Data Science for Mathematicians

Lesson 04: Model Evaluation and Statistical Inference

Department of Mathematics and Computer Science

Outline

From Fitting to Evaluating

In previous lessons we derived OLS and Naive Bayes—both focused on **fitting** models to data.

The central question now:

Having fit a model, is it any good?

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The central question now:

Having fit a model, is it any good?

- Low training error $\neq$ good model
- The dataset $D = \{(x_i, y_i)\}_{i=1}^{n}$ is a **sample**, not the population
- The estimator $\hat{\beta} = (X^T X)^{-1} X^T y$ is a **random variable**—it depends on which sample we drew

Training Error vs. Generalization Error

- **Training error:** Performance on the data used to fit the model

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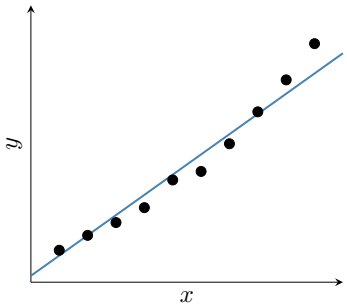
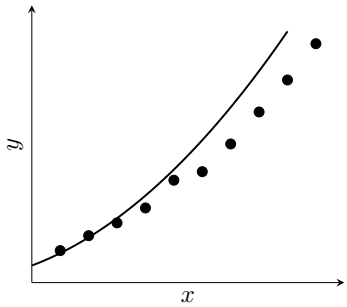
Our true objective: minimize **generalization error**, not training error.

Memorization vs. Generalization

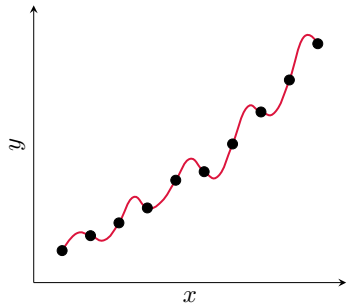
Overfitting: the model fits the noise, not the signal.



Underfitting
(High Bias)



Good Fit



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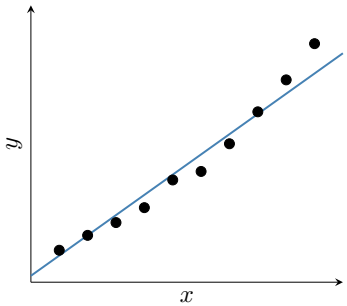

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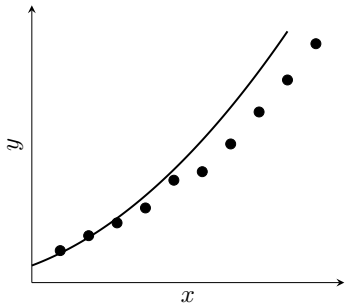

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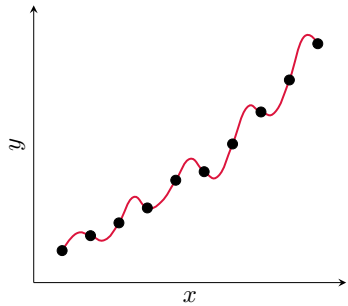

Overfitting
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Goal: capture stable, repeatable patterns while ignoring stochastic noise.

Lecture Roadmap

Three pillars of model evaluation:

1. **Theoretical Framework:** Bias-Variance Decomposition
   - Why does error arise? What are its components?

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   - How do we measure error in practice?

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2. **Practical Metrics:** MSE, R^2, Precision, Recall, F_1, AUC
   - How do we measure error in practice?
3. **Estimation Procedure:** Cross-Validation
   - How do we reliably estimate generalization error?

The Data Generating Process

Definition: Data Generating Process

We assume observed data arises from:

$$y = f(x) + \epsilon$$

where $f : \mathbb{R}^p \to \mathbb{R}$ is the true (unknown) function and ϵ is random noise with:

1. $\mathbb{E}[\epsilon] = 0$ (unbiased noise)
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- f is the **signal** we wish to learn
- ϵ is the **noise** (measurement error, unmodeled variables, randomness)
- Our estimator $\hat{f}(x; D)$ is a **random quantity**—it depends on the training set D

Expected Prediction Error

Consider a new, unseen point (x_0, y_0) with $y_0 = f(x_0) + \epsilon_0$.

