

Introduction & Linear Regression

Deep Dive: Mathematics and Implementation

Methods and Algorithms

MSc Data Science

Spring 2026

Outline

- 1 Mathematical Foundations
- 2 Gradient Descent
- 3 Model Evaluation
- 4 Regularization
- 5 Bias-Variance Tradeoff
- 6 Decision Framework
- 7 Summary

By the end of this session, you will be able to:

1. **Derive** the OLS estimator and prove its optimality under Gauss-Markov assumptions
2. **Analyze** gradient descent convergence and evaluate learning rate selection
3. **Evaluate** regression diagnostics to identify assumption violations
4. **Compare** regularization strategies (Ridge, Lasso, Elastic Net) for different problem structures

Finance Applications: Property valuation, asset pricing (CAPM)

Foundation for all supervised learning methods

Finance Use Case: House Price Prediction

- Banks need accurate property valuations for mortgage decisions
- Insurers must estimate replacement costs
- Investors evaluate real estate portfolios

Why Linear Regression?

- Interpretable coefficients (how much does each feature matter?)
- Regulatory requirement for explainable models
- Fast, well-understood baseline

Linear regression: the workhorse of quantitative finance since the 1800s

Capital Asset Pricing Model – Linear Regression in Finance

$$R_i - R_f = \alpha_i + \beta_i(R_m - R_f) + \varepsilon_i \quad (1)$$

- R_i : Return of asset i
- R_f : Risk-free rate (e.g., T-bill)
- R_m : Market return (e.g., S&P 500)
- β_i : Systematic risk (market sensitivity)
- α_i : Abnormal return (should be zero if CAPM holds)

Interpretation: $\beta = 1.2$ means 10% market rise \Rightarrow 12% expected asset rise

CAPM: The original factor model – basis for portfolio management

The Model in Matrix Form

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\varepsilon} \quad (2)$$

- $\mathbf{y} \in \mathbb{R}^n$: Response vector
- $\mathbf{X} \in \mathbb{R}^{n \times (p+1)}$: Design matrix (with intercept column)
- $\boldsymbol{\beta} \in \mathbb{R}^{p+1}$: Coefficient vector
- $\boldsymbol{\varepsilon} \in \mathbb{R}^n$: Error vector

Matrix notation enables elegant derivations and efficient computation

Design Matrix Structure

The Design Matrix \mathbf{X}

$$\mathbf{X} = \begin{bmatrix} 1 & x_{11} & x_{12} & \cdots & x_{1p} \\ 1 & x_{21} & x_{22} & \cdots & x_{2p} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_{n1} & x_{n2} & \cdots & x_{np} \end{bmatrix} \quad (3)$$

- First column of 1s for intercept β_0
- Each row is one observation
- Each column (after first) is one feature

n observations, *p* features, *p* + 1 parameters

Classical Assumptions for Valid Inference

1. **Linearity:** $E[y|X] = X\beta$ (correct functional form)
2. **Exogeneity:** $E[\varepsilon|X] = 0$ (no omitted variables)
3. **Homoscedasticity:** $\text{Var}(\varepsilon|X) = \sigma^2 I$ (constant variance)
4. **No multicollinearity:** $\text{rank}(X) = p + 1$ (full rank)
5. **Normality** (for inference): $\varepsilon \sim N(0, \sigma^2 I)$

Violations? Robust standard errors, transformations, regularization

Assumptions 1-4 needed for unbiased estimates; 5 for t-tests and CIs

Why OLS is Special

Under assumptions 1-4 (linearity, exogeneity, homoscedasticity, no perfect multicollinearity):

OLS is BLUE – Best Linear Unbiased Estimator

What BLUE Means:

- **Best:** Lowest variance among all linear unbiased estimators
- **Linear:** Estimator is linear function of y
- **Unbiased:** $E[\hat{\beta}] = \beta$

Implication: You cannot find a better linear unbiased estimator than OLS

Gauss-Markov justifies why OLS is the default choice for linear regression

Goal: Show OLS $\hat{\beta}$ has minimum variance among all linear unbiased estimators.

Proof: Let $\tilde{\beta} = \mathbf{C}\mathbf{y}$ be any other linear unbiased estimator. Write $\mathbf{C} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}' + \mathbf{D}$ for some matrix \mathbf{D} .

