COMS4995W32
Applied Machine Learning

Dr. Spencer W. Luo

Columbia University | Fall 2025

Announcement

Mid-term 😮

Week 6

Duration: 1.5 hours

Format:

- Multiple Choice ✅
- Short Answer ✏️
- Calculation / Problem Solving 🔢

Cheat Sheet:

- 1-page A4 (double-sided allowed)
- Handwritten or printed

What You Need to Know 🧠

Course 1 - 5:

- Data prep & feature engineering
- Generative vs. Discriminative models
- Model evaluation & bias - variance
- Ensemble

Focus on:

- Understanding concepts
- Applying formulas
- Explaining scenarios

Assignment 1

https://www.gradescope.com/courses/1138767/assignments/6799370

Due: Oct 6, 2025 12:00 AM EST

Late Due: Oct 8, 2025 12:00 AM EST

Recitation 1

Next week

More details will be released on Ed soon

Model Evaluation
Bias-Variance

Agenda

- Motivation
- Train / Validation / Test Split
- Common Evaluation Metrics
- Bias - Variance Tradeoff
- Model Selection Strategies

Motivation

Supervised vs. Unsupervised Learning

Supervised Learning

- Learn mapping $f: X \to Y$
- Given data (x_i, y_i)
- Example: Spam Email (label = spam / ham)

Unsupervised Learning

- Discover hidden structures in data
- Only x_i, no labels
- Example: Customer Segmentation

What is Machine Learning (ML)?

- Learn patterns from **data** 🧩
- Make **predictions** on new data 🔮
- **Generalize** beyond training 🌍

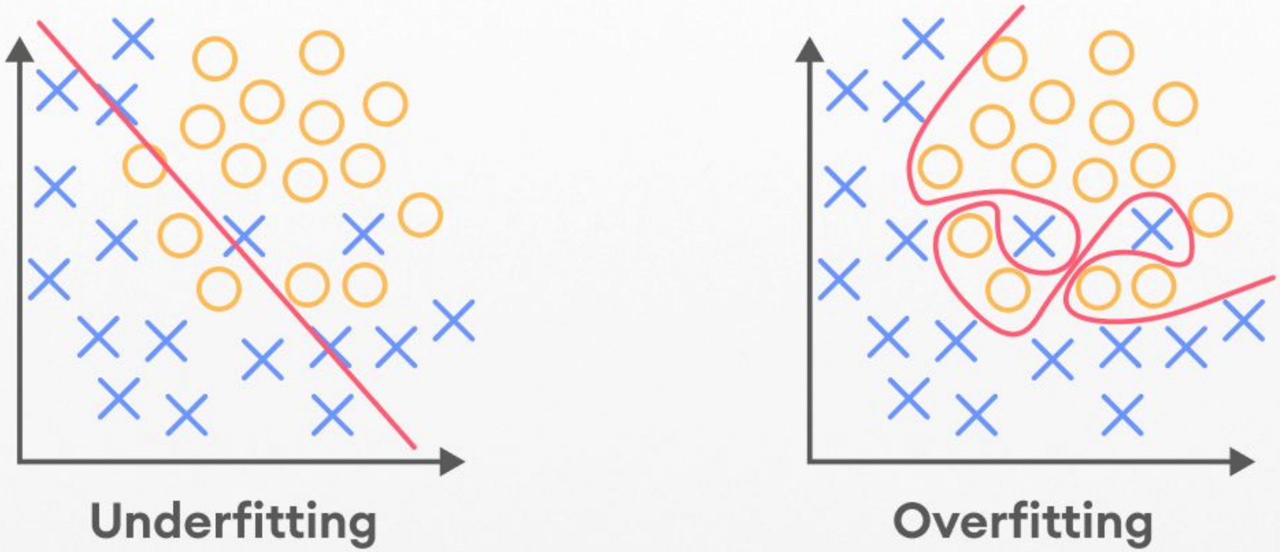
Why Do We Need Model Evaluation? 🤔

Training accuracy ≠ Real-world performance

Without proper evaluation:

- Models may memorize training data (overfitting)
- Models may be too simple to capture patterns (underfitting)

Wrong evaluation → Wrong decisions → Costly mistakes 💸


Underfitting
Overfitting

Overfitting vs Underfitting 📉📈

Overfitting definition:

- Model fits the training data too closely - including random noise
- Symptom:
  - Training Accuracy ≈ 100%
  - Test Accuracy ≪ Training Accuracy

Like a student who:

📖 Memorizes every word from lecture slides (training set)

❌ Cannot answer slightly different questions in mid-term (test set)

Overfitting vs Underfitting 📉📈

Underfitting definition:

- Model is too simple to capture the underlying patterns in data.
- Symptom:
  - Low Training Accuracy
  - Low Test Accuracy

Like a student who:

📖 Barely skimmed the textbook

❌ Cannot even handle problems in the textbook (training set)

❌ Naturally also fails in mid-term (test set)

Why Wrong Metrics Can Be Dangerous 🚨

Accuracy is misleading when data is imbalanced

Example: disease detection dataset

- 99% healthy, 1% sick
- A model that always predicts “healthy” → 99% accuracy but useless ❌

Need metrics that capture what matters: precision, recall, etc.

Key Takeaway 💡

- Evaluation is not optional, it is essential
- Good evaluation = Fair model comparison
- Good evaluation = Reliable deployment in real world

Train / Validation / Test Split

Why Split Data? 🍰

Goal: measure generalization ability

If we only check training accuracy:

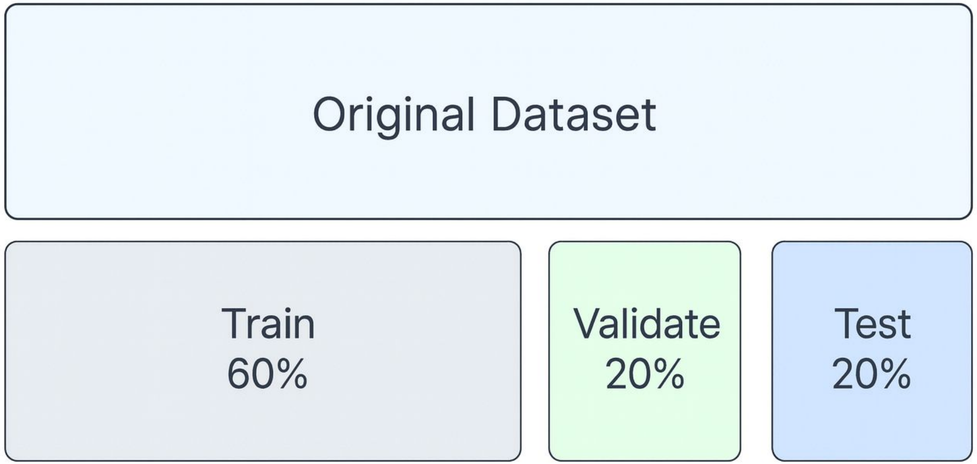
- Might think model is “perfect” → but actually memorizing 📖

Solution: keep separate sets

- Train → learn patterns
- Validation → tune hyperparameters
- Test → simulate unseen real-world data

Why Split Data? 🍰

Multiple Models
Percentage Split



Typical Splits 📊

Common ratios:

- Train: 60 - 80%
- Validation: 10 - 20%
- Test: 10 - 20%

Important rule: Test set is locked 🔒

Hold-Out Method ✂️

One-time split (Train / Val / Test)