Definition: Expected Prediction Error

The expected squared prediction error at x_0:

$$\mathbb{E}\left[(y_0 - \hat{f}(x_0))^2\right]$$

where the expectation is over:

- the random training dataset D
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Can we decompose this error into interpretable components?

The Bias-Variance Decomposition

Theorem: Bias-Variance Decomposition

For $y = f(x) + \epsilon$ with $\mathbb{E}[\epsilon] = 0$, $\text{Var}(\epsilon) = \sigma^2$:

$$\mathbb{E}[(y_0 - \hat{f}(x_0))^2] = \underbrace{\left(\mathbb{E}[\hat{f}(x_0)] - f(x_0)\right)^2}_{\text{Squared Bias}} + \underbrace{\text{Var}(\hat{f}(x_0))}_{\text{Variance}} + \underbrace{\sigma^2}_{\text{Irreducible Error}}$$

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Three distinct, additive sources of error:

- **Bias**^{2}: systematic error from model assumptions
- **Variance**: sensitivity to the particular training set
- $\boldsymbol{\sigma^2}$: noise inherent to the process (cannot be reduced)

Proof Sketch: Setup

Write $\hat{f} = \hat{f}(x_0; D)$ and $f = f(x_0)$. Add and subtract $\mathbb{E}[\hat{f}]$:

$$\mathbb{E}[(y_0 - \hat{f})^2] = \mathbb{E}\left[\left((y_0 - \mathbb{E}[\hat{f}]) + (\mathbb{E}[\hat{f}] - \hat{f})\right)^2\right]$$

$$= \underbrace{\mathbb{E}[(y_0 - \mathbb{E}[\hat{f}])^2]}_{\text{Term 1}} + \underbrace{\mathbb{E}[(\hat{f} - \mathbb{E}[\hat{f}])^2]}_{\text{Term 2}} + \underbrace{2\mathbb{E}[(y_0 - \mathbb{E}[\hat{f}])(\mathbb{E}[\hat{f}] - \hat{f})]}_{\text{Term 3}}$$

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Term 2 $= \mathrm{Var}(\hat{f})$ (by definition)

Term 3 $= 0$ (y_0 and $\hat{f}$ are independent; $\mathbb{E}_D[\mathbb{E}[\hat{f}] - \hat{f}] = 0$)

Proof Sketch: Term 1

For Term 1, substitute $y_0 = f + \epsilon_0$:

$$\begin{aligned}
\mathbb{E}[(y_0 - \mathbb{E}[\hat{f}])^2] &= \mathbb{E}\left[\left((f - \mathbb{E}[\hat{f}]) + \epsilon_0\right)^2\right] \\
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\end{aligned}$$

Combining all terms:

$$\mathbb{E}[(y_0 - \hat{f})^2] = \text{Bias}^2(\hat{f}) + \text{Var}(\hat{f}) + \sigma^2 \qquad \square$$

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Component 1: Irreducible Error

Definition: Irreducible Error

$$\sigma^2 = \text{Var}(\epsilon) = \mathbb{E}[\epsilon^2]$$

A **uniform lower bound** on the expected prediction error for *any* estimator $\hat{f}$.

- Inherent to the data-generating process
- Arises from measurement error, unmodeled variables, intrinsic randomness
- **No model can eliminate it**—the price of modeling a stochastic world

Component 2: Bias

Definition: Bias

$$\text{Bias}(\hat{f}(x_0)) = \mathbb{E}_D[\hat{f}(x_0)] - f(x_0)$$

$$\text{Bias}^2(\hat{f}(x_0)) = \left(\mathbb{E}_D[\hat{f}(x_0)] - f(x_0)\right)^2$$