- Unbiasedness requires $E[\tilde{\beta}] = \beta$, which forces $\mathbf{DX} = \mathbf{0}$
- Then: $\text{Var}(\tilde{\beta}) = \sigma^2(\mathbf{X}'\mathbf{X})^{-1} + \sigma^2\mathbf{DD}'$
- Since $\mathbf{DD}' \succeq \mathbf{0}$ (positive semi-definite), we have:

$$\text{Var}(\tilde{\beta}) - \text{Var}(\hat{\beta}) = \sigma^2\mathbf{DD}' \succeq \mathbf{0} \quad (4)$$

Therefore OLS has the smallest variance among all linear unbiased estimators. \square

The key insight: any deviation \mathbf{D} from OLS adds noise (\mathbf{DD}') without reducing bias.

Sum of Squared Residuals (SSR)

$$L(\beta) = \sum_{i=1}^n (y_i - \hat{y}_i)^2 = (\mathbf{y} - \mathbf{X}\beta)^\top (\mathbf{y} - \mathbf{X}\beta) \quad (5)$$

Expanding:

$$L(\beta) = \mathbf{y}^\top \mathbf{y} - 2\beta^\top \mathbf{X}^\top \mathbf{y} + \beta^\top \mathbf{X}^\top \mathbf{X}\beta \quad (6)$$

Quadratic function in β – has unique minimum (if X full rank)

Deriving the Normal Equation

Taking the Derivative

$$\frac{\partial L}{\partial \beta} = -2\mathbf{X}^\top \mathbf{y} + 2\mathbf{X}^\top \mathbf{X}\beta \quad (7)$$

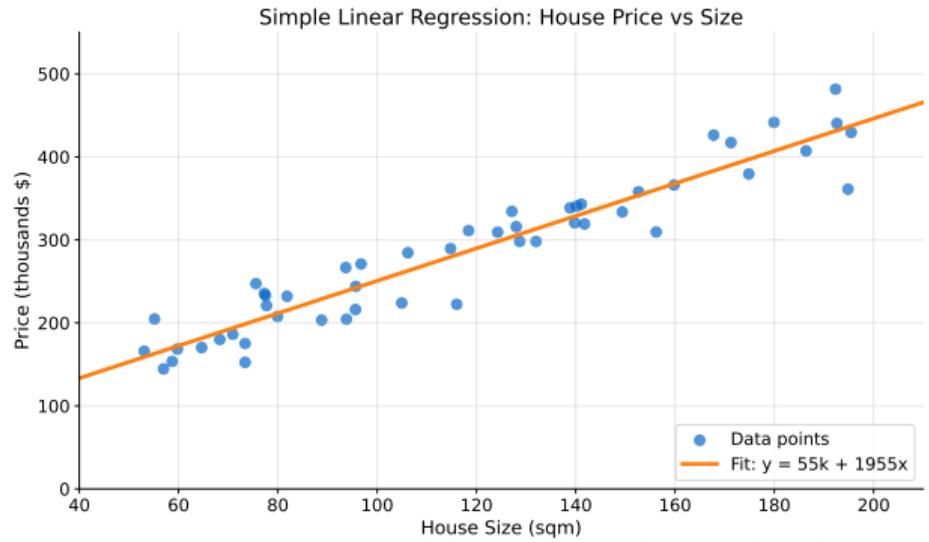
Setting to Zero:

$$\mathbf{X}^\top \mathbf{X}\hat{\beta} = \mathbf{X}^\top \mathbf{y} \quad (8)$$

$$\hat{\beta} = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{y} \quad (9)$$

This is the closed-form OLS solution – the “normal equation”

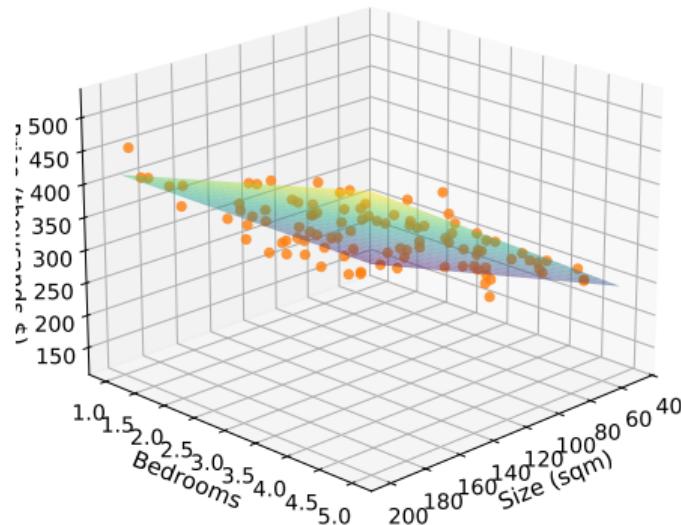
Simple Regression Visualization



The fitted line minimizes vertical distances squared

Multiple Regression Surface

Multiple Regression: Price = $f(\text{Size}, \text{Bedrooms})$



https://github.com/Digital-AI-Finance/methods-algorithms/tree/master/slides/L01_Introduction_Linear_Regression/02_multiple_regression_3d

With 2 features, we fit a plane; with p features, a hyperplane

Standardization: Zero Mean, Unit Variance

$$x_j^{\text{scaled}} = \frac{x_j - \bar{x}_j}{s_j} \quad (10)$$

Why Scale Features?