- Pros: simple, fast
- Cons:
  - depends heavily on the random split
  - unstable on small data

k-Fold Cross-Validation 🔄

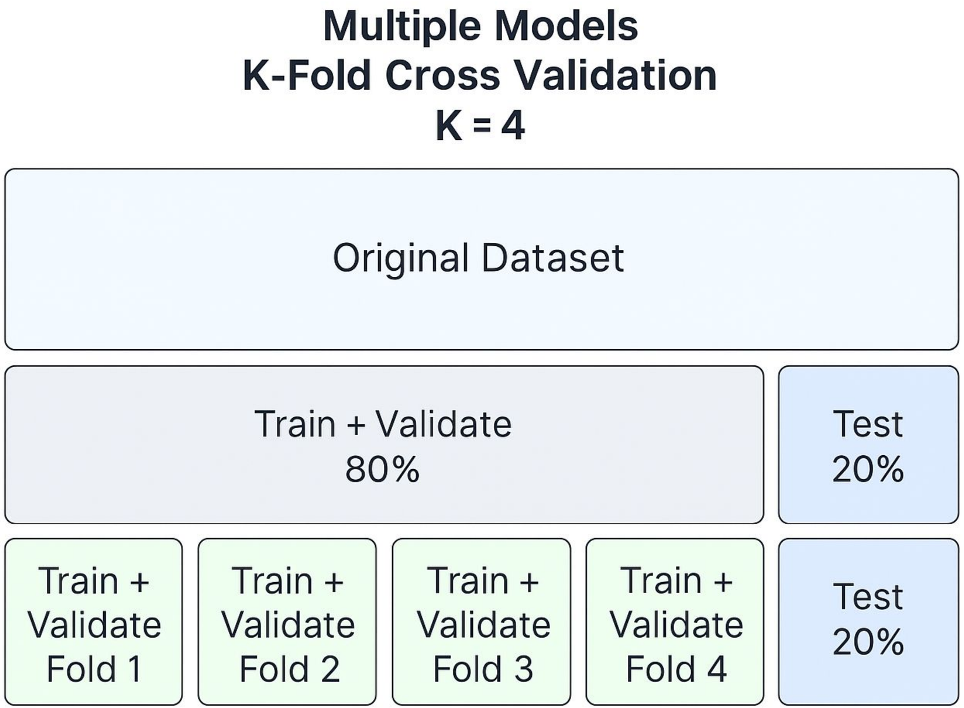
💡 Idea: Rotate the validation set

Steps:

- Split into k equal folds
- Train on (k–1) folds, validate on the remaining one
- Repeat k times, average results

Pros: robust, uses all data
Cons: more compute ⏱️

k-Fold Cross-Validation 🔄



Common Evaluation Metrics

Why Metrics Matter 🎯

Different problems need different metrics

Example:

- Credit card fraud detection → catch rare cases
- Recommender system → focus on ranking quality

⚠️ Accuracy is not enough ❌

Regression Metrics 📉

Mean Squared Error (MSE)

- Penalizes large errors more

$$\mathrm{MSE} = \overset{\text{Mean}}{\boxed{\frac{1}{n}\sum_{i=1}^{n}}}\left(\overset{\text{Error}}{\boxed{Y_i - \hat{Y}_i}}\right)^{\overset{\text{Squared}}{\boxed{2}}}$$

Regression Metrics 📉

Mean Absolute Error (MAE)

- Less sensitive to outliers

$$MAE = \overset{\text{Divide by the total number of data points}}{\boxed{\frac{1}{n}}} \underset{\text{Sum of}}{\sum} \underbrace{\left| \overset{\text{Actual output value}}{\boxed{y}} - \overset{\text{Predicted output value}}{\boxed{\widehat{y}}} \right|}_{\text{The absolute value of the residual}}$$

Classification Metrics ✅/❌

Accuracy

- Proportion of correct predictions
- Simple but misleading on imbalanced data

Confusion Matrix 🔢

	Predicted Class: **Positive**	Predicted Class: **Negative**	
Actual Class: **Positive**	True Positive (TP)	False Negative (FN) **Type II Error**	**Recall** $\frac{TP}{(TP + FN)}$
Actual Class: **Negative**	False Positive (FP) **Type I Error**	True Negative (TN)	**Specificity** $\frac{TN}{(TN + FP)}$
	Precision $\frac{TP}{(TP + FP)}$	**Negative Predictive Value** $\frac{TN}{(TN + FN)}$	**Accuracy** $\frac{TP + TN}{(TP + TN + FP + FN)}$

Precision, Recall, F1 ⚖️

Precision (Purity)

- Out of predicted positives, how many are correct?

