

# **Model Selection**

# **& Ensembles**

## **Choosing, Tuning, and Combining Models**

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# Learning Goals

By the end of this lecture, you will:

| Goal              | What You'll Learn                        |
|-------------------|--|
| <b>Understand</b> | Why models fail (bias vs variance)       |
| <b>Implement</b>  | Cross-validation for reliable evaluation |
| <b>Tune</b>       | Hyperparameters with Grid/Random search  |
| <b>Build</b>      | Ensemble models (Random Forest, XGBoost) |
| <b>Apply</b>      | Clustering when no labels exist          |

# The Story So Far

We know several algorithms:

| Algorithm           | Type           | When to Use          |
|---------------------|----------------|----------------------|
| Linear Regression   | Regression     | Linear relationships |
| Logistic Regression | Classification | Binary decisions     |
| Decision Trees      | Both           | Interpretable rules  |
| K-NN                | Both           | Similar items        |

**But how do we choose? And can we do better?**

# Today's Questions

1. Why does my model perform poorly on new data?
2. How do I reliably compare models?
3. How do I find the best settings for a model?
4. Can I combine models to get better results?
5. What if I don't have labels?

# **Part 1: Bias-Variance Tradeoff**

**The Fundamental Reason Models Fail**

# A Story of Two Mistakes

Imagine you're estimating someone's weight from their height.

| Mistake Type  | What Happened                       | The Problem |
|---------------|-------------------------------------|-------------|
| High Bias     | Used a flat line (everyone = 70 kg) | Too simple  |
| High Variance | Memorized every person exactly      | Too complex |

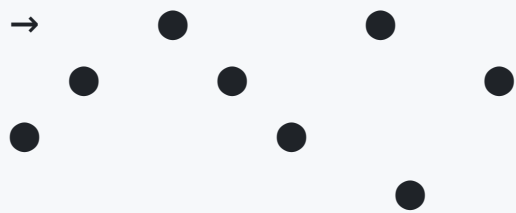
Every ML mistake is one of these two types!

# Underfitting: The Too-Simple Model

**Definition:** Model is too simple to capture the pattern.

Reality: Weight increases with height

Height →



Your Model: \_\_\_\_\_ (flat line: always predict average)

Problem: Doesn't capture the upward trend!

# Underfitting: Symptoms

| Symptom        | Value      |
|----------------|------------|
| Training Error | HIGH       |
| Test Error     | HIGH       |
| Model          | Too simple |

**Both errors are high** because the model can't even fit the training data!



# Overfitting: The Memorizer

**Definition:** Model is too complex and memorizes noise.

Training Data:

Height →  (with some measurement noise)

Your Model: ~~~~~ (wiggly line hitting every point)

Problem: When a new person comes, prediction is garbage!

# Overfitting: Symptoms

| Symptom        | Value               |
|----------------|---------------------|
| Training Error | LOW (near perfect!) |
| Test Error     | HIGH                |
| Model          | Too complex         |

**Big gap** between training and test error!

# The Goldilocks Model

**Goal:** A model that's "just right"



Captures the pattern, ignores the noise!

| Symptom        | Value |
|----------------|-------|
| Training Error | Low   |
| Test Error     | Low   |
| Gap            | Small |

