Ridge Regression

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September 11, 2025

Outline

Motivation: The Problem of Overfitting

The Problem: Overfitting in Linear Regression

Important: Overfitting Challenge

As model complexity increases (higher polynomial degree), we often observe:

- Training error decreases
- Test error increases
- Model coefficients become very large

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Key Points: Key Insight

Large coefficient magnitudes often indicate overfitting!

The Problem: Overfitting in Linear Regression

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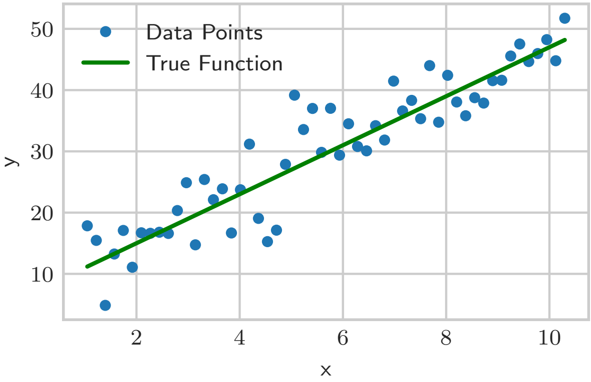
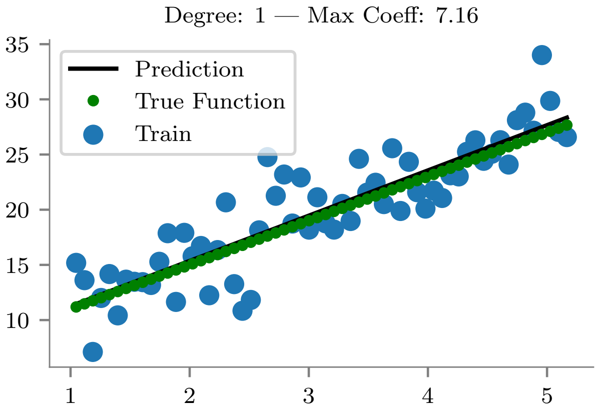
In polynomial $f(x) = c_0 + c_1 x + c_2 x^2 + \cdots + c_d x^d$, watch $\max |c_i|$

Demonstration: Polynomial Degree vs Overfitting



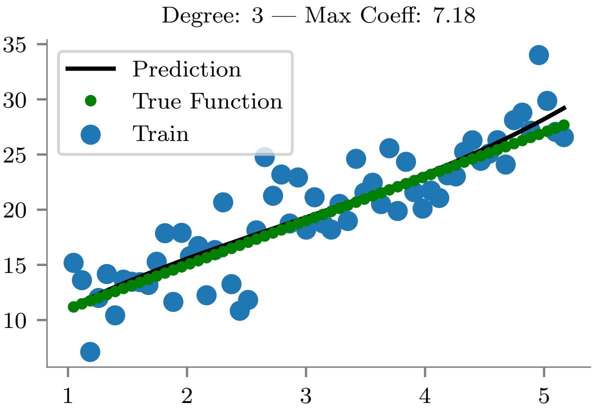
Base Data Set

Demonstration: Polynomial Degree vs Overfitting



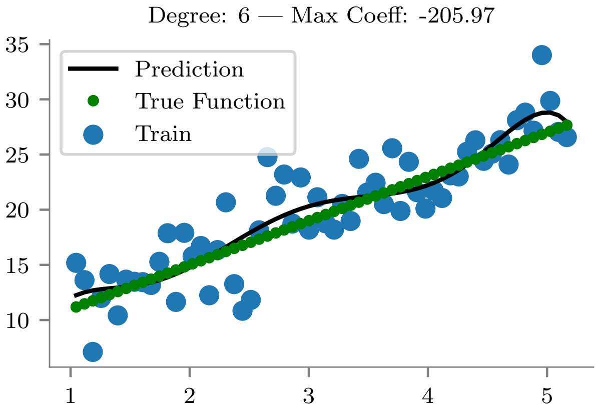
Fit with Degree 1 - Underfitting

Demonstration: Polynomial Degree vs Overfitting



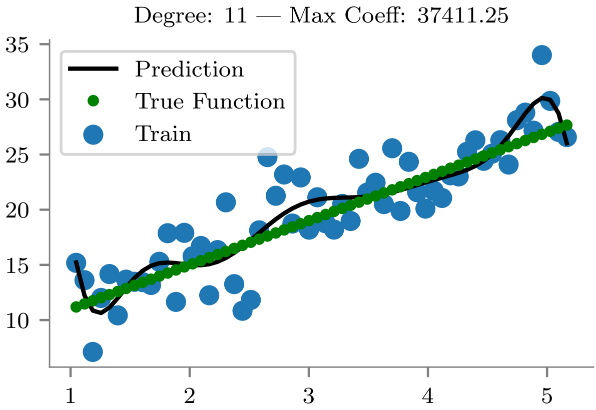
Fit with Degree 3 - Good Fit

Demonstration: Polynomial Degree vs Overfitting



Fit with Degree 6 - Starting to Overfit

Demonstration: Polynomial Degree vs Overfitting

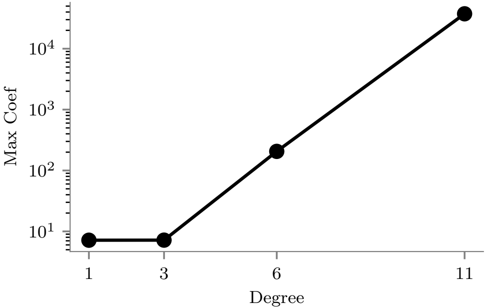


Fit with Degree 11 - Severe Overfitting

Coefficient Explosion with Overfitting

Key Points: Key Observation

As polynomial degree increases → coefficients grow exponentially!



Coefficient Magnitudes vs Polynomial Degree

The Central Question

Important: Critical Question

How can we control coefficient magnitudes to prevent overfitting?

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How can we control coefficient magnitudes to prevent overfitting?

Key Points: Answer Preview

Ridge regression adds a penalty term to shrink coefficients!

Pop Quiz 1

Answer this!

Which statement about overfitting is TRUE?

A) Higher polynomial degree always improves generalization
B) Large coefficients indicate good model fit
C) Overfitting occurs when training error $>>$ test error
D) Overfitting occurs when training error $<<$ test error

Answer: Pop Quiz 1

Answer this!