Recall (Coverage)

- Out of actual positives, how many did we find?

Example: Disease detection 🧪

- High recall = fewer missed cases
- High precision = fewer false alarms

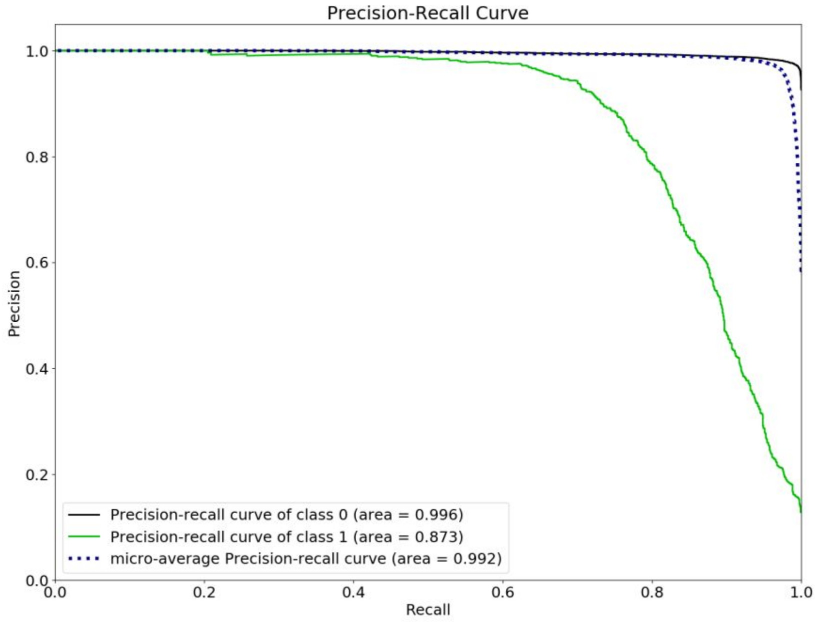
Precision, Recall, F1 ⚖️

F1 combines Precision and Recall into one metric

$$\text{F1 Score} = 2 \cdot \frac{\text{Precision} \cdot \text{Recall}}{\text{Precision} + \text{Recall}}$$

AUCPR

AUC = Area Under Curve



Choosing the Right Metric 🧭

- Regression → MSE, MAE, RMSE
- Balanced classification → Accuracy, F1
- Imbalanced classification → Precision, Recall, PR Curve
- Unsupervised tasks → Normalized Mutual Information (later lectures)

Bias - Variance Tradeoff

Bias–Variance Decomposition 🎯

Bias

- Error caused by simplifying assumptions in the model, leading to a systematic difference between prediction and ground truth

Symptom

- Model is too simple to capture the true relationship
- Leads to underfitting
- Example: Using a straight line to fit a curved pattern

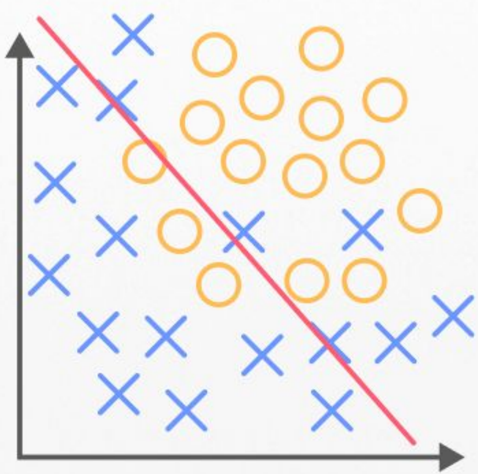
Bias–Variance Decomposition 🎯

Variance

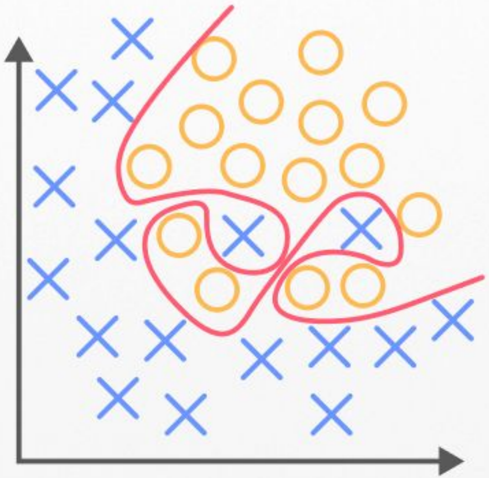
- Error caused by a model's sensitivity to small fluctuations in the training data, leading to inconsistent predictions across different datasets.