1. **Coefficient comparison:** After scaling, $|\beta_j|$ reflects relative importance
2. **Gradient descent:** Converges faster with similar feature scales
3. **Regularization:** Fair penalty across all features

Caution: Standardized coefficients lose original units (trade-off)

Always standardize for regularization; optional for OLS if only predicting

Why Gradient Descent?

Normal Equation Limitations

- Computing $(\mathbf{X}^\top \mathbf{X})^{-1}$ is $O(p^3)$
- Memory: Need to store $p \times p$ matrix
- For large p (millions of features): infeasible

Gradient Descent Advantages

- Memory efficient: process one sample at a time
- Scales to big data (SGD)
- Generalizes to non-linear models

For $p > 10,000$, gradient descent usually faster

Gradient of the Loss Function

$$\nabla L(\beta) = -2\mathbf{X}^\top (\mathbf{y} - \mathbf{X}\beta) = -2\mathbf{X}^\top \mathbf{r} \quad (11)$$

where $\mathbf{r} = \mathbf{y} - \mathbf{X}\beta$ is the residual vector.

Intuition:

- Gradient points in direction of steepest ascent
- We move opposite to gradient (steepest descent)
- Scale by learning rate α

Gradient is a $p + 1$ dimensional vector

Update Rule

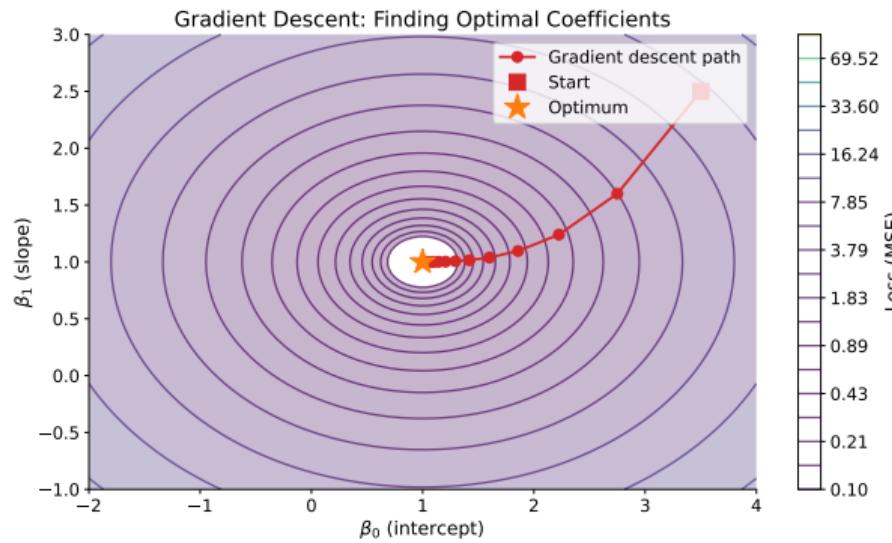
$$\beta^{(t+1)} = \beta^{(t)} - \alpha \nabla L(\beta^{(t)}) \quad (12)$$

Algorithm:

1. Initialize $\beta^{(0)}$ (often zeros or random)
2. Compute gradient $\nabla L(\beta^{(t)})$
3. Update: $\beta^{(t+1)} = \beta^{(t)} - \alpha \nabla L$
4. Repeat until convergence

Convergence: $\|\beta^{(t+1)} - \beta^{(t)}\| < \epsilon$ or max iterations

Gradient Descent Visualization



Contours show loss surface; path shows optimization trajectory

The Critical Hyperparameter

- **Too small:** Slow convergence, many iterations
- **Too large:** Divergence, oscillation
- **Just right:** Fast, stable convergence

Convergence Theory:

- Convex: $O(1/t)$ convergence rate
- Strongly convex: $O(\rho^t)$ where $\rho < 1$ (linear rate)
- Learning rate condition: $\eta < 2/L$ where L is Lipschitz constant of ∇L