D) Overfitting occurs when training error $<<$ test error

Explanation:

- Training error becomes very small (model memorizes training data)
- Test error remains large (model fails to generalize)
- Large gap indicates overfitting

Ridge Regression Formulation

Solution: Regularization

Theorem: Ridge Regression Approach

Add a penalty term to control coefficient magnitudes:

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Theorem: Ridge Regression Approach

Add a penalty term to control coefficient magnitudes:

Definition: Constrained Formulation

$$\begin{aligned} \min_{\boldsymbol{\theta}} \quad & (\mathbf{y} - \mathbf{X}\boldsymbol{\theta})^T (\mathbf{y} - \mathbf{X}\boldsymbol{\theta}) \\ \text{subject to} \quad & \boldsymbol{\theta}^T \boldsymbol{\theta} \leq S \end{aligned}$$

where $S > 0$ controls the size of the coefficient vector.

Lagrangian Formulation

Theorem: Equivalence Theorem

The constrained problem is equivalent to the unconstrained:

$$\min_{\boldsymbol{\theta}} \quad (\mathbf{y} - \mathbf{X}\boldsymbol{\theta})^T (\mathbf{y} - \mathbf{X}\boldsymbol{\theta}) + \lambda \boldsymbol{\theta}^T \boldsymbol{\theta}$$

where $\lambda \geq 0$ is the regularization parameter.

Lagrangian Formulation

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where $\lambda \geq 0$ is the regularization parameter.

Key Points: Key Insight

This transforms a constrained optimization into an unconstrained one with a penalty term.

Understanding the Ridge Penalty

$$J(\boldsymbol{\theta}) = \underbrace{(\mathbf{y} - \mathbf{X}\boldsymbol{\theta})^T(\mathbf{y} - \mathbf{X}\boldsymbol{\theta})}_{\text{Fit to data (MSE)}} + \underbrace{\lambda\boldsymbol{\theta}^T\boldsymbol{\theta}}_{\text{Penalty term}} \quad (1)$$

$$= \mathsf{MSE}(\boldsymbol{\theta}) + \lambda\|\boldsymbol{\theta}\|_2^2 \quad (2)$$

Understanding the Ridge Penalty

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$$= \mathsf{MSE}(\boldsymbol{\theta}) + \lambda\|\boldsymbol{\theta}\|_2^2 \tag{2}$$

Key Points: Key Components

- **Data fitting term**: Ensures good fit to training data
- **Regularization term**: L_2 penalty shrinks coefficients toward zero
- λ: Controls trade-off between fitting vs. regularization

Effect of Regularization Parameter λ

Key Points: Parameter Effects

- $\lambda = 0$: No regularization (standard linear regression)
- λ small: Light regularization (slight shrinkage)
- λ large: Heavy regularization (strong shrinkage)
- $\lambda \to \infty$: Extreme regularization (coefficients $\to 0$)

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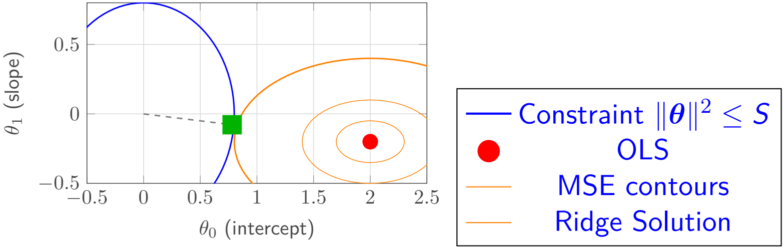
Important: Key Trade-off

Higher λ = more regularization = more bias, less variance

Geometric Interpretation



Ridge solution where MSE contours touch constraint region

Key Points: Key Insight

Ridge finds the minimum MSE point within the constraint $\|\boldsymbol{\theta}\|_2^2 \leq S$

Mathematical Derivation

Mathematical Derivation: Step 1

Step 1: Set up the Lagrangian

For the constrained optimization problem:

$$\min_{\boldsymbol{\theta}} \quad (\mathbf{y} - \mathbf{X}\boldsymbol{\theta})^T (\mathbf{y} - \mathbf{X}\boldsymbol{\theta})$$
$$\text{s.t.} \quad \boldsymbol{\theta}^T\boldsymbol{\theta} \leq S$$

The Lagrangian is:

$$L(\boldsymbol{\theta}, \lambda) = (\mathbf{y} - \mathbf{X}\boldsymbol{\theta})^T (\mathbf{y} - \mathbf{X}\boldsymbol{\theta}) + \lambda \left(\boldsymbol{\theta}^T\boldsymbol{\theta} - S\right)$$

where $\lambda \geq 0$ is the Lagrange multiplier.

Mathematical Derivation: Step 2

Step 2: Apply KKT Conditions

For optimality, we need:

$$\frac{\partial L}{\partial \boldsymbol{\theta}} = 0 \quad \text{(stationarity)} \tag{3}$$

$$\lambda \geq 0 \quad \text{(dual feasibility)} \tag{4}$$

$$\boldsymbol{\theta}^T\boldsymbol{\theta} - S \leq 0 \quad \text{(primal feasibility)} \tag{5}$$

$$\lambda(\boldsymbol{\theta}^T\boldsymbol{\theta} - S) = 0 \quad \text{(complementary slackness)} \tag{6}$$

Mathematical Derivation: Step 2

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$$\lambda(\boldsymbol{\theta}^T\boldsymbol{\theta} - S) = 0 \quad \text{(complementary slackness)} \tag{6}$$

Key Points: Two Cases

- **Case 1:** $\lambda = 0 \Rightarrow$ No constraint active (standard OLS)
- **Case 2:** $\lambda > 0 \Rightarrow \boldsymbol{\theta}^T\boldsymbol{\theta} = S$ (constraint is tight)

Mathematical Derivation: Step 3

Step 3: Compute the Gradient

Taking the derivative of the Lagrangian with respect to $\boldsymbol{\theta}$:

$$\frac{\partial L}{\partial \boldsymbol{\theta}} = \frac{\partial}{\partial \boldsymbol{\theta}} \left[(\mathbf{y} - \mathbf{X}\boldsymbol{\theta})^T (\mathbf{y} - \mathbf{X}\boldsymbol{\theta}) + \lambda \boldsymbol{\theta}^T \boldsymbol{\theta} \right] \tag{7}$$

$$= \frac{\partial}{\partial \boldsymbol{\theta}} \left[\mathbf{y}^T \mathbf{y} - 2\mathbf{y}^T \mathbf{X}\boldsymbol{\theta} + \boldsymbol{\theta}^T \mathbf{X}^T \mathbf{X}\boldsymbol{\theta} + \lambda \boldsymbol{\theta}^T \boldsymbol{\theta} \right] \tag{8}$$

$$= -2\mathbf{X}^T \mathbf{y} + 2\mathbf{X}^T \mathbf{X}\boldsymbol{\theta} + 2\lambda \boldsymbol{\theta} \tag{9}$$