Symptom

- Model is too complex, changes a lot with small noises in data
- Leads to overfitting



Underfitting



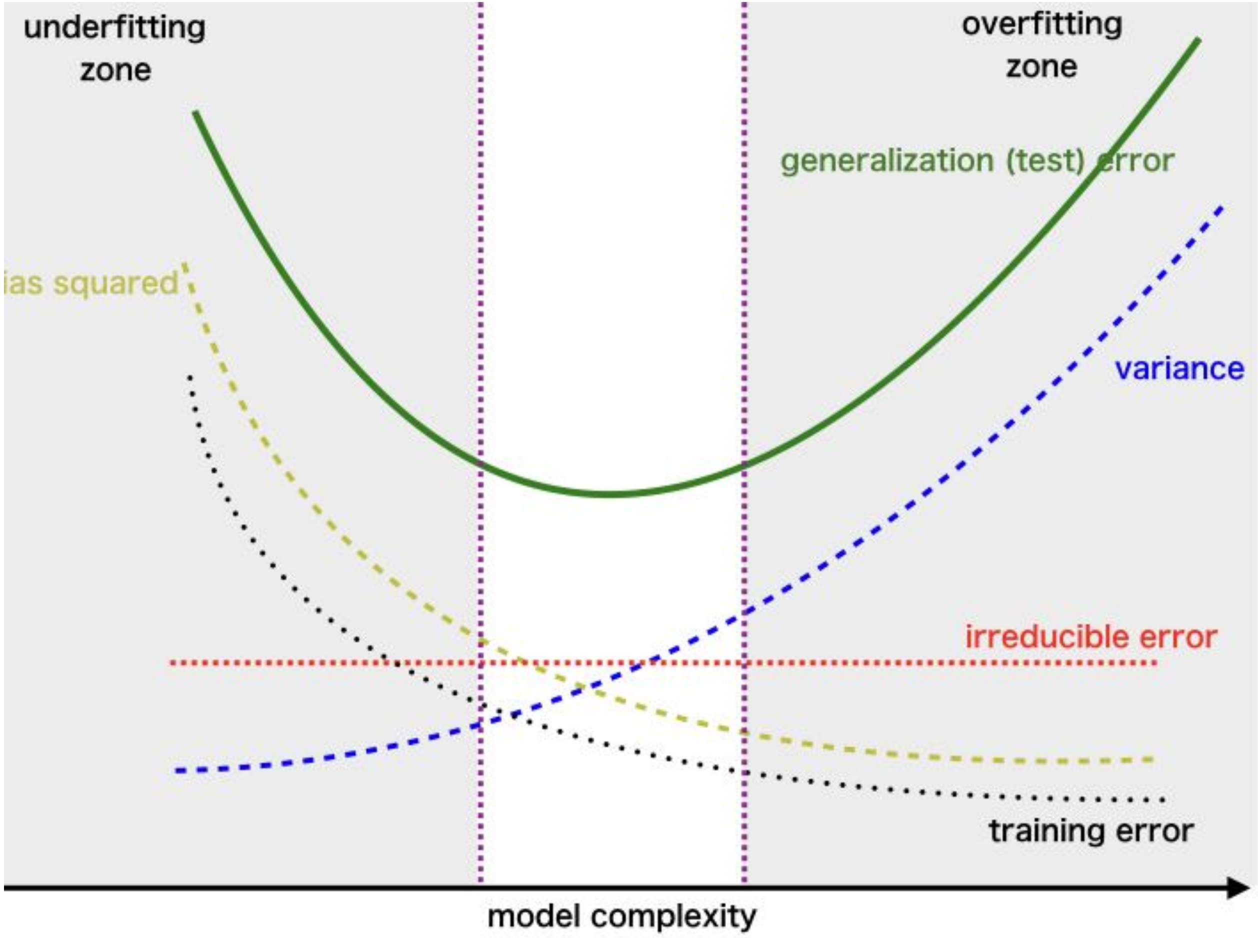
Overfitting

Bias–Variance Tradeoff

Generalization Error = Bias^2 + Variance + Noise

- Generalization Error == Expected Test Error

Goal = balance between Bias (too simple → underfit) and Variance (too complex → overfit)


underfitting zone
overfitting zone
generalization (test) error
ias squared
variance
irreducible error
training error
model complexity

Bias vs Variance — Key Takeaways 🎯

Opposite failure modes

- High Bias → Underfitting, model too rigid
- High Variance → Overfitting, model too sensitive

Tradeoff is unavoidable

- Reducing bias usually increases variance
- Reducing variance usually increases bias

What we really want

- Minimize expected test error (generalization error)
- Balance both terms + accept some irreducible noise

Model Selection Strategies

Why Model Selection? 🎯

We have mastered:

- How to split data 🍰
- How to measure performance 📊
- Why bias & variance matter ⚖️

Next challenge:

- Choosing the best model among candidates

Cross-Validation for Model Choice 🔄