Practical: Start with $\eta = 0.01$, use adaptive methods (Adam, AdaGrad)

For OLS, optimal $\eta = 1/\lambda_{\max}(X^\top X)$

Stochastic Gradient Descent (SGD)

Mini-Batch Gradient Descent

Instead of full gradient:

$$\nabla L(\beta) = -\frac{2}{n} \mathbf{X}^\top \mathbf{r} \quad (13)$$

Use mini-batch of size m :

$$\nabla L_B(\beta) = -\frac{2}{m} \mathbf{X}_B^\top \mathbf{r}_B \quad (14)$$

- $m = 1$: Stochastic GD (noisy but fast)
- $m = n$: Batch GD (stable but slow)
- $m \in [32, 256]$: Mini-batch (good tradeoff)

SGD: Process data once per epoch, update many times

R-Squared (R^2)

Coefficient of Determination

$$R^2 = 1 - \frac{SS_{\text{res}}}{SS_{\text{tot}}} = 1 - \frac{\sum(y_i - \hat{y}_i)^2}{\sum(y_i - \bar{y})^2} \quad (15)$$

Interpretation:

- Proportion of variance explained by model
- $R^2 = 0$: Model no better than mean
- $R^2 = 1$: Perfect fit
- $R^2 = 0.7$: 70% of variance explained

R^2 always increases with more features – use Adjusted R^2

Penalizing Model Complexity

$$R_{\text{adj}}^2 = 1 - \frac{(1 - R^2)(n - 1)}{n - p - 1} \quad (16)$$

Properties:

- Adjusts for number of predictors p
- Can decrease when adding irrelevant features
- Better for model comparison

Use R_{adj}^2 when comparing models with different p

Error Metrics in Original Units

$$\text{RMSE} = \sqrt{\frac{1}{n} \sum (y_i - \hat{y}_i)^2} \quad (17)$$

$$\text{MAE} = \frac{1}{n} \sum |y_i - \hat{y}_i| \quad (18)$$

Comparison:

- RMSE: Penalizes large errors more (sensitive to outliers)
- MAE: More robust, easier to interpret
- Units: Same as target variable (e.g., dollars)

Report both for comprehensive evaluation

Quantifying Uncertainty in Estimates

$$\text{Var}(\hat{\beta}) = \sigma^2(\mathbf{X}^\top \mathbf{X})^{-1} \quad (19)$$

Standard Error of $\hat{\beta}_j$:

$$\text{SE}(\hat{\beta}_j) = \hat{\sigma} \sqrt{[(\mathbf{X}^\top \mathbf{X})^{-1}]_{jj}} \quad (20)$$

where $\hat{\sigma}^2 = \frac{1}{n-p-1} \sum (y_i - \hat{y}_i)^2$ (unbiased variance estimate)

SE tells us how much $\hat{\beta}_j$ would vary across different samples

Is Feature j Significant?

- $H_0 : \beta_j = 0$ (feature has no effect)
- $H_1 : \beta_j \neq 0$ (feature matters)

t-Statistic:

$$t_j = \frac{\hat{\beta}_j - 0}{\text{SE}(\hat{\beta}_j)} \sim t_{n-p-1} \quad (21)$$

Decision Rule:

- p-value < 0.05: Reject H_0 , coefficient is significant
- p-value ≥ 0.05 : Cannot reject H_0

Always check p-values before interpreting coefficients

95% CI for Coefficient β_j :

$$\hat{\beta}_j \pm t_{n-p-1, 0.975} \times \text{SE}(\hat{\beta}_j) \quad (22)$$

Interpretation: If we repeated the study many times, 95% of intervals would contain the true β_j

Prediction Intervals:

- **Confidence interval for mean:** $\hat{y} \pm t \cdot \text{SE}(\hat{y})$
- **Prediction interval for new observation:** Wider (includes σ^2)

CI for mean is narrower; prediction interval accounts for individual variability

F-Test for Overall Model Significance

Null hypothesis: $H_0 : \beta_1 = \beta_2 = \dots = \beta_p = 0$ (model has no explanatory power)

$$F = \frac{R^2/p}{(1 - R^2)/(n - p - 1)} \sim F_{p,n-p-1} \quad (23)$$

- Tests whether the model **as a whole** explains significant variance
- Reject H_0 if $F > F_{\alpha,p,n-p-1}$ (or equivalently, if p-value < α)
- Complements individual t-tests: possible to have no significant t-tests but a significant F-test (multicollinearity)

Equivalently (using sums of squares):

$$F = \frac{(TSS - RSS)/p}{RSS/(n - p - 1)} = \frac{MSR}{MSE} \quad (24)$$

Every regression output table reports the F-statistic. Always check it before interpreting individual coefficients.