Mathematical Derivation: Step 4

Step 4: Set Gradient to Zero

Setting $\frac{\partial L}{\partial \boldsymbol{\theta}} = 0$:

$$-2\mathbf{X}^T\mathbf{y} + 2\mathbf{X}^T\mathbf{X}\boldsymbol{\theta} + 2\lambda\boldsymbol{\theta} = 0 \tag{10}$$

$$-\mathbf{X}^T\mathbf{y} + (\mathbf{X}^T\mathbf{X} + \lambda\mathbf{I})\boldsymbol{\theta} = 0 \tag{11}$$

$$(\mathbf{X}^T\mathbf{X} + \lambda\mathbf{I})\boldsymbol{\theta} = \mathbf{X}^T\mathbf{y} \tag{12}$$

Mathematical Derivation: Step 4

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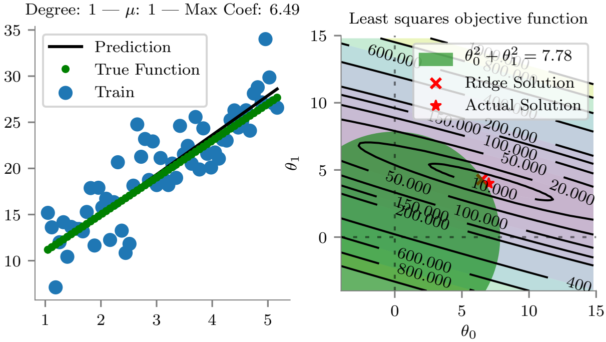
$$(\mathbf{X}^T\mathbf{X} + \lambda\mathbf{I})\boldsymbol{\theta} = \mathbf{X}^T\mathbf{y} \tag{12}$$

Theorem: Ridge Regression Solution

$$\hat{\boldsymbol{\theta}}_{\text{ridge}} = (\mathbf{X}^T\mathbf{X} + \lambda\mathbf{I})^{-1}\mathbf{X}^T\mathbf{y}$$

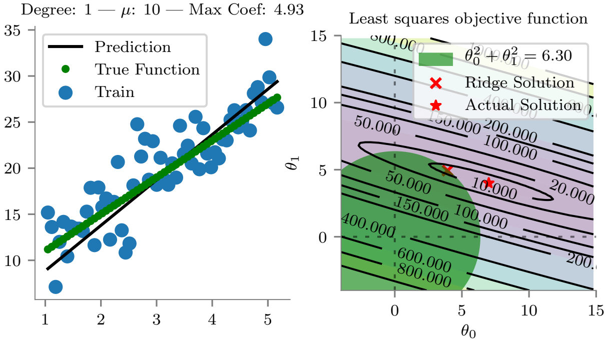
Compare with OLS: $\hat{\boldsymbol{\theta}}_{\text{OLS}} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}$

Effect of Regularization Parameter λ



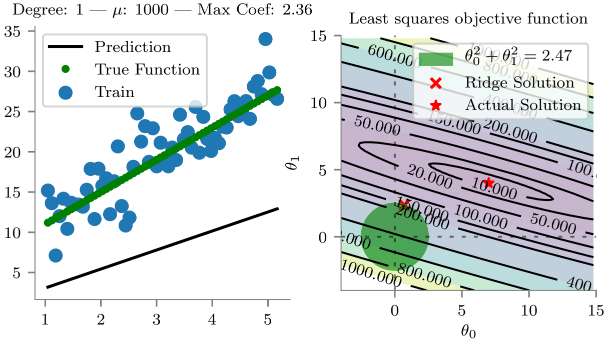
$\lambda = 1$ - Mild Regularization

Effect of Regularization Parameter λ



$\lambda = 10$ - Moderate Regularization

Effect of Regularization Parameter λ



$\lambda = 1000$ - Heavy Regularization

Pop Quiz 2

Answer this!

What happens to the Ridge regression solution as $\lambda \to \infty$?

A) Coefficients approach the OLS solution
B) Coefficients approach zero
C) Solution becomes undefined
D) Training error becomes zero

Answer: Pop Quiz 2

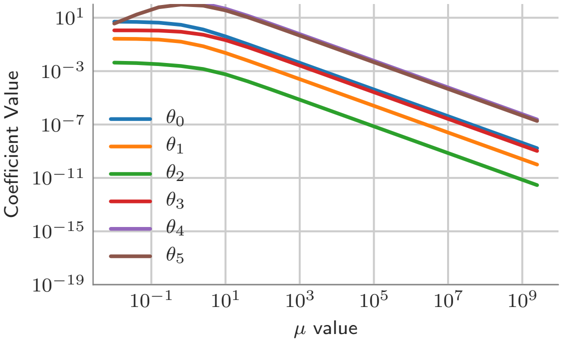
Answer this!

B) Coefficients approach zero

As $\lambda \to \infty$, the penalty term dominates:

$$\hat{\boldsymbol{\theta}}_{\text{ridge}} = (\mathbf{X}^T\mathbf{X} + \lambda\mathbf{I})^{-1}\mathbf{X}^T\mathbf{y} \approx \lambda^{-1}\mathbf{I}\mathbf{X}^T\mathbf{y} \to \mathbf{0}$$

Coefficient Shrinkage: Visual Evidence

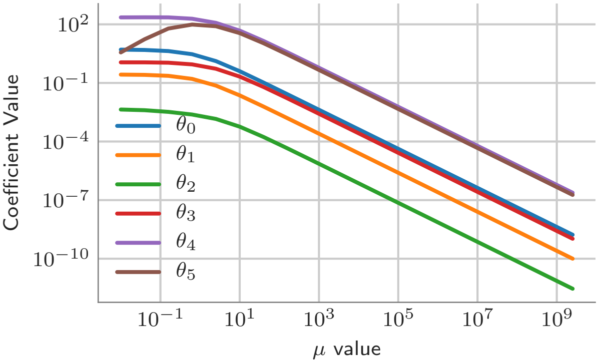


Coefficient Magnitudes vs λ (Real Estate Dataset)

Important: Important Question

Do coefficients ever become exactly zero?

Ridge Coefficient Behavior



Ridge Coefficients Shrink but Never Reach Zero

Ridge vs. Lasso: Key Difference

Key Points: Coefficient Behavior Comparison

- **Ridge (L_2):** Coefficients shrink toward zero but remain non-zero
- **Lasso (L_1):** Coefficients can become exactly zero (feature selection)

Ridge vs. Lasso: Key Difference

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Important: Important Insight

Ridge provides shrinkage, Lasso provides selection!