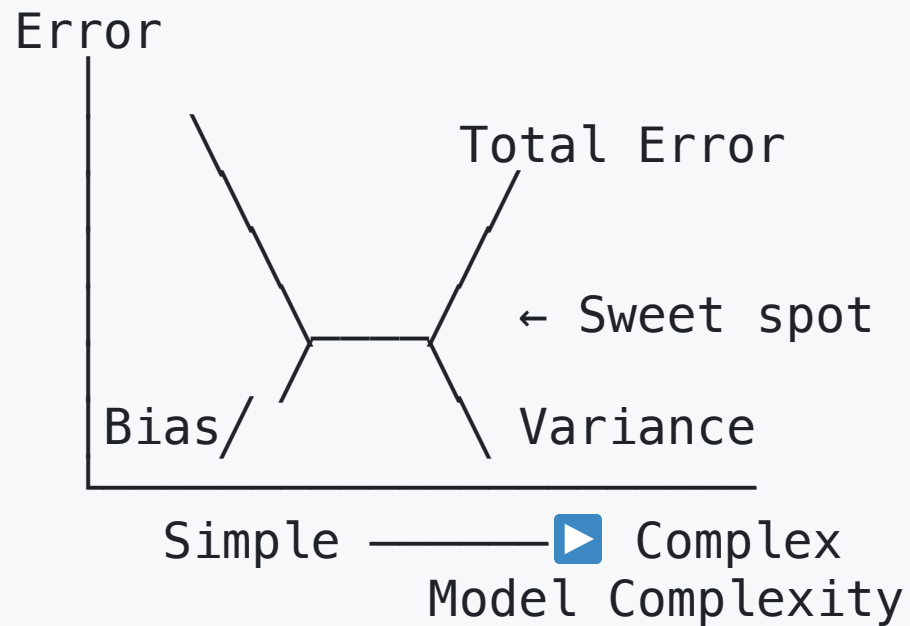
# Bias-Variance Decomposition

Mathematical view:

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

| Component               | What It Means                | Source            |
|-------------------------|------------------------------|-------------------|
| <b>Bias<sup>2</sup></b> | Error from wrong assumptions | Model too simple  |
| <b>Variance</b>         | Sensitivity to training data | Model too complex |
| <b>Noise</b>            | Random error in data         | Can't reduce      |

# The Tradeoff Visualized



**You can't minimize both simultaneously!**

# Bias-Variance in Different Models

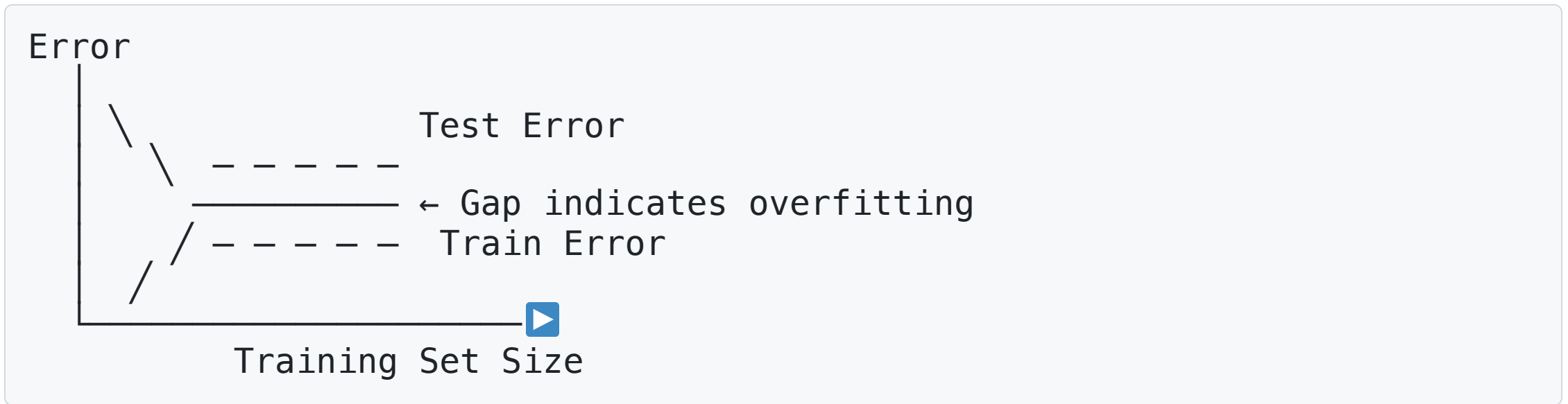
| Model                    | Complexity | Bias   | Variance |
|--------------------------|------------|--------|----------|
| Linear Regression        | Low        | High   | Low      |
| Polynomial (degree 2)    | Medium     | Medium | Medium   |
| Polynomial (degree 20)   | High       | Low    | High     |
| Decision Tree (depth 3)  | Low        | High   | Low      |
| Decision Tree (depth 50) | High       | Low    | High     |

# Diagnosing Your Model

| Train Error | Test Error | Diagnosis       | Fix             |
|-------------|------------|-----------------|-----------------|
| High        | High       | Underfitting    | More complexity |
| Low         | High       | Overfitting     | Less complexity |
| Low         | Low        | Good fit!       | Deploy it       |
| High        | Low        | Something weird | Check for bugs  |

# Learning Curves

Plot error vs training set size:



**More data helps reduce overfitting!**



# Solutions for Overfitting

| Technique        | How It Helps             |
|------------------|--------------------------|
| More data        | Harder to memorize       |
| Simpler model    | Less capacity to overfit |
| Regularization   | Penalize complexity      |
| Early stopping   | Stop before memorizing   |
| Cross-validation | Better evaluation        |
| Ensemble methods | Average out variance     |

# Solutions for Underfitting

| Technique           | How It Helps                |
|---------------------|-----------------------------|
| More features       | Give model more information |
| More complex model  | Increase capacity           |
| Less regularization | Let model be more flexible  |
| Feature engineering | Create better features      |
| Polynomial features | Capture non-linear patterns |

## **Part 2: Cross-Validation**

### **Getting Reliable Performance Estimates**

# The Problem with Train/Test Split

```
from sklearn.model_selection import train_test_split

# Try different random seeds
for seed in [1, 2, 3, 4, 5]:
    X_train, X_test, y_train, y_test = train_test_split(
        X, y, test_size=0.2, random_state=seed)
    model.fit(X_train, y_train)
    print(f"Seed {seed}: {model.score(X_test, y_test):.2%}")
```

```
Seed 1: 87%
Seed 2: 92% ← Which one should we believe?
Seed 3: 84%
Seed 4: 90%
Seed 5: 88%
```

# The Lucky/Unlucky Split Problem

What if your test set happened to contain:

| Scenario              | Accuracy | Reality            |
|-----------------------|----------|--------------------|
| Easy examples only    | 95%      | Overly optimistic  |
| Hard examples only    | 80%      | Overly pessimistic |
| Representative sample | 88%      | Realistic          |

**One split = One roll of the dice**

# K-Fold Cross-Validation

**Idea:** Use EVERY data point for both training AND testing!

Data: [1] [2] [3] [4] [5] [6] [7] [8] [9] [10]

Fold 1: [TEST 1-2] [TRAIN 3-10] → Score: 0.87

Fold 2: [TRAIN 1-2] [TEST 3-4] [TRAIN 5-10] → Score: 0.89

Fold 3: [TRAIN 1-4] [TEST 5-6] [TRAIN 7-10] → Score: 0.91

Fold 4: [TRAIN 1-6] [TEST 7-8] [TRAIN 9-10] → Score: 0.88

Fold 5: [TRAIN 1-8] [TEST 9-10] → Score: 0.90

Final Score: 0.89 ± 0.01

## Visual: 5-Fold Cross-Validation

| Data:     | Fold 1 | Fold 2 | Fold 3 | Fold 4 | Fold 5 |
|-----------|--------|--------|--------|--------|--------|
| Portion 1 | TEST   | Train  | Train  | Train  | Train  |
| Portion 2 | Train  | TEST   | Train  | Train  | Train  |
| Portion 3 | Train  | Train  | TEST   | Train  | Train  |
| Portion 4 | Train  | Train  | Train  | TEST   | Train  |
| Portion 5 | Train  | Train  | Train  | Train  | TEST   |

Every portion is used for testing exactly ONCE

# K-Fold in sklearn

```
from sklearn.model_selection import cross_val_score
from sklearn.tree import DecisionTreeClassifier

model = DecisionTreeClassifier(max_depth=5)

# 5-fold cross-validation
scores = cross_val_score(model, X, y, cv=5)

print(f"Fold scores: {scores}")
# [0.87, 0.89, 0.91, 0.88, 0.90]

print(f"Mean: {scores.mean():.3f}") # 0.890
print(f"Std: {scores.std():.3f}") # 0.015
```



# Interpreting Cross-Validation Results

```
scores = [0.87, 0.89, 0.91, 0.88, 0.90]
```

| Metric | Value | Meaning              |
|--------|-------|----------------------|
| Mean   | 0.890 | Expected performance |
| Std    | 0.015 | Model stability      |
| Min    | 0.87  | Worst case           |
| Max    | 0.91  | Best case            |

**Low std = Stable model**

**High std = Model performance varies a lot**

# Choosing K

| K  | Name          | Pros           | Cons          |
|----|---------------|----------------|---------------|
| 5  | 5-Fold        | Fast, standard | Less reliable |
| 10 | 10-Fold       | More reliable  | Slower        |
| n  | Leave-One-Out | Uses all data  | Very slow     |