Not just for evaluation → also for model selection

Use k-fold CV to estimate performance

Pick model with best average validation score

Hyper-parameter Tuning 🔧

Models often have parameters not learned directly

- Regularization strength (α)
- Decision tree depth
- Neural network depth

Strategies

- Grid search 🗂️
- Random search 🎲

Regularization 📉

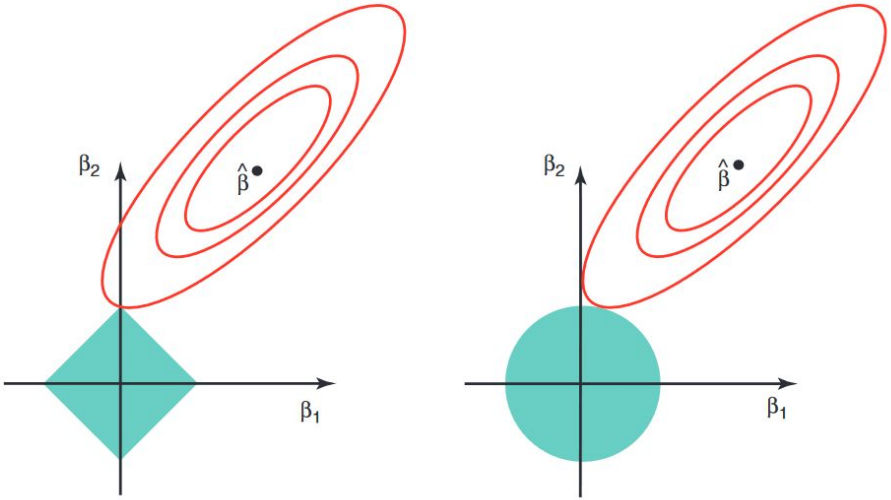
Problem: overly complex models → high variance

Solution: add penalty terms

- Ridge (L2): penalize large weights smoothly
- Lasso (L1): shrink some weights to zero → feature selection

Ridge vs Lasso (Geometry)

Lasso	Ridge
diamond constraint → corners	circular constraint → smooth shrinkage



Early Stopping 🛑

Common in neural networks

Idea:

- Stop training when validation error starts increasing
- Prevents overfitting from too many epochs

Ensemble Methods 🤝

Combine multiple models to reduce variance

Examples:

- Bagging / Random Forests 🌲
- Boosting (AdaBoost, XGBoost) 🚀

Analogy: “wisdom of the crowd”

Practical Workflow 🔄

- Split data into Train / Val / Test
- Define candidate models + hyperparameters
- Use Cross-validation for fair comparison
- Regularize or stop early if variance too high