# Introduction to Statistical Learning

Omid Safarzadeh

January 18, 2022

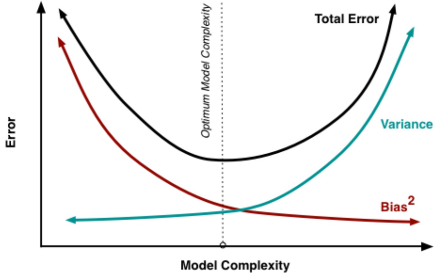
# Table of contents

# Regularization

**Properties of the least squares estimate:**

- When relation between $Y$ and $X = [X_1, ..., X_p]^T$ is almost linear, least squares estimate have low bias
- But it can have high variance. Ex: when $p \approx n$ or $p \geq n$
- Shrinking regression coefficients results in better fit

**Reducing the complexity of linear regression**



# Two method for regularization

**Ordinary leas squares:**

$$RSS(\beta) = \sum_{i=1}^{n}(y_i - \beta_0 - \sum_{j=1}^{p}\beta_j x_{ij})^2$$

**Ridge regression:**

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

$$= RSS(\beta) + \lambda\sum_{j=1}^{p}\beta_j^2$$

**Lasso:**

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

$$= RSS(\beta) + \lambda\sum_{j=1}^{p}|\beta_j|$$

# Ridge regression

$$Loss_R(\beta, \lambda) = \sum_{i=1}^{n} (y_i - \beta_0 - \sum_{j=1}^{p} \beta_j x_{ij})^2 + \underbrace{\lambda}_{\text{tuning parameter}} \underbrace{\sum_{j=1}^{p} \beta_j^2}_{penalty}$$

$$\hat{\beta}^R = \text{arg}_\beta \min Loss_R(\beta, \lambda)$$

$$\underset{\beta}{minimize} \{ \sum_{i=1}^{n} (y_i - \beta_0 - \sum_{j=1}^{p} \beta_j X_{ij})^2 \} \quad \text{subject to} \quad \sum_{j=1}^{p} \beta_j^2 \leq s$$

**What happens when**

- $\lambda \to 0$
- $\lambda \to \infty$

**How to select $\lambda$?**

# Ridge regression

## Example 2.1

**Credit card balance prediction**:

- $Y =$ card balance
- $X =$ (income, limit, rating, student, ...)
- Lines show estimated regression coefficients $\hat{\beta}^R$ by ridge regression.

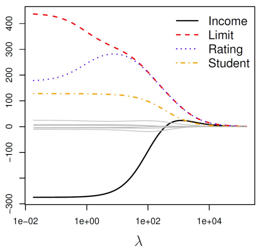



Figure: James et al., 2013

# Scale invariance

- Least squares linear regression is scale invariant
- Is ridge regression scale invariant?

Making ridge regression fair:

- Standardize the predictors:

$$\underset{ij}{\overset{\sim}{X}} = \frac{X_{ij} - \bar{X}_j}{\sqrt{\frac{1}{n}\Sigma_{i=1}^{n}(X_{ij} - \bar{X}_j)^2}}$$

where $\bar{X}_j = \frac{1}{n}\Sigma_{i=1}^{n} X_{ij}$

Properties of standardized predictors:

1. $\frac{1}{n}\Sigma_{i=1}^{n}\, X_{ij}^{\sim} = 0$ (zero mean)
2. $\frac{1}{n}\Sigma_{i=1}^{n}\, X_{ij}^{\sim}\, 2 = 1$ (unit variance)

# Bias-variance tradeoff

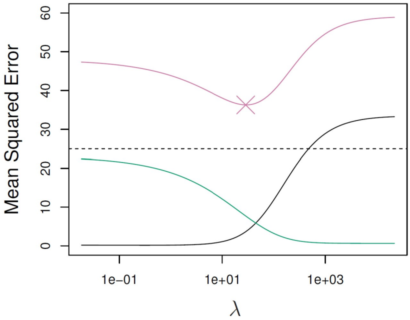



Figure: James et al., 2013

- bias: black, variance: green, MSE: red

$$MSE := \frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{f}(\mathbf{x}_i))^2$$

# How to solve ridge regression?

$$Loss_R(\beta, \lambda) = \sum_{i=1}^{n}(y_i - \beta_0 - \sum_{j=1} 6p\beta_j X_{ij})^2 + \lambda \sum_{j=1} 6p\beta_j^2$$

$$\hat{\beta}^R = \arg_\beta \min Loss_R(\beta, \lambda)$$

- Center the predictors and the response (centering makes the intercept $\hat{\beta}_0^R$)
- Standardize the predictors

# How to solve ridge regression?

**Some notation:** $y$ and $\mathbf{X}$ centered

$$\mathbf{y}_{n*1} \quad \beta_{p*1} \quad \mathbf{X}_{n*p}$$

Linear algebra and matrix calculus gives:

$$\hat{\beta}^{R} = (\mathbf{X}^T\mathbf{X} + \lambda\mathbf{I})^{-1}\mathbf{X}^T\mathbf{y}$$

Hence given a new (centered and scaled) input $\mathbf{x}$, (centered prediction) $\hat{y} = \mathbf{x}^T\hat{\beta}^R$
**Compare with least squares solution:**

$$\hat{\beta}^{RSS} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}$$

# Pros and cons of ridge regression

**Pros:**

- Reduces variance
- $\mathbf{X}^T\mathbf{X} + \lambda\mathbf{I}$, $\lambda > 0$ is invertable even when $\mathbf{X}^T\mathbf{X}$ is not invertable.

**Cons:**

- Coefficients will be small but still almost all of them will be nonzero

# Lasso

$$Loss_L(\beta, \lambda) = RSS(\beta) + \lambda \sum_{j=1}^{p} |\beta_j|$$

$$\hat{\beta}^L = \text{arg}_\beta \min Loss_L(\beta, \lambda)$$

$$\underset{\beta}{minimize}\{\sum_{i=1}^{n}(y_i - \beta_0 - \sum_{j=1}^{p} \beta_j X_{ij})^2\} \quad \text{subject to} \quad \sum_{j=1}^{p} |\beta_j| \leq s$$

- Bad news: no closed form solution like ridge regression
- Good news: no derivation

**What happens when**

- $\lambda \to 0$
- $\lambda \to \infty$

## Example 2.2

**Credit card balance prediction**:

- $Y =$ card balance
- $X =$ (income, limit, rating, student, ...)
- Lines show estimated regression coefficients $\hat{\beta}^L$ by lasso.
- Lasso performs variable selection (results in a sparse model)

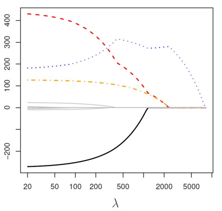



Figure: James et al., 2013

# Geometric interpretation

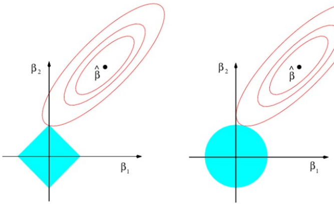


Figure: James et al., 2013

- Red lines: error contours for RSS (same error for all $\beta$ values on the same contour)
- $\hat{\beta}$: least square solution
- Blue areas: region for which $|\beta_1| + |\beta_2| \leq S$ or $\beta_1^2 + \beta_2^2 \leq S$

# References

James, G., Witten, D., Hastie, T., & Tibshirani, R. (2013). *An introduction to statistical learning: With applications in r*. Springer New York. https://books.google.fr/books?id=qcI%5C_AAAAQBAJ