## Rule of thumb:

- Small dataset (< 1000): Use 10-fold
- Medium dataset: Use 5-fold
- Large dataset (> 10000): Even 3-fold is fine

# Stratified K-Fold

**Problem:** What if your classes are imbalanced?

```
# Original data: 900 class 0, 100 class 1  
# Random fold might get: 200 class 0, 0 class 1 ← Bad!
```

**Solution:** Stratified K-Fold maintains class proportions

```
from sklearn.model_selection import cross_val_score, StratifiedKFold  
  
skf = StratifiedKFold(n_splits=5, shuffle=True, random_state=42)  
scores = cross_val_score(model, X, y, cv=skf)
```

# Comparing Models with Cross-Validation

```
from sklearn.linear_model import LogisticRegression
from sklearn.tree import DecisionTreeClassifier
from sklearn.neighbors import KNeighborsClassifier

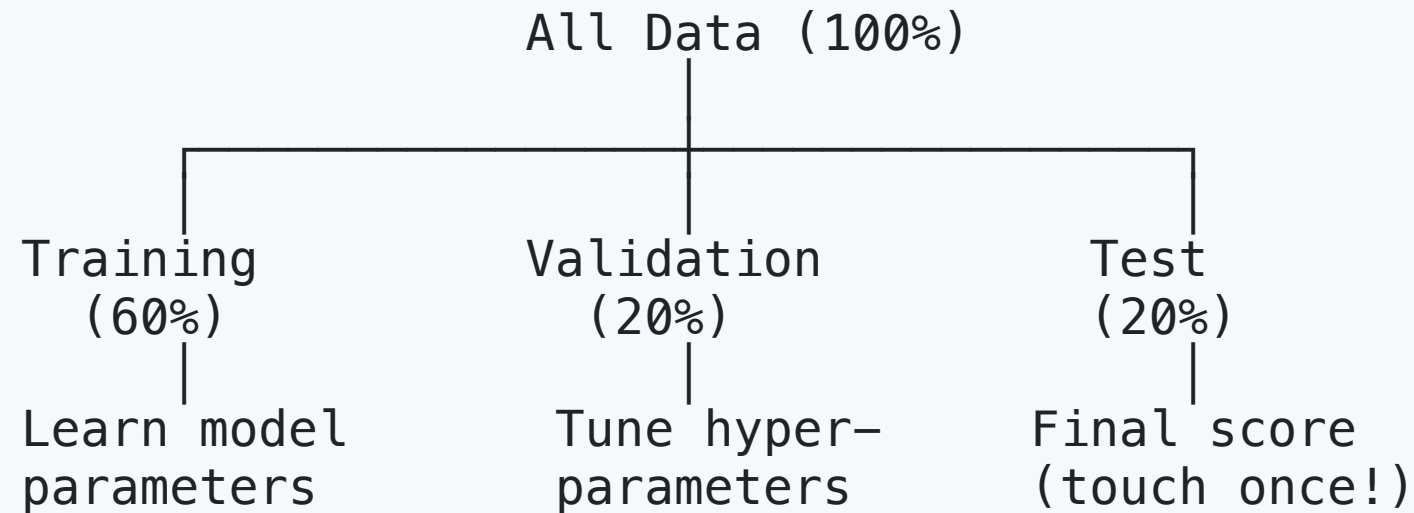
models = {
    'Logistic': LogisticRegression(),
    'Tree': DecisionTreeClassifier(max_depth=5),
    'KNN': KNeighborsClassifier(n_neighbors=5)
}

for name, model in models.items():
    scores = cross_val_score(model, X, y, cv=5)
    print(f"{name}: {scores.mean():.3f} ± {scores.std():.3f}")
```

```
Logistic: 0.850 ± 0.020
Tree:      0.890 ± 0.015 ← Winner
KNN:       0.870 ± 0.025
```

# The Three-Way Split

For model selection AND final evaluation:



# Why Three Sets?

| Set        | Purpose                                | When to Use           |
|------------|--|-----------------------|
| Training   | Learn model parameters                 | During fit()          |
| Validation | Choose hyperparameters, compare models | During tuning         |
| Test       | Final evaluation                       | Only at the very end! |