Ridge Regression Solution

Theorem: Ridge Solution Formula

$$\hat{\boldsymbol{\theta}}_{\text{ridge}} = (\mathbf{X}^T\mathbf{X} + \lambda\mathbf{I})^{-1}\mathbf{X}^T\mathbf{y}$$

Key Property 1: Always Invertible

Theorem: Invertibility Guarantee

$(\mathbf{X}^T\mathbf{X} + \lambda\mathbf{I})$ is always positive definite for $\lambda > 0$

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Theorem: Invertibility Guarantee

$(\mathbf{X}^T\mathbf{X} + \lambda\mathbf{I})$ is always positive definite for $\lambda > 0$

Key Points: Why This Matters

- No singularity issues (unlike OLS)
- Always has unique solution
- Handles multi-collinearity gracefully

Key Property 2: Coefficient Shrinkage

Theorem: Shrinkage Effect

Ridge regression shrinks coefficients toward zero (but not exactly zero)

Key Property 2: Coefficient Shrinkage

Theorem: Shrinkage Effect

Ridge regression shrinks coefficients toward zero (but not exactly zero)

Key Points: Shrinkage Benefits

- Reduces overfitting
- Stabilizes coefficient estimates
- Improves generalization

Key Property 3: Bias-Variance Trade-off

Theorem: Trade-off Effect

Ridge regression increases bias but reduces variance

Key Property 3: Bias-Variance Trade-off

Theorem: Trade-off Effect

Ridge regression increases bias but reduces variance

Key Points: Net Effect

- Total error often decreases
- Better generalization to new data
- Controlled by λ parameter

Hyperparameter Selection

Choosing the Regularization Parameter λ

Important: Hyperparameter Selection

How do we choose the optimal value of λ?

Choosing the Regularization Parameter λ

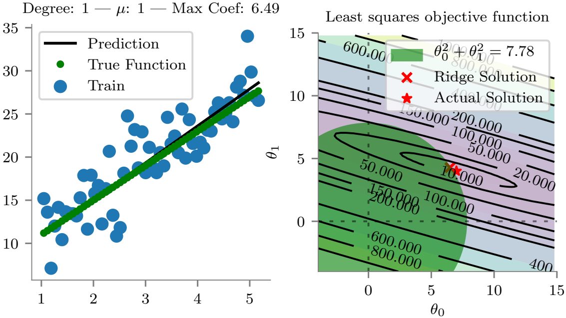
Important: Hyperparameter Selection

How do we choose the optimal value of λ?

Theorem: Cross-Validation Approach

1. Split data into training and validation sets (k-fold CV)
2. For each candidate λ value:
   - Train ridge model on training data
   - Compute validation error
3. Select λ that minimizes validation error
4. Retrain on full dataset with chosen λ

Cross-Validation for Ridge Regression



Cross-validation curve showing optimal λ

Key Points: CV Pattern

Small λ: Overfitting   Large λ: Underfitting   Optimal λ: Best trade-off

Bias-Variance Trade-off in Ridge Regression

Theorem: Bias-Variance Decomposition

$$\text{Total Error} = \text{Bias}^2 + \text{Variance} + \text{Irreducible Error}$$

Bias-Variance Trade-off in Ridge Regression

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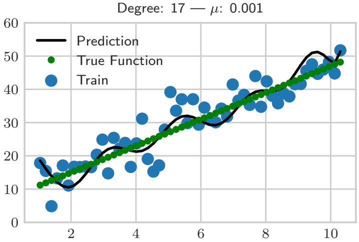
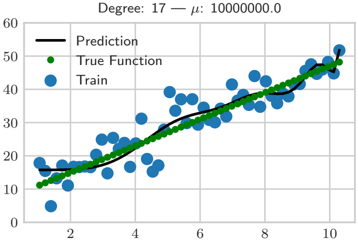
Key Points: Ridge Effect

Regularization increases bias but reduces variance, often leading to lower total error.

Small vs Large Regularization





Small λ ($\lambda \to 0$):

- Low bias
- High variance
- Risk of overfitting

Large λ ($\lambda \to \infty$):

- High bias
- Low variance
- Risk of underfitting

Pop Quiz 3

Answer this!

In ridge regression, as we increase λ, what happens to model bias and variance?

A) Both bias and variance increase
B) Both bias and variance decrease
C) Bias increases, variance decreases
D) Bias decreases, variance increases

Answer: Pop Quiz 3

Answer this!

C) Bias increases, variance decreases

Explanation:

- Increasing λ constrains coefficients more severely
- Model becomes simpler (higher bias)
- Less sensitive to training data variations (lower variance)
- This is the fundamental bias-variance trade-off!

Examples and Applications

Worked Example: Setup

Example: Ridge Regression Example

Given the following simple dataset, compare OLS vs. Ridge regression with $\lambda = 2$:

Data: $(x_1, y_1) = (1, 1)$, $(x_2, y_2) = (2, 2)$, $(x_3, y_3) = (3, 3)$, $(x_4, y_4) = (4, 0)$
Model: $y = \theta_0 + \theta_1 x$

Worked Example: Setup

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Step 1: Set up matrices

$$\mathbf{X} = \begin{bmatrix} 1 & 1 \\ 1 & 2 \\ 1 & 3 \\ 1 & 4 \end{bmatrix}, \quad \mathbf{y} = \begin{bmatrix} 1 \\ 2 \\ 3 \\ 0 \end{bmatrix}, \quad \boldsymbol{\theta} = \begin{bmatrix} \theta_0 \\ \theta_1 \end{bmatrix}$$

Worked Example: OLS Setup

Step 2: Ordinary Least Squares

$$\hat{\boldsymbol{\theta}}_{\mathsf{OLS}} = (\mathbf{X}^T\mathbf{X})^{-1}(\mathbf{X}^T\mathbf{y})$$

Worked Example: OLS Setup

Step 2: Ordinary Least Squares

$$\hat{\boldsymbol{\theta}}_{\mathsf{OLS}} = (\mathbf{X}^T\mathbf{X})^{-1}(\mathbf{X}^T\mathbf{y})$$

Step 3: Compute matrix products

$$\mathbf{X}^T\mathbf{X} = \begin{bmatrix} 4 & 10 \\ 10 & 30 \end{bmatrix}$$

$$\mathbf{X}^T\mathbf{y} = \begin{bmatrix} 6 \\ 14 \end{bmatrix}$$

Worked Example: Matrix Inverse

Step 4: Compute the inverse

For $\mathbf{X}^T\mathbf{X} = \begin{bmatrix} 4 & 10 \\ 10 & 30 \end{bmatrix}$:

$\det(\mathbf{X}^T\mathbf{X}) = 4 \cdot 30 - 10 \cdot 10 = 20$

$$(\mathbf{X}^T\mathbf{X})^{-1} = \frac{1}{20}\begin{bmatrix} 30 & -10 \\ -10 & 4 \end{bmatrix}$$

Worked Example: OLS Calculation

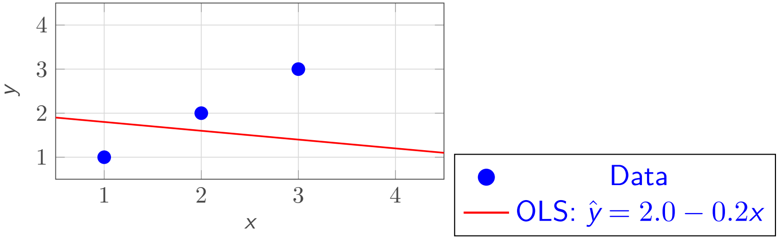
Step 5: Final matrix multiplication

$$
\begin{aligned}
\hat{\boldsymbol{\theta}}_{\mathsf{OLS}} &= (\mathbf{X}^T\mathbf{X})^{-1}(\mathbf{X}^T\mathbf{y}) \\
&= \frac{1}{20}\begin{bmatrix} 30 & -10 \\ -10 & 4 \end{bmatrix}\begin{bmatrix} 6 \\ 14 \end{bmatrix} \\
&= \frac{1}{20}\begin{bmatrix} 180 - 140 \\ -60 + 56 \end{bmatrix} = \frac{1}{20}\begin{bmatrix} 40 \\ -4 \end{bmatrix} = \begin{bmatrix} 2.0 \\ -0.2 \end{bmatrix}
\end{aligned}
$$

OLS Final Result

Theorem: OLS Result

$\hat{y} = 2.0 - 0.2x$ (No regularization)



OLS fit to our example data

Worked Example: Ridge Setup

Step 5: Ridge regression with $\lambda = 2$

$$\hat{\boldsymbol{\theta}}_{\text{ridge}} = (\mathbf{X}^T\mathbf{X} + \lambda\mathbf{I})^{-1}(\mathbf{X}^T\mathbf{y})$$

Worked Example: Ridge Setup

Step 5: Ridge regression with $\lambda = 2$

$$\hat{\boldsymbol{\theta}}_{\text{ridge}} = (\mathbf{X}^T\mathbf{X} + \lambda\mathbf{I})^{-1}(\mathbf{X}^T\mathbf{y})$$

Step 6: Add regularization term

$$\mathbf{X}^T\mathbf{X} + \lambda\mathbf{I} = \begin{bmatrix} 4 & 10 \\ 10 & 30 \end{bmatrix} + 2\mathbf{I}$$
$$= \begin{bmatrix} 6 & 10 \\ 10 & 32 \end{bmatrix}$$

Worked Example: Matrix Inverse

Step 7: Compute inverse

$\det(\mathbf{X}^T\mathbf{X} + \lambda\mathbf{I}) = 6 \cdot 32 - 10 \cdot 10 = 92$

$$(\mathbf{X}^T\mathbf{X} + \lambda\mathbf{I})^{-1} = \frac{1}{92}\begin{bmatrix} 32 & -10 \\ -10 & 6 \end{bmatrix}$$

Worked Example: Ridge Calculation

Step 8: Matrix multiplication

$$\hat{\boldsymbol{\theta}}_{\text{ridge}} = (\mathbf{X}^T\mathbf{X} + \lambda\mathbf{I})^{-1}(\mathbf{X}^T\mathbf{y})$$
$$= \frac{1}{92}\begin{bmatrix} 32 & -10 \\ -10 & 6 \end{bmatrix}\begin{bmatrix} 6 \\ 14 \end{bmatrix}$$

Worked Example: Ridge Calculation

Step 8: Matrix multiplication

$$\begin{aligned}\hat{\boldsymbol{\theta}}_{\text{ridge}} &= (\mathbf{X}^T\mathbf{X} + \lambda\mathbf{I})^{-1}(\mathbf{X}^T\mathbf{y}) \\ &= \frac{1}{92}\begin{bmatrix} 32 & -10 \\ -10 & 6 \end{bmatrix}\begin{bmatrix} 6 \\ 14 \end{bmatrix}\end{aligned}$$

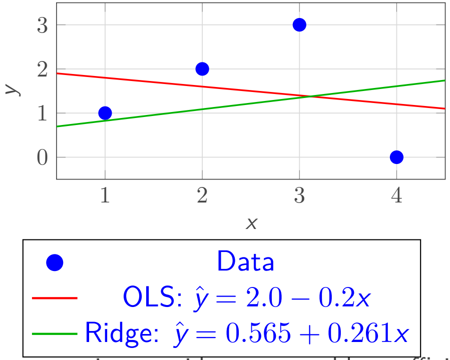
Step 9: Compute products

$$\begin{aligned}&= \frac{1}{92}\begin{bmatrix} 32 \cdot 6 + (-10) \cdot 14 \\ (-10) \cdot 6 + 6 \cdot 14 \end{bmatrix} \\ &= \frac{1}{92}\begin{bmatrix} 192 - 140 \\ -60 + 84 \end{bmatrix} = \frac{1}{92}\begin{bmatrix} 52 \\ 24 \end{bmatrix} = \begin{bmatrix} 0.565 \\ 0.261 \end{bmatrix}\end{aligned}$$

Ridge vs OLS: Final Comparison

Theorem: Ridge Result

$\hat{y} = 0.565 + 0.261x$ (With $\lambda = 2$)



Ridge regression provides more stable coefficients

Coefficient Magnitude Comparison

Theorem: OLS vs Ridge Solutions

- **OLS**: $\theta_{OLS} = \begin{bmatrix} 2.0 \\ -0.2 \end{bmatrix}$
- **Ridge**: $\theta_{Ridge} = \begin{bmatrix} 0.565 \\ 0.261 \end{bmatrix}$

Coefficient Magnitude Comparison

Theorem: OLS vs Ridge Solutions

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- **Ridge**: $\theta_{Ridge} = \begin{bmatrix} 0.565 \\ 0.261 \end{bmatrix}$

L2 Norm Calculation

$$\|\boldsymbol{\theta}_{OLS}\|_2^2 = (2.0)^2 + (-0.2)^2 = 4.04 \tag{13}$$

$$\|\boldsymbol{\theta}_{Ridge}\|_2^2 = (0.565)^2 + (0.261)^2 = 0.387 \tag{14}$$

Ridge Coefficient Shrinkage Result

Important: Key Result

Ridge regression achieved a **90.4% reduction** in coefficient magnitude!

$$\frac{0.387}{4.04} = 0.096 \quad \text{(Ridge is 9.6\% of OLS magnitude)}$$

Key Points: Shrinkage Effect

Ridge systematically produces smaller coefficient magnitudes while maintaining prediction accuracy.