Under the normality assumption $\varepsilon_i \sim \mathcal{N}(0, \sigma^2)$, the likelihood is:

$$L(\beta, \sigma^2) = \prod_{i=1}^n \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(y_i - \mathbf{x}'_i \beta)^2}{2\sigma^2}\right) \quad (25)$$

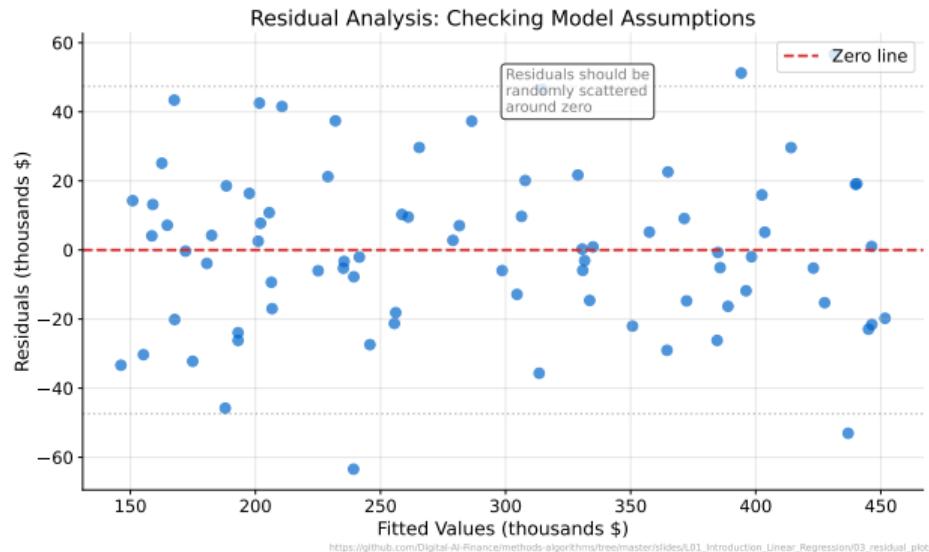
Maximizing the log-likelihood $\ell = -\frac{n}{2} \ln(2\pi\sigma^2) - \frac{1}{2\sigma^2} \sum(y_i - \mathbf{x}'_i \beta)^2$:

- $\frac{\partial \ell}{\partial \beta} = 0$ gives the **same normal equations as OLS**
- $\hat{\sigma}_{MLE}^2 = \frac{RSS}{n}$ (biased; OLS uses $n - p - 1$)
- This connection enables likelihood ratio tests, AIC/BIC model comparison

Key insight: OLS \equiv MLE under normality \Rightarrow all MLE properties (efficiency, asymptotic normality) transfer to OLS.

This bridges to L02 (Logistic Regression), where MLE is the only estimation method.

Residual Analysis



Good: random scatter. Bad: patterns indicate model misspecification

Assumption	Test	H_0
Homoscedasticity	Breusch-Pagan	Constant variance
	White test	Constant variance (robust)
No autocorrelation	Durbin-Watson	No serial correlation
Normality	Shapiro-Wilk	Residuals are normal
	Jarque-Bera	Skewness=0, kurtosis=3
Functional form	Ramsey RESET	No omitted nonlinearities

When assumptions fail:

- Heteroscedasticity \Rightarrow White/HC robust standard errors
- Autocorrelation \Rightarrow Newey-West standard errors, GLS
- Non-normality \Rightarrow Bootstrap inference (large n : CLT helps)

In finance/banking, regulators require formal test results – “the residuals looked fine” is insufficient.

The **hat matrix** maps observed to fitted values: $\hat{\mathbf{y}} = \mathbf{H}\mathbf{y}$ where

$$\mathbf{H} = \mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}' \quad (26)$$

Leverage: $h_{ii} \in [1/n, 1]$ measures how far \mathbf{x}_i is from the center of the design space. High leverage ($h_{ii} > 2p/n$): observation *could* be influential.

Cook's Distance combines leverage and residual:

$$D_i = \frac{e_i^2}{p \cdot \text{MSE}} \cdot \frac{h_{ii}}{(1 - h_{ii})^2} \quad (27)$$

- $D_i > 1$: observation substantially changes $\hat{\boldsymbol{\beta}}$ when removed
- Critical in finance: a single crisis observation can distort the entire model

Rule of thumb: investigate points with $D_i > 4/n$ or leverage $h_{ii} > 2(p + 1)/n$.