**Never tune on test set!** It defeats the purpose of having one.

# **Part 3: Hyperparameter Tuning**

## **Finding the Best Model Settings**

# Parameters vs Hyperparameters

| Type            | Set By    | When            | Example                |
|-----------------|-----------|-----------------|------------------------|
| Parameters      | Algorithm | During training | Weights in regression  |
| Hyperparameters | You       | Before training | max_depth, n_neighbors |

```
# Hyperparameter (you choose)
model = DecisionTreeClassifier(max_depth=5)

# Parameters (learned automatically)
model.fit(X, y)
print(model.tree_.feature) # Learned split features
```



# Common Hyperparameters

| Model         | Hyperparameter   | What It Controls | Range        |
|---------------|------------------|------------------|--------------|
| Decision Tree | max_depth        | Tree depth       | 1 to 20+     |
| Decision Tree | min_samples_leaf | Leaf size        | 1 to 50      |
| K-NN          | n_neighbors      | Neighbors to use | 1 to 50      |
| Logistic Reg  | C                | Regularization   | 0.001 to 100 |
| Random Forest | n_estimators     | Number of trees  | 10 to 500    |

# Manual Tuning: Trial and Error

```
# Try different max_depth values
for depth in [3, 5, 7, 10, 15]:
    model = DecisionTreeClassifier(max_depth=depth)
    scores = cross_val_score(model, X, y, cv=5)
    print(f"depth={depth}: {scores.mean():.3f}")
```

```
depth=3:    0.820
depth=5:    0.870
depth=7:    0.890 ← Best
depth=10:   0.880
depth=15:   0.840 ← Overfitting starts
```

**Works but tedious for multiple hyperparameters!**

# Grid Search: Automated Tuning

Try ALL combinations systematically:

| max_depth | min_samples_leaf | Score              |
|-----------|------------------|--------------------|
| 3         | 1                | 0.82               |
| 3         | 5                | 0.83               |
| 3         | 10               | 0.81               |
| 5         | 1                | 0.87               |
| 5         | 5                | 0.88               |
| 5         | 10               | <b>0.89</b> ← Best |
| 7         | 1                | 0.86               |
| ...       | ...              | ...                |

# GridSearchCV in sklearn

```
from sklearn.model_selection import GridSearchCV
from sklearn.tree import DecisionTreeClassifier

# Define the grid of values to try
param_grid = {
    'max_depth': [3, 5, 7, 10],
    'min_samples_leaf': [1, 5, 10, 20]
}

# Create and run the search
grid_search = GridSearchCV(
    DecisionTreeClassifier(),
    param_grid,
    cv=5,                    # 5-fold cross-validation
    scoring='accuracy'      # Metric to optimize
)
grid_search.fit(X_train, y_train)
```

# GridSearchCV Results

```
# Best hyperparameters
print(f"Best params: {grid_search.best_params_}")
# {'max_depth': 5, 'min_samples_leaf': 10}

# Best cross-validation score
print(f"Best CV score: {grid_search.best_score_:.3f}")
# 0.890

# Get the best model (already fitted!)
best_model = grid_search.best_estimator_

# Evaluate on test set
test_score = best_model.score(X_test, y_test)
print(f"Test score: {test_score:.3f}")
# 0.885
```

# Viewing All Results

```
import pandas as pd

results = pd.DataFrame(grid_search.cv_results_)
print(results[['param_max_depth', 'param_min_samples_leaf',
               'mean_test_score', 'rank_test_score']])
```

|     | param_max_depth | param_min_samples_leaf | mean_test_score | rank_test_score |        |
|-----|-----------------|------------------------|-----------------|-----------------|--------|
| 0   | 3               | 1                      | 0.820           | 12              |        |
| 1   | 3               | 5                      | 0.830           | 10              |        |
| 2   | 3               | 10                     | 0.810           | 14              |        |
| 3   | 5               | 1                      | 0.870           | 6               |        |
| 4   | 5               | 5                      | 0.880           | 3               |        |
| 5   | 5               | 10                     | 0.890           | 1               | ← Best |
| ... |                 |                        |                 |                 |        |

# The Explosion Problem

Grid search with 5 hyperparameters, 10 values each:

$$10 \times 10 \times 10 \times 10 \times 10 = 100,000 \text{ combinations!}$$

With 5-fold CV: 500,000 model trainings!

| Combinations | Time (1 sec/train) |
|--------------|--------------------|
| 100          | 8 minutes          |
| 1,000        | 1.4 hours          |
| 10,000       | 14 hours           |
| 100,000      | 6 days             |

# Random Search: Smart Sampling

**Idea:** Don't try everything, sample randomly!

```
from sklearn.model_selection import RandomizedSearchCV
from scipy.stats import randint

param_dist = {
    'max_depth': randint(1, 20),           # Random 1–20
    'min_samples_leaf': randint(1, 50),    # Random 1–50
    'min_samples_split': randint(2, 50)    # Random 2–50
}

random_search = RandomizedSearchCV(
    DecisionTreeClassifier(),
    param_dist,
    n_iter=50,      # Only try 50 random combinations
    cv=5,
    random_state=42
)
random_search.fit(X_train, y_train)
```



# Grid vs Random Search

| Aspect            | Grid Search          | Random Search         |
|-------------------|----------------------|-----------------------|
| Coverage          | All combinations     | Sample of space       |
| Time              | Slow for large grids | Controllable (n_iter) |
| Continuous params | Must discretize      | Can sample directly   |
| Best for          | Few params           | Many params           |

Random search often finds good solutions faster than grid search!

# Practical Tuning Strategy

| Step             | What to Do                              |
|------------------|---|
| 1. Baseline      | Train with defaults, get baseline score |
| 2. Coarse search | Random search with wide ranges          |
| 3. Fine search   | Grid search around best area            |
| 4. Final eval    | Test on held-out test set               |

```
# Start wide
RandomizedSearchCV(model, wide_params, n_iter=100)

# Then narrow down
GridSearchCV(model, narrow_params, cv=5)
```

# **Part 4: Ensemble Methods**

## **The Wisdom of Crowds**

# Why Ensembles Work

One person guessing jar of marbles: Often wrong

1000 people averaging guesses: Usually close!

| Individual | Guess |
|------------|-------|
| Person 1   | 520   |
| Person 2   | 680   |
| Person 3   | 450   |
| ...        | ...   |
| Average    | 503   |
| Actual     | 500   |

Errors cancel out!

# The Same Idea in ML

**One decision tree:** May overfit, unstable

**100 decision trees averaged:** Robust, accurate

| Single Model         | Ensemble             |
|----------------------|----------------------|
| High variance        | Reduced variance     |
| Biased view          | Diverse perspectives |
| One mistake ruins it | Errors average out   |
| Unstable             | Stable               |

# Two Ensemble Strategies

| Strategy        | Key Idea                     | How It Reduces Error |
|-----------------|------------------------------|----------------------|
| <b>Bagging</b>  | Average many parallel models | Reduces variance     |
| <b>Boosting</b> | Build models sequentially    | Reduces bias         |

# Bagging: Bootstrap Aggregating

## Steps:

1. **Bootstrap:** Create random subsets of data (with replacement)
2. **Train:** Fit a model on each subset
3. **Aggregate:** Average predictions (regression) or vote (classification)

Original Data: [1, 2, 3, 4, 5, 6, 7, 8, 9, 10]

Bootstrap 1: [1, 1, 3, 4, 6, 6, 7, 9, 9, 10] → Model 1

Bootstrap 2: [2, 2, 3, 5, 5, 6, 8, 8, 9, 10] → Model 2

Bootstrap 3: [1, 3, 4, 4, 5, 7, 7, 8, 10, 10] → Model 3

Final: Average(Model 1, Model 2, Model 3)

# Random Forest

## Bagging + Decision Trees + Feature Randomization

| Component        | What It Does           |
|------------------|------------------------|
| Many trees       | Reduce variance        |
| Random samples   | Different perspectives |
| Random features  | Decorrelate trees      |
| Voting/Averaging | Combine predictions    |

```
from sklearn.ensemble import RandomForestClassifier

model = RandomForestClassifier(
    n_estimators=100,      # 100 trees
    max_depth=10,         # Limit tree depth
    random_state=42
```



# Why Random Forest Works

```
Tree 1: Uses features [A, B, C] → Predicts: Class 1
Tree 2: Uses features [B, D, E] → Predicts: Class 0
Tree 3: Uses features [A, C, F] → Predicts: Class 1
Tree 4: Uses features [D, E, F] → Predicts: Class 1
...
Tree 100: Uses features [A, E, G] → Predicts: Class