Multi-collinearity

$(\mathbf{X}^T\mathbf{X})^{-1}$ is not computable when $|\mathbf{X}^T\mathbf{X}| = 0$.
This was a drawback of using linear regression

$$\mathbf{X} = \begin{bmatrix} 1 & 1 & 2 \\ 1 & 2 & 4 \\ 1 & 3 & 6 \end{bmatrix}$$

The matrix $\mathbf{X}$ is not full rank.

Ridge Solution to Multi-collinearity

Key Points: Ridge Advantage

With ridge regression, we invert $\mathbf{X}^T\mathbf{X} + \mu\mathbf{I}$ instead of $\mathbf{X}^T\mathbf{X}$

$$\mathbf{X}^T\mathbf{X} + \mu\mathbf{I} = \begin{bmatrix} 3+\mu & 6 & 12 \\ 6 & 14+\mu & 28 \\ 12 & 28 & 56+\mu \end{bmatrix}$$

Why Ridge Fixes Singularity

Theorem: Key Result

The matrix $\mathbf{X}^T\mathbf{X} + \mu\mathbf{I}$ is always full rank for $\mu > 0$

Why Ridge Fixes Singularity

Theorem: Key Result

The matrix $\mathbf{X}^T\mathbf{X} + \mu\mathbf{I}$ is always full rank for $\mu > 0$

Important: Another Interpretation

Ridge regression = regularization = fixing singularity issues!

Why Ridge Fixes Singularity

Theorem: Key Result

The matrix $\mathbf{X}^T\mathbf{X} + \mu\mathbf{I}$ is always full rank for $\mu > 0$

Important: Another Interpretation

Ridge regression = regularization = fixing singularity issues!

Key Points: Summary

Ridge regression elegantly handles multi-collinearity problems!

The Intercept Penalty Problem

Important: Critical Issue

Should we penalize the intercept θ_0 in ridge regression?

Key Points: Two Approaches

- **Standard Ridge**: $\hat{\boldsymbol{\theta}} = (\mathbf{X}^T\mathbf{X} + \lambda\mathbf{I})^{-1}\mathbf{X}^T\mathbf{y}$ (penalizes intercept)
- **No-intercept penalty**: $\hat{\boldsymbol{\theta}} = (\mathbf{X}^T\mathbf{X} + \lambda\mathbf{I}^*)^{-1}\mathbf{X}^T\mathbf{y}$

Modified Identity Matrix $\mathbf{I}^*$

Definition of $\mathbf{I}^*$

$$\mathbf{I}^* = \begin{bmatrix} \color{red}{0} & 0 & 0 & \dots & 0 \\ 0 & 1 & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \dots & 1 \end{bmatrix}$$

Important: Key Point

Zero in first position means NO penalty on intercept θ_0

Demonstration: Two Simple Functions

Example: Setup

Compare two functions with different intercepts:

- **Function 1**: $f_1(x) = x$ (small intercept)
- **Function 2**: $f_2(x) = x + 100$ (large intercept)

Data Generation and Test Question

Data Generation

For each function, generate data at $x = 1, 2$:

$$\text{Function 1:} \quad (1, 1), (2, 2) \tag{15}$$

$$\text{Function 2:} \quad (1, 101), (2, 102) \tag{16}$$

Data Generation and Test Question

Data Generation

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$$\text{Function 1:} \quad (1, 1), (2, 2) \tag{15}$$

$$\text{Function 2:} \quad (1, 101), (2, 102) \tag{16}$$

Important: Test Question

How well can we predict y at $x = 0$ using ridge regression with $\lambda = 100$?

Function 1: Setup and Data

Theorem: Function 1: $y = x$

True value at $x = 0$: $y = 0$

Data matrices

$$\mathbf{X} = \begin{bmatrix} 1 & 1 \\ 1 & 2 \end{bmatrix}, \quad \mathbf{y} = \begin{bmatrix} 1 \\ 2 \end{bmatrix}$$

Function 1: Matrix Computations

Matrix computations

$$\mathbf{X}^T\mathbf{X} = \begin{bmatrix} 2 & 3 \\ 3 & 5 \end{bmatrix} \tag{17}$$

$$\mathbf{X}^T\mathbf{y} = \begin{bmatrix} 3 \\ 5 \end{bmatrix} \tag{18}$$

Function 1: Ridge with Standard $\mathbf{I}$

Standard Ridge: $\mathbf{I}$ penalties both θ_0 and θ_1

$$\mathbf{X}^T\mathbf{X} + \lambda\mathbf{I} = \begin{bmatrix} 2 & 3 \\ 3 & 5 \end{bmatrix} + 100 \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} = \begin{bmatrix} 102 & 3 \\ 3 & 105 \end{bmatrix}$$

Function 1: Standard Ridge Solution

Solution

$$\hat{\boldsymbol{\theta}} = \begin{bmatrix} 102 & 3 \\ 3 & 105 \end{bmatrix}^{-1} \begin{bmatrix} 3 \\ 5 \end{bmatrix} \tag{19}$$

$$\approx \begin{bmatrix} 0.029 \\ 0.047 \end{bmatrix} \tag{20}$$

Function 1: Standard Ridge Solution

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$$\hat{\boldsymbol{\theta}} = \begin{bmatrix} 102 & 3 \\ 3 & 105 \end{bmatrix}^{-1} \begin{bmatrix} 3 \\ 5 \end{bmatrix} \tag{19}$$

$$\approx \begin{bmatrix} 0.029 \\ 0.047 \end{bmatrix} \tag{20}$$

Theorem: Prediction at $x = 0$

$\hat{y}(0) = 0.029 + 0.047 \times 0 = 0.029$

Error: $|0.029 - 0| = 0.029$

Function 1: Ridge with Modified $\mathbf{I}^*$

Modified Ridge: $\mathbf{I}^*$ does NOT penalize θ_0

$$\mathbf{X}^T\mathbf{X} + \lambda\mathbf{I}^* = \begin{bmatrix} 2 & 3 \\ 3 & 5 \end{bmatrix} + 100 \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix} = \begin{bmatrix} 2 & 3 \\ 3 & 105 \end{bmatrix}$$