Evaluating Generalization

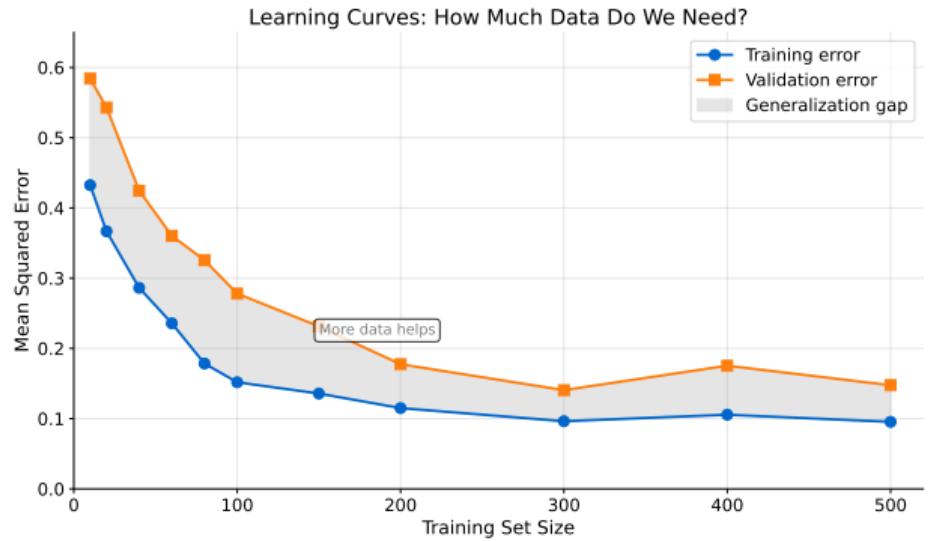
- Never evaluate on training data alone
- Split: 70-80% train, 20-30% test
- Report test set metrics

Cross-Validation (K-Fold):

- Split into K folds (typically $K = 5$ or 10)
- Train on $K - 1$ folds, validate on 1
- Repeat K times, average results

CV gives more reliable estimate with limited data

Learning Curves



Gap between curves indicates overfitting; convergence shows saturation

The Overfitting Problem

When Models Memorize Instead of Learn

- High-dimensional data ($p \approx n$ or $p > n$)
- Coefficients become very large
- Perfect fit on training data, poor generalization

Solution: Add Penalty to Loss Function

$$L_{\text{reg}}(\beta) = \|\mathbf{y} - \mathbf{X}\beta\|^2 + \lambda \cdot \text{penalty}(\beta) \quad (28)$$

λ controls strength of regularization

Ridge Regression (L2)

L2 Penalty: Sum of Squared Coefficients

$$L_{\text{ridge}}(\boldsymbol{\beta}) = \|\mathbf{y} - \mathbf{X}\boldsymbol{\beta}\|^2 + \lambda \|\boldsymbol{\beta}\|_2^2 \quad (29)$$

Closed-Form Solution:

$$\hat{\boldsymbol{\beta}}_{\text{ridge}} = (\mathbf{X}^\top \mathbf{X} + \lambda \mathbf{I})^{-1} \mathbf{X}^\top \mathbf{y} \quad (30)$$

- Shrinks all coefficients toward zero
- Never sets coefficients exactly to zero
- Always invertible (even when $p > n$)