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- Systematic error from the model's simplifying assumptions
- Discrepancy between the **average prediction** (over all possible datasets) and the **true value**
- High bias $\Rightarrow$ model is too rigid $\Rightarrow$ **underfitting**
- Example: fitting a linear model to a cubic relationship

Component 3: Variance

Definition: Variance of an Estimator

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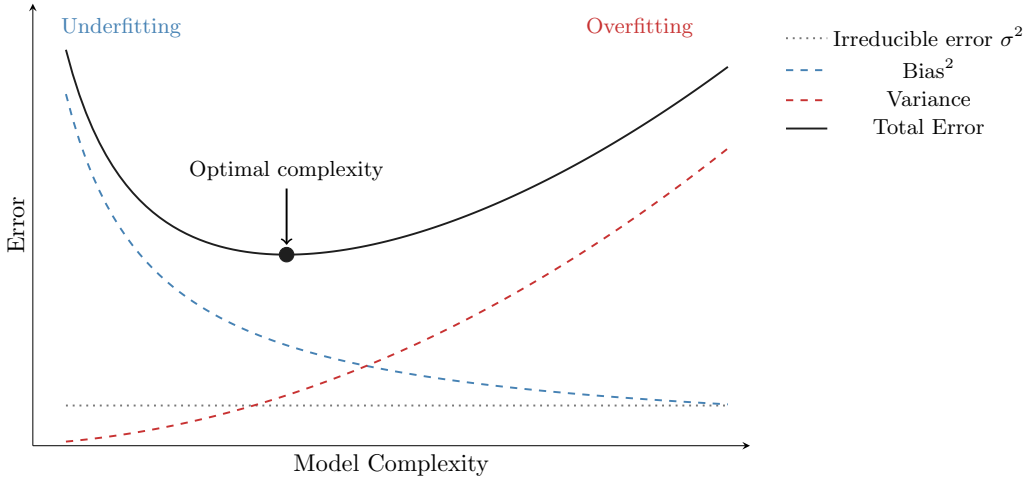
- Sensitivity to the particular training dataset
- How much does $\hat{f}(x_0)$ **fluctuate** across different training samples?
- High variance $\Rightarrow$ model is too flexible $\Rightarrow$ **overfitting**
- Example: a 20th-degree polynomial changes shape dramatically with each training set

The Tradeoff Curve



A slightly biased model can have lower total error than an unbiased but high-variance one.

Why Simpler Models Can Win

The decomposition justifies preferring a simpler, slightly *wrong* model:

	Simple Model	**Complex Model**
Bias^2	High	Low
Variance	Low	High
Total Reducible Error	Can be lower	Can be higher

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Regularization (Ridge, LASSO) intentionally introduces bias to reduce variance:

$$\text{Reducible Error} = \text{Bias}^2 + \text{Var}$$

The goal is not to eliminate bias, but to minimize the **sum**.

Mean Squared Error (MSE)

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Given n observations (y_i) and predictions $(\hat{y}_i)$:

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- Direct empirical analogue of the theoretical expected prediction error
- OLS minimizes MSE on training data *by construction*
- **Limitation:** units are squared (e.g., $\$^2$)

Root Mean Squared Error (RMSE)

Definition: Root Mean Squared Error

$$\text{RMSE} = \sqrt{\text{MSE}} = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2}$$

- Same units as y — directly interpretable
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Example

MSE $= 25{,}000{,}000$ \$^{2} is hard to interpret.
RMSE $=$ \$5,000 immediately tells you the typical error scale.

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Definition: Total Sum of Squares

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Error of the baseline **mean-only model** $\hat{y}_i = \bar{y}$ for all i.

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Definition: Residual Sum of Squares

$$\mathrm{SS}_{\mathrm{res}} = \sum_{i=1}^{n} (y_i - \hat{y}_i)^2$$

Variation left **unexplained** by the model.

The Coefficient of Determination (R^2)

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Definition: Coefficient of Determination

$$R^2 = 1 - \frac{SS_{res}}{SS_{tot}}$$

Interpretation: proportion of variance **explained** by the model.

- $R^2 = 1.0$: perfect fit ($SS_{res} = 0$)
- $R^2 = 0.0$: no better than predicting $\bar{y}$ ($SS_{res} = SS_{tot}$)
- $R^2 < 0$: **worse** than predicting $\bar{y}$

Critical Limitations of R^2

Lemma

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Consequence: R^2 *actively encourages overfitting*—adding pure noise variables increases R^2.

Further Limitations of R^2

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The uncritical pursuit of high R^2 is a common anti-pattern in data analysis.

Adjusted R^2

Definition: Adjusted R^2

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where n = number of samples, p = number of predictors.

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- Penalizes model complexity through the ratio $\frac{n-1}{n-p-1}$
- Only increases if the new variable reduces SS_{res} *enough* to overcome the penalty
- More suitable for comparing models with **different numbers of predictors**
- Rewards **parsimony**

The Pitfall of Accuracy

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Example: Credit Card Fraud Detection

Dataset: 1,000,000 transactions, 100 fraudulent (0.01%).

A model that *always predicts "not fraud"*:

$$\text{Accuracy} = \frac{999{,}900}{1{,}000{,}000} = 99.99\%$$

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Yet it detects **zero** fraud cases—completely useless!

The Confusion Matrix

Definition: Confusion Matrix

For binary classification with true labels $y_i \in \{0, 1\}$ and predictions $\hat{y}_i \in \{0, 1\}$:

$$\text{TP} = |\{i : y_i = 1,\ \hat{y}_i = 1\}| \qquad \text{FN} = |\{i : y_i = 1,\ \hat{y}_i = 0\}|$$
$$\text{FP} = |\{i : y_i = 0,\ \hat{y}_i = 1\}| \qquad \text{TN} = |\{i : y_i = 0,\ \hat{y}_i = 0\}|$$

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	Predicted +	**Predicted −**
Actual +	TP	FN
Actual −	FP	TN

$$\mathrm{TP} + \mathrm{TN} + \mathrm{FP} + \mathrm{FN} = n \quad \text{and} \quad \text{Accuracy} = \frac{\mathrm{TP} + \mathrm{TN}}{n}$$

Confusion Matrix: Medical Test Example

Example

$n = 200$ patients: 50 sick, 150 healthy. Model predicts positive for 60.

	Predicted +	**Predicted −**
Actual +	TP $= 40$	FN $= 10$
Actual −	FP $= 20$	TN $= 130$

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	Predicted +	**Predicted −**
Actual +	TP $= 40$	FN $= 10$
Actual −	FP $= 20$	TN $= 130$

- 40/50 sick patients correctly identified
- 20 false alarms among healthy patients
- Verify: $40 + 130 + 20 + 10 = 200$

Precision

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Only 2/3 of flagged patients actually have the disease. The remaining 1/3 are false alarms.

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Optimize for precision when FP is costly (e.g., spam filter—don't lose legitimate emails).

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$$\text{Recall} = \frac{40}{40 + 10} = \frac{4}{5} = 0.80$$

The model catches 80% of sick patients, but misses 10 (1 in 5 go undiagnosed).

Optimize for recall when FN is costly (e.g., disease screening—don't miss sick patients).

The Precision-Recall Tradeoff

Most classifiers output a score $p(y{=}1|x)$, thresholded at τ:

$$\hat{y} = \begin{cases} 1 & \text{if } p(y{=}1|x) > \tau \\ 0 & \text{otherwise} \end{cases}$$

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Increase τ (e.g., 0.9):

- More conservative
- Fewer FP $\Rightarrow$ **higher precision**
- More FN $\Rightarrow$ **lower recall**

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The optimal threshold is a **domain decision**, not a purely statistical one.

Why the Harmonic Mean?

Lemma: Property of the Harmonic Mean

For positive a, b:

$$H(a,b) = \frac{2ab}{a+b}$$

is always closer to $\min\{a,b\}$ than the arithmetic mean $A(a,b) = \frac{a+b}{2}$.

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Why this matters:

- The harmonic mean is **low if either input is low**
- A model cannot score well by having perfect recall but terrible precision
- This makes it ideal for combining Precision and Recall

The F_1-Score

Definition: F_1-Score

The harmonic mean of Precision and Recall:

$$\boxed{\mathrm{F}_1 = \frac{2 \cdot \text{Precision} \cdot \text{Recall}}{\text{Precision} + \text{Recall}}}$$

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Example

With Precision $= 2/3$ and Recall $= 4/5$:

$$F_1 = \frac{2 \cdot \frac{2}{3} \cdot \frac{4}{5}}{\frac{2}{3} + \frac{4}{5}} = \frac{\frac{16}{15}}{\frac{22}{15}} = \frac{16}{22} = \frac{8}{11} \approx 0.727$$

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Compare: arithmetic mean ≈ 0.733. The F_1 is pulled toward the **lower** value.

The F_β-Score

Definition: F_β-Score

For $\beta > 0$, the weighted harmonic mean:

$$\mathrm{F}_\beta = \frac{(1+\beta^2) \cdot \text{Precision} \cdot \text{Recall}}{\beta^2 \cdot \text{Precision} + \text{Recall}}$$

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- $\beta = 1$: equal weight $\Rightarrow$ recovers F_1
- $\beta > 1$: **recall weighted more** (penalizes FN)
- $\beta < 1$: **precision weighted more** (penalizes FP)

F_β-Score: Choosing β by Context

With Precision $= 2/3$, Recall $= 4/5$:

Metric	Value	Use Case
$F_{0.5}$	≈ 0.690	Spam filter (precision matters)
F_1	≈ 0.727	Balanced
F_2	≈ 0.769	Disease screening (recall matters)

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Since Recall $>$ Precision for this model:

- Higher β rewards the model's stronger recall $\Rightarrow$ higher score
- Lower β penalizes the model's weaker precision $\Rightarrow$ lower score

The ROC Curve

Definition: ROC Curve

Plot of TPR vs. FPR as threshold τ varies:

$$\mathrm{TPR} = \frac{\mathrm{TP}}{\mathrm{TP} + \mathrm{FN}}, \quad \mathrm{FPR} = \frac{\mathrm{FP}}{\mathrm{FP} + \mathrm{TN}}$$

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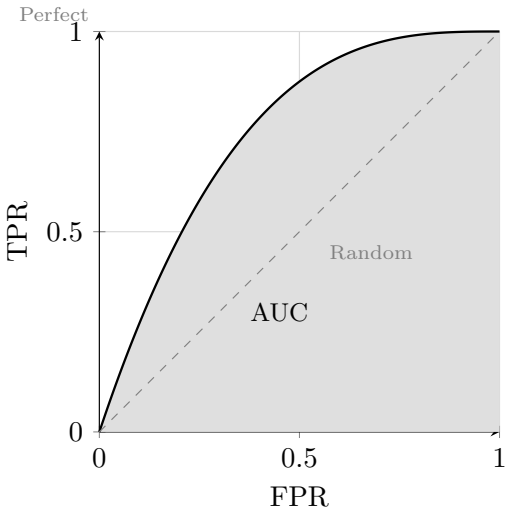
Key reference points:

- $\tau = 1$: all negative $\Rightarrow (0, 0)$
- $\tau = 0$: all positive $\Rightarrow (1, 1)$
- Diagonal = random guessing
- Top-left corner = perfect



Area Under the ROC Curve (AUC)

Definition: AUC

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AUC	**Interpretation**
1.0	Perfect classifier
0.5	Random guessing (no discriminative power)
< 0.5	Worse than random (invert predictions)

ROC Curve: Worked Example

Example

10 patients, $P = 5$, $N = 5$, sorted by score:

τ	TP	FP	TPR	FPR
> 0.95	0	0	0.0	0.0
0.95	1	0	0.2	0.0
0.90	2	0	0.4	0.0
0.82	2	1	0.4	0.2
0.65	4	1	0.8	0.2
0.40	5	2	1.0	0.4
≤ 0.10	5	5	1.0	1.0

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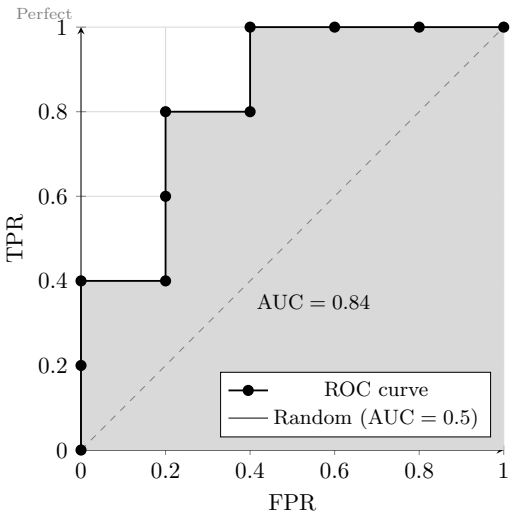
$\mathrm{AUC} = \mathbf{0.84}$



ROC vs. Precision-Recall Curves

- The ROC curve can be **overly optimistic** under class imbalance
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	ROC/AUC	**PR Curve**
Balanced classes	Appropriate	Appropriate
Imbalanced classes	Can be misleading	Preferred

The Flaw of Evaluating on Training Data

Training error is a **systematically optimistic** estimate of generalization error.

- A complex model can achieve near-perfect training scores yet fail on new data
- Training error $\neq$ generalization error
- We need a procedure to estimate performance on **unseen data**

The Simple Validation Set

Split data into two disjoint parts:

1. Train $\hat{f}$ on D_{train} (e.g., 80%)
2. Evaluate on D_{val} (e.g., 20%)

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Two critical drawbacks:

1. **High variance:** The estimate depends heavily on the random split
2. **Data inefficiency:** The model is trained on less data $\Rightarrow$ systematically worse

Validation Set: Instability Example

Example

Dataset: $n = 10$, linear model. Two different 80/20 splits:

Split A (val $= \{(5, 11), (6, 12)\}$):

$$\mathrm{MSE}^{(A)} \approx 0.71$$

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A **12$\times$ difference** from the same model on the same data—the estimate is unreliable!

k-Fold Cross-Validation

Definition: k-Fold Cross-Validation

1. **Partition** D into k disjoint folds $D_1, \ldots, D_k$
2. **For each** $i = 1, \ldots, k$:
   - Train $\hat{f}_i$ on $D \setminus D_i$
   - Evaluate metric M_i on D_i
3. **Average:**

$$\boxed{\mathrm{CV}_k = \frac{1}{k} \sum_{i=1}^{k} M_i}$$

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Every data point is used for validation **exactly once**. Common choices: $k = 5$ or $k = 10$.

k-Fold CV: Visual Representation

$$\mathrm{CV}_k = \frac{1}{k} \sum_{i=1}^{k} M_i$$

5-Fold CV: Worked Example

Example

Same dataset ($n = 10$), linear model, 5 folds of size 2:

Fold	Validation set	OLS on remaining	M_i
1	$\{(1,3),\ (2,5)\}$	$\hat{y} \approx -0.86 + 2.29x$	2.06
2	$\{(3,7),\ (4,8)\}$	$\hat{y} \approx 0.29 + 2.14x$	0.40
3	$\{(5,11),\ (6,12)\}$	$\hat{y} \approx 0.29 + 2.15x$	0.71
4	$\{(7,15),\ (8,16)\}$	$\hat{y} \approx 0.08 + 2.21x$	1.68
5	$\{(9,19),\ (10,24)\}$	$\hat{y} \approx 1.11 + 1.89x$	8.35

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$$\mathrm{CV}_5 = \frac{2.06 + 0.40 + 0.71 + 1.68 + 8.35}{5} = \mathbf{2.64}$$

More representative than either Split A (0.71) or Split B (8.35).

Bias and Variance of the CV Estimator

The CV score CV_k is itself an **estimator**—it has its own bias and variance.

Bias of CV_k:

- Each fold trains on $\frac{k-1}{k} \cdot n$ data
- Less data $\Rightarrow$ worse model $\Rightarrow$ pessimistic estimate
- Small k: high bias
- Large k: low bias

Variance of CV_k:

- Large k: training sets highly overlap
- Models $\hat{f}_i$ are correlated
- Averaging correlated estimates $\Rightarrow$ variance doesn't decrease much
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A **meta-level** bias-variance tradeoff in the choice of k!

Leave-One-Out Cross-Validation (LOOCV)

Definition: LOOCV

Special case $k = n$: each fold is a single observation.

$$\mathrm{CV}_n = \frac{1}{n}\sum_{i=1}^{n} e_i, \qquad e_i = L\big(y_i,\ \hat{f}_{-i}(x_i)\big)$$

where $\hat{f}_{-i}$ is trained on all data except (x_i, y_i).

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- Training size $= n - 1 \Rightarrow$ approximately **zero bias**
- Training sets overlap in $n - 2$ points $\Rightarrow$ **high variance**
- Requires training n models $\Rightarrow$ **computationally expensive**

Stratified k-Fold Cross-Validation

Definition: Stratified k-Fold CV

Variant where each fold preserves the **class proportions** of D:

$$\frac{|\{(x_i, y_i) \in D_j : y_i = c\}|}{|D_j|} \approx \frac{n_c}{n} \quad \text{for all folds } j \text{ and classes } c.$$

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Example

$n = 100$: 80 class-0, 20 class-1 (80/20 split), $k = 5$.

- **Unstratified:** some folds might get 0–1 minority instances
- **Stratified:** each fold gets exactly 16 class-0 and 4 class-1

Essential for **imbalanced classification** to get stable metric estimates.

Comparison of CV Methods

	Validation	**5/10-Fold**	**LOOCV**	**Stratified**
Training Size	$0.8n$	$\frac{k-1}{k}n$	$n-1$	$\frac{k-1}{k}n$
Bias	High	Moderate	Low	Moderate
Variance	High	Moderate	High	Moderate
Cost	Low	Moderate	High	Moderate
Best For	Large data	General	Small data	Imbalanced

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Default recommendation: 5- or 10-fold CV (stratified for classification).

CV for Model Selection

Example: Model Selection

Choose among polynomial degrees using 5-fold CV:

	M_1	M_2	M_3	M_4	M_5	CV_5
Linear ($d = 1$)	2.06	0.40	0.71	1.68	8.35	2.64
Quadratic ($d = 2$)	0.52	0.18	0.33	0.41	1.06	**0.50**
Cubic ($d = 3$)	0.61	0.25	0.40	0.55	1.89	0.74

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- Linear underfits; cubic overfits; **quadratic wins**
- Training MSE would favor the cubic model—CV correctly identifies overfitting!

CV for Hyperparameter Tuning

Example: Tuning Polynomial Degree

Test $d \in \{1, 2, 3, 4, 5\}$:

Degree d	CV_5 (MSE)
1	2.64
2	**0.50**
3	0.74
4	1.35
5	3.92

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- CV error is **U-shaped**: bias-variance tradeoff in action!
- Optimal: $d^* = 2$

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- Optimal: $d^* = 2$

Crucial step: After selecting d^*, retrain on the *entire* dataset D using $d = d^*$.

Key Takeaways

1. **Bias-Variance Decomposition:**

$$\mathbb{E}[(y_0 - \hat{f}(x_0))^2] = \text{Bias}^2 + \text{Var} + \sigma^2$$

   Error = systematic assumptions + instability + irreducible noise

2. **Regression Metrics:** MSE/RMSE measure absolute error; R^2 measures relative explained variance but *inflates with complexity*—use $\mathrm{R}^2_{\text{adj}}$

3. **Classification Metrics:** Accuracy fails under imbalance. Use the confusion matrix to derive Precision, Recall, and F_β. AUC provides threshold-independent evaluation

4. **Cross-Validation:** Never evaluate on training data. *k*-Fold CV provides a robust, nearly unbiased estimate of generalization error

5. **After selecting a model via CV:** Retrain on the *full* dataset before deployment