Function 1: Modified Ridge Solution

Solution

$$\hat{\boldsymbol{\theta}} = \begin{bmatrix} 2 & 3 \\ 3 & 105 \end{bmatrix}^{-1} \begin{bmatrix} 3 \\ 5 \end{bmatrix} \tag{21}$$

$$\approx \begin{bmatrix} -0.001 \\ 0.048 \end{bmatrix} \tag{22}$$

Function 1: Modified Ridge Solution

Solution

$$\hat{\boldsymbol{\theta}} = \begin{bmatrix} 2 & 3 \\ 3 & 105 \end{bmatrix}^{-1} \begin{bmatrix} 3 \\ 5 \end{bmatrix} \tag{21}$$

$$\approx \begin{bmatrix} -0.001 \\ 0.048 \end{bmatrix} \tag{22}$$

Theorem: Prediction at $x = 0$

$\hat{y}(0) = -0.001 + 0.048 \times 0 = -0.001$

Error: $|-0.001 - 0| = 0.001$

Function 2: Setup and Data

Theorem: Function 2: $y = x + 100$

True value at $x = 0$: $y = 100$

Data matrices

$$\mathbf{X} = \begin{bmatrix} 1 & 1 \\ 1 & 2 \end{bmatrix}, \quad \mathbf{y} = \begin{bmatrix} 101 \\ 102 \end{bmatrix}$$

Function 2: Matrix Computations

Matrix computations

$$\mathbf{X}^T\mathbf{X} = \begin{bmatrix} 2 & 3 \\ 3 & 5 \end{bmatrix} \quad \text{(same as Function 1)} \tag{23}$$

$$\mathbf{X}^T\mathbf{y} = \begin{bmatrix} 203 \\ 305 \end{bmatrix} \tag{24}$$

Function 2: Ridge with Standard $\mathbf{I}$

Standard Ridge: penalizes large intercept heavily

$$\mathbf{X}^T\mathbf{X} + \lambda\mathbf{I} = \begin{bmatrix} 102 & 3 \\ 3 & 105 \end{bmatrix} \quad \text{(same matrix)}$$

Function 2: Standard Ridge Solution

Solution

$$\hat{\boldsymbol{\theta}} = \begin{bmatrix} 102 & 3 \\ 3 & 105 \end{bmatrix}^{-1} \begin{bmatrix} 203 \\ 305 \end{bmatrix} \tag{25}$$

$$\approx \begin{bmatrix} 1.98 \\ 2.89 \end{bmatrix} \tag{26}$$

Function 2: Standard Ridge Solution

Solution

$$\hat{\boldsymbol{\theta}} = \begin{bmatrix} 102 & 3 \\ 3 & 105 \end{bmatrix}^{-1} \begin{bmatrix} 203 \\ 305 \end{bmatrix} \tag{25}$$

$$\approx \begin{bmatrix} 1.98 \\ 2.89 \end{bmatrix} \tag{26}$$

Theorem: Prediction at $x = 0$

$\hat{y}(0) = 1.98 + 2.89 \times 0 = 1.98$
Error: $|1.98 - 100| = 98.02$ **(TERRIBLE!)**

Function 2: Ridge with Modified $\mathbf{I}^*$

Modified Ridge: does NOT penalize intercept

$$\mathbf{X}^T\mathbf{X} + \lambda\mathbf{I}^* = \begin{bmatrix} 2 & 3 \\ 3 & 105 \end{bmatrix} \quad \text{(same as Function 1)}$$

Function 2: Modified Ridge Solution

Solution

$$\hat{\boldsymbol{\theta}} = \begin{bmatrix} 2 & 3 \\ 3 & 105 \end{bmatrix}^{-1} \begin{bmatrix} 203 \\ 305 \end{bmatrix} \tag{27}$$

$$\approx \begin{bmatrix} 99.91 \\ 1.05 \end{bmatrix} \tag{28}$$

Function 2: Modified Ridge Solution

Solution

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$$\approx \begin{bmatrix} 99.91 \\ 1.05 \end{bmatrix} \tag{28}$$

Theorem: Prediction at $x = 0$

$\hat{y}(0) = 99.91 + 1.05 \times 0 = 99.91$

Error: $|99.91 - 100| = 0.09$ **(EXCELLENT!)**

Results Summary

Function	**True** $y(0)$	**Standard** $\mathbf{I}$	**Modified** $\mathbf{I}^*$
$f_1 : y = x$	0	0.029	-0.001
Error		0.029	0.001
$f_2 : y = x + 100$	100	1.98	99.91
Error		98.02	0.09

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Important: Key Insight

Penalizing the intercept creates **biased predictions** when data has non-zero mean!

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Important: Key Insight

Penalizing the intercept creates **biased predictions** when data has non-zero mean!

Key Points: Solution

Use $\mathbf{I}^*$ to avoid penalizing the intercept, or normalize data first.

Alternative: Data Normalization

Theorem: Normalization Approach

Center the data to have zero mean, then use standard $\mathbf{I}$

Function 2 with normalization

Original: $(1, 101), (2, 102)$
Mean: $\bar{x} = 1.5, \bar{y} = 101.5$
Centered: $(-0.5, -0.5), (0.5, 0.5)$

Benefits of Data Normalization

Key Points: Why Normalize?

- Can use standard $\mathbf{I}$ without bias
- Intercept becomes meaningful (deviation from mean)
- All features on similar scale
- More numerically stable

Important: Best Practice

Always normalize data OR use $\mathbf{I}^*$ for unbiased ridge regression!

Implementation Details

Ridge Regression via Gradient Descent

Theorem: Gradient Descent Update Rule

Standard gradient descent step for ridge regression:

$$\boldsymbol{\theta}^{(t+1)} = \boldsymbol{\theta}^{(t)} - \alpha \nabla J(\boldsymbol{\theta}^{(t)})$$

Ridge Regression via Gradient Descent

Theorem: Gradient Descent Update Rule

Standard gradient descent step for ridge regression:

$$\boldsymbol{\theta}^{(t+1)} = \boldsymbol{\theta}^{(t)} - \alpha \nabla J(\boldsymbol{\theta}^{(t)})$$

Ridge Gradient Computation

$$\begin{aligned}
\nabla J(\boldsymbol{\theta}) &= \nabla \left[\frac{1}{2} \|\mathbf{y} - \mathbf{X}\boldsymbol{\theta}\|_2^2 + \frac{\lambda}{2} \|\boldsymbol{\theta}\|_2^2 \right] && (29) \\
&= -\mathbf{X}^T(\mathbf{y} - \mathbf{X}\boldsymbol{\theta}) + \lambda\boldsymbol{\theta} && (30) \\
&= -\mathbf{X}^T\mathbf{y} + \mathbf{X}^T\mathbf{X}\boldsymbol{\theta} + \lambda\boldsymbol{\theta} && (31)
\end{aligned}$$