Ridge adds λ to diagonal – stabilizes inversion

L1 Penalty: Sum of Absolute Coefficients

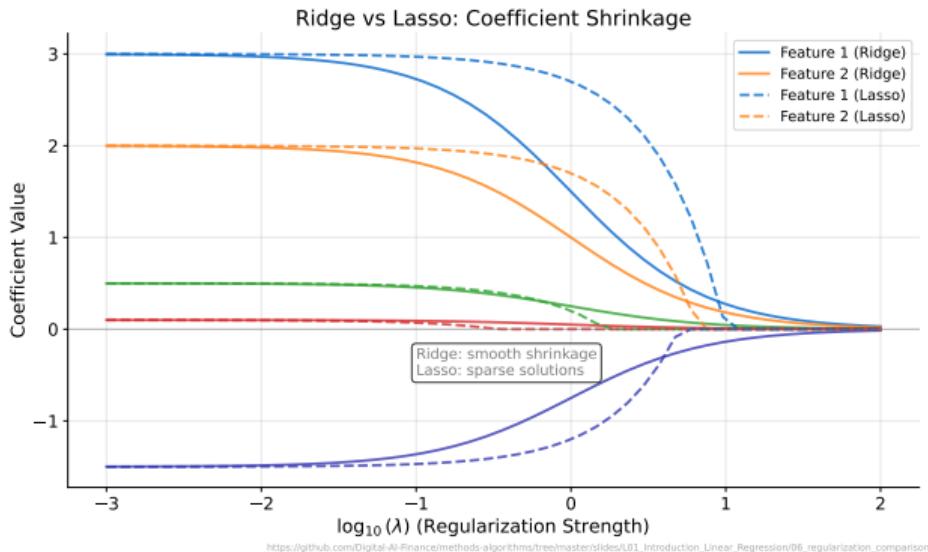
$$L_{\text{lasso}}(\boldsymbol{\beta}) = \|\mathbf{y} - \mathbf{X}\boldsymbol{\beta}\|^2 + \lambda\|\boldsymbol{\beta}\|_1 \quad (31)$$

Properties:

- Produces sparse solutions (some $\beta_j = 0$)
- Automatic feature selection
- No closed-form solution (use coordinate descent)

Lasso: Least Absolute Shrinkage and Selection Operator

Ridge vs Lasso Comparison



Ridge: smooth shrinkage. Lasso: sparse (feature selection)

Combining L1 and L2 Penalties (Zou & Hastie, 2005)

$$\min_{\beta} \frac{1}{2N} \|\mathbf{y} - \mathbf{X}\beta\|_2^2 + \lambda \left(\alpha \|\beta\|_1 + \frac{1-\alpha}{2} \|\beta\|_2^2 \right) \quad (32)$$

where $\alpha \in [0, 1]$ is the mixing parameter.

Benefits:

- Sparsity from L1 when $\alpha > 0$
- Stability from L2 (handles correlated features)
- $\alpha = 1$: pure Lasso; $\alpha = 0$: pure Ridge

Often best of both worlds for correlated features

Cross-Validation for Hyperparameter Tuning

1. Define grid of λ values (e.g., 10^{-4} to 10^4)
2. For each λ , perform K-fold CV
3. Select λ with lowest CV error
4. Refit on full training data

In Practice:

- `sklearn.linear_model.RidgeCV`
- `sklearn.linear_model.LassoCV`

Larger λ = more regularization = simpler model

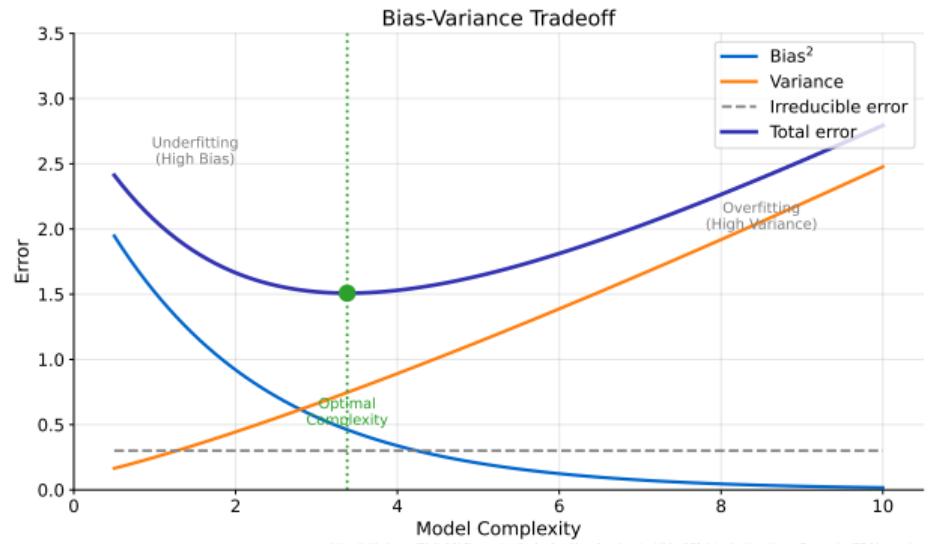
Expected Prediction Error

$$E[(y - \hat{f}(x))^2] = \text{Bias}^2(\hat{f}) + \text{Var}(\hat{f}) + \sigma^2 \quad (33)$$

- **Bias:** Error from wrong assumptions (underfitting)
- **Variance:** Error from sensitivity to training data (overfitting)
- σ^2 : Irreducible noise in data

We can't reduce irreducible error – focus on bias and variance

The Tradeoff Illustrated



Optimal complexity minimizes total error

How Regularization Helps

- Increasing λ : **increases bias, decreases variance**
- Decreasing λ : decreases bias, increases variance
- Optimal λ : minimizes total error

In Practice:

- Use CV to find optimal λ
- Regularization almost always helps when p is large

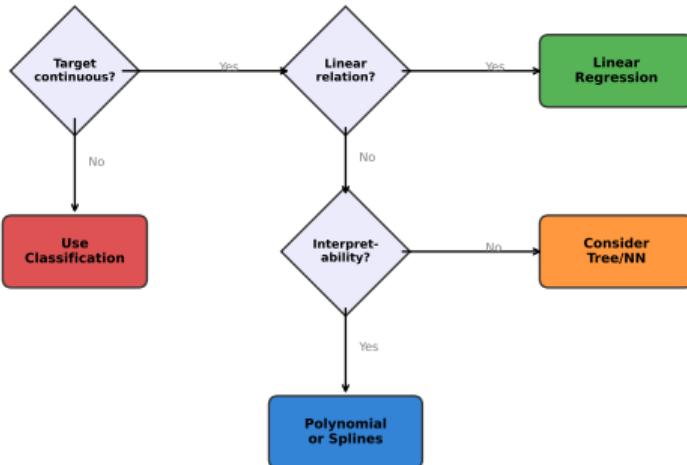
Regularization trades a little bias for a lot of variance reduction

Open the Colab Notebook

- Exercise 1: Implement OLS from scratch
- Exercise 2: Use scikit-learn LinearRegression
- Exercise 3: Compare with gradient descent

Link: See course materials on GitHub

Linear Regression Decision Guide



https://github.com/Digital-AI-Finance/methods-algorithms/tree/master/slides/L01_Introduction_Linear_Regression/08_decision_flowchart

Use this framework when choosing regression methods

Use When:

- Continuous target variable
- Approximate linear relationships
- Interpretability is critical
- Inference on coefficients needed
- Fast prediction required

Avoid When:

- Target is categorical
- Strong non-linear patterns
- Many outliers present
- Features highly correlated
- Prediction accuracy paramount

When in doubt, linear regression is a strong baseline

Variance Inflation Factor (VIF)

$$\text{VIF}_j = \frac{1}{1 - R_j^2} \quad (34)$$

where R_j^2 is from regressing x_j on all other features.

Interpretation:

- VIF = 1: No correlation with other features
- VIF > 5: Moderate concern
- VIF > 10: Serious multicollinearity

Remedies:

- Remove highly correlated features
- Use Ridge regression ($\lambda > 0$ stabilizes)
- Apply PCA before regression

Always check VIF before trusting coefficient estimates

Key Equations Summary

$$\text{Model: } \mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\varepsilon} \quad (35)$$

$$\text{OLS Solution: } \hat{\boldsymbol{\beta}} = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{y} \quad (36)$$

$$\text{Gradient: } \nabla L = -2\mathbf{X}^\top (\mathbf{y} - \mathbf{X}\boldsymbol{\beta}) \quad (37)$$

$$\text{GD Update: } \boldsymbol{\beta}^{(t+1)} = \boldsymbol{\beta}^{(t)} - \alpha \nabla L \quad (38)$$

$$\text{Ridge: } \hat{\boldsymbol{\beta}} = (\mathbf{X}^\top \mathbf{X} + \lambda \mathbf{I})^{-1} \mathbf{X}^\top \mathbf{y} \quad (39)$$

$$R^2 : 1 - \frac{\sum (y_i - \hat{y}_i)^2}{\sum (y_i - \bar{y})^2} \quad (40)$$

Key Takeaways

1. Linear regression minimizes squared error – closed form or GD
2. Matrix notation enables efficient computation
3. Gradient descent scales to large datasets
4. Regularization (Ridge/Lasso) prevents overfitting
5. The bias-variance tradeoff guides model complexity
6. Always evaluate on held-out test data

Next Session: Logistic Regression for Classification

References

- James, Witten, Hastie, Tibshirani (2021). *Introduction to Statistical Learning*. Chapter 3.
- Hastie, Tibshirani, Friedman (2009). *Elements of Statistical Learning*. Chapter 3.
- Bishop (2006). *Pattern Recognition and Machine Learning*. Chapter 3.

Online Resources:

- scikit-learn: https://scikit-learn.org/stable/modules/linear_model.html
- Stanford CS229: <https://cs229.stanford.edu/>