$ to the least squares objective, scaled by $\lambda \geq 0$
 - Shrinks β_j more strongly as λ grows, stabilizing estimates
- **Bias-variance tradeoff:**
 - Larger $\lambda \Rightarrow$ higher bias but lower variance
 - Especially helpful when OLS has high variance (e.g. large p , or $p > n$)
- **Computation:**
 - Efficient to solve for all λ at roughly the cost of one OLS fit
- **Limitation:**
 - Coefficients seldom reach exactly zero \implies no direct variable selection

The lasso: 1) Formulation

The lasso: Find $\hat{\beta}_0, \dots, \hat{\beta}_p$ that minimize

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

- $\lambda \geq 0$ is a tuning parameter
- Each choice of λ gives a different set of Lasso estimates $\hat{\beta}_\lambda^L$

Remarks:

- No penalty on β_0 (the intercept)
- As $\lambda \rightarrow 0$, lasso \rightarrow standard least squares
- As λ grows, many β_j shrink toward zero, and some exactly become 0

Unlike ridge, the lasso can yield exact zero estimates \implies **variable selection!**

The lasso: 2) Credit dataset example

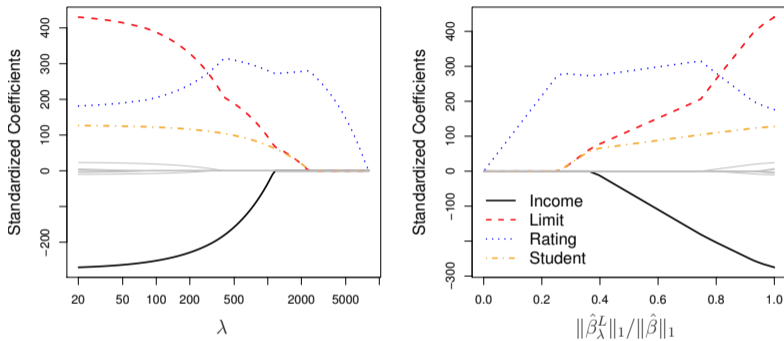


Figure: Standardized lasso coefficients for **Credit**, plotted vs. λ and the shrinkage level $\|\hat{\beta}_\lambda^R\|_2 / \|\hat{\beta}\|_2$ [JWHT21, Figure 6.6].

- Lasso can force some coefficients to zero as λ increases
- Achieves *variable selection* directly (predictors with $\hat{\beta}_j^L = 0$ are excluded)

The lasso: 3) Example with a toy dataset (R script)

- **Setup:**
 - $n = 5$, $p = 2$
 - Compare lasso vs. OLS at $\lambda = 1$
- **Objective:** See how lasso can shrink coefficients to zero

```
# Toy data: 5 obs, 2 predictors, no intercept
df <- data.frame(
  x1 = c(1,2,3,4,5),
  x2 = c(2,1,3,1,2),
  y = c(2,2.5,6,4,6.5)
)
```

```
# OLS fit
ols_fit <- lm(y ~ x1 + x2, data=df)
cat("OLS Coeffs:\n", coef(ols_fit), "\n")

# If needed: install.packages("glmnet")
library(glmnet)

# Prepare X, y
X <- as.matrix(df[, c("x1","x2")])
y <- df$y

# Lasso with alpha=1, lambda=1
lasso_fit <- glmnet(X, y,
                    alpha=1,
                    lambda=1,
                    intercept=TRUE,
                    standardize=TRUE)
cat("Lasso Coeffs (lambda=1):\n",
    as.matrix(coef(lasso_fit)), "\n")
```

The lasso: 4) Selecting λ

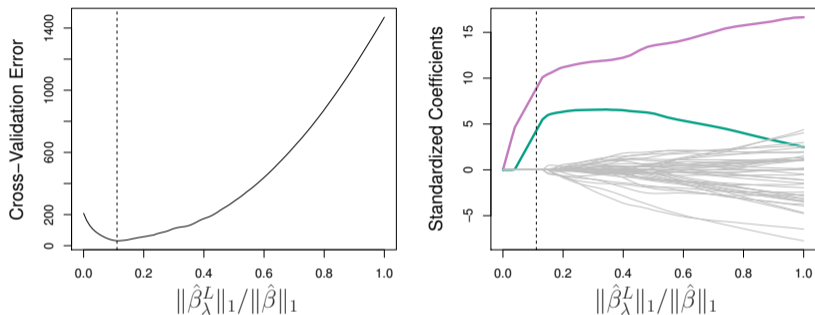


Figure: **Left:** Ten-fold cross-validation MSE for the lasso, applied to the sparse simulated data. **Right:** The corresponding lasso coefficient estimates, with the two *signal* variables in color and the *noise* variables in gray. The vertical dashed line indicates the fit that minimizes the cross-validation error [JWHT21, Figure 6.13].

- The lasso cleanly separates two *signal* variables from *noise* variables
- In contrast, standard least squares (far right, with $\|\hat{\beta}_\lambda^L\|_1 / \|\hat{\beta}\|_1 = 1$) only identifies the **purple** variable without discarding the noise predictors

The lasso: 5) Summary

- **Lasso formulation:**
 - Penalty term $\sum_{j=1}^p |\beta_j|$ scaled by λ
 - As λ grows, some β_j become exactly zero \implies variable selection
- **Lasso advantages:**
 - Encourages a *sparse* model for interpretability
 - Computationally efficient in practice, though slightly more complex to solve than ridge
- **Ridge vs. lasso:**
 - Lasso can set some coefficients to *exact zeros*, while ridge generally does not
 - Ridge tends to be more stable especially when predictors are highly correlated
 - Both typically tune λ via cross-validation

Wrap-up & Takeaways

Regularization:

- **Ridge:** l_2 penalty shrinks all coefficients toward zero, good if many have modest nonzero effects
- **The lasso:** l_1 penalty can set some coefficients exactly to zero (variable selection)
- **Tuning** λ typically via cross-validation for both

	Ridge	Lasso
Penalty	$\sum_{j=1}^p \beta_j^2$	$\sum_{j=1}^p \beta_j $
Effect	shrinks coefficients	shrinks and can set to zero
Variable selection	No	Yes
Often useful when	many small/moderate effects	only some predictors matter
Tuning	λ typically chosen by cross-validation	

Takeaway: Ridge stabilizes estimates; lasso can produce sparse, interpretable models.

References



Gareth James, Daniela Witten, Trevor Hastie, and Robert Tibshirani.

An Introduction to Statistical Learning: with Applications in R, volume 112 of *Springer Texts in Statistics*.

Springer, New York, NY, 2nd edition, 2021.