Ridge vs OLS: Gradient Descent Updates

Theorem: Ridge Update (with shrinkage)

$$\begin{aligned}\boldsymbol{\theta}^{(t+1)} &= \boldsymbol{\theta}^{(t)} - \alpha(-\mathbf{X}^T\mathbf{y} + \mathbf{X}^T\mathbf{X}\boldsymbol{\theta}^{(t)} + \lambda\boldsymbol{\theta}^{(t)}) \\ &= (1-\alpha\lambda)\boldsymbol{\theta}^{(t)} - \alpha(-\mathbf{X}^T\mathbf{y} + \mathbf{X}^T\mathbf{X}\boldsymbol{\theta}^{(t)})\end{aligned}$$

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Theorem: OLS Update (no shrinkage)

$$\boldsymbol{\theta}^{(t+1)} = \boldsymbol{\theta}^{(t)} - \alpha(-\mathbf{X}^T\mathbf{y} + \mathbf{X}^T\mathbf{X}\boldsymbol{\theta}^{(t)})$$

Ridge vs OLS: Gradient Descent Updates

Theorem: Ridge Update (with shrinkage)

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$$\boldsymbol{\theta}^{(t+1)} = \boldsymbol{\theta}^{(t)} - \alpha(-\mathbf{X}^T\mathbf{y} + \mathbf{X}^T\mathbf{X}\boldsymbol{\theta}^{(t)})$$

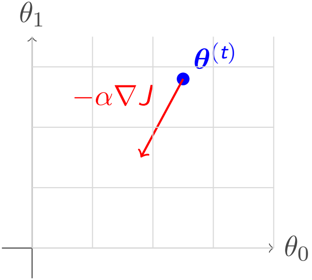
Key Points: Key Insight

The $(1-\alpha\lambda)$ factor **shrinks** coefficients at each step!

Visual: OLS Gradient Descent Step

Theorem: OLS Update

$$\boldsymbol{\theta}^{(t+1)} = \boldsymbol{\theta}^{(t)} - \alpha \nabla J(\boldsymbol{\theta}^{(t)})$$



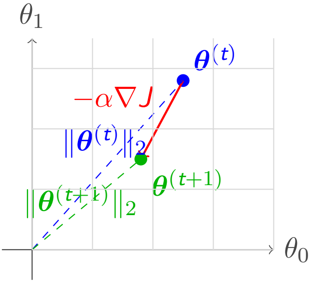
Important: Step 1

Start at $\boldsymbol{\theta}^{(t)}$ and compute negative gradient direction

Visual: OLS Gradient Descent - Vector Sum

Theorem: Vector Addition

$$\boldsymbol{\theta}^{(t+1)} = \boldsymbol{\theta}^{(t)} + (-\alpha \nabla J)$$



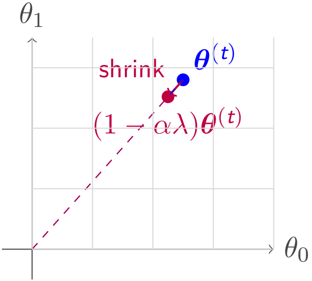
Key Points: Result

OLS: $\|\boldsymbol{\theta}^{(t+1)}\|_2$ depends only on gradient direction

Visual: Ridge Gradient Descent - Shrinkage Step

Theorem: Ridge Shrinkage

First: $\boldsymbol{\theta}^{(t)} \to (1 - \alpha\lambda)\boldsymbol{\theta}^{(t)}$



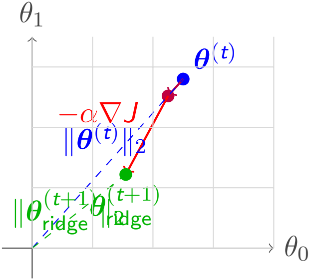
Important: Ridge Step 1

Shrink current parameters by factor $(1 - \alpha\lambda) < 1$

Visual: Ridge Gradient Descent - Complete Update

Theorem: Ridge Complete Update

$\boldsymbol{\theta}^{(t+1)} = (1 - \alpha\lambda)\boldsymbol{\theta}^{(t)} - \alpha\nabla J$

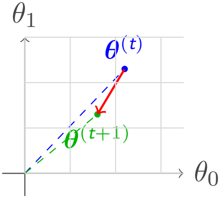


Key Points: Key Insight

Ridge: $\|\boldsymbol{\theta}^{(t+1)}_{\text{ridge}}\|_2 < \|\boldsymbol{\theta}^{(t+1)}_{\text{OLS}}\|_2$ (smaller coefficients!)

Side-by-Side Comparison: OLS vs Ridge Updates

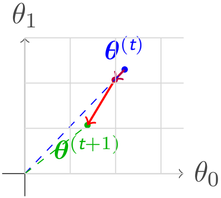
OLS Gradient Descent



No shrinkage

$\|\boldsymbol{\theta}^{(t+1)}\|_2 = 1.98$

Ridge Gradient Descent



With shrinkage

$\|\boldsymbol{\theta}^{(t+1)}\|_2 = 1.72 <$ OLS

Important: Ridge Effect

Ridge regression systematically produces **smaller coefficient magnitudes** at every gradient descent step!

Summary: What We Learned

Key Points: Ridge Regression Key Points

- **Problem**: Overfitting in linear regression with large coefficients
- **Solution**: Add L_2 penalty $\lambda\|\boldsymbol{\theta}\|_2^2$ to loss function
- **Effect**: Shrinks coefficients, improves generalization
- **Trade-off**: Higher bias, lower variance

Key Formula & Next Steps

Theorem: Ridge Regression Solution

$$\hat{\boldsymbol{\theta}}_{\text{ridge}} = (\mathbf{X}^T\mathbf{X} + \lambda\mathbf{I})^{-1}\mathbf{X}^T\mathbf{y}$$

Key Formula & Next Steps

Theorem: Ridge Regression Solution

$$\hat{\boldsymbol{\theta}}_{\text{ridge}} = (\mathbf{X}^T\mathbf{X} + \lambda\mathbf{I})^{-1}\mathbf{X}^T\mathbf{y}$$

Important: Next Steps

- Compare with Lasso regression (L_1 penalty)
- Explore elastic net (combines L_1 and L_2)
- Apply to real-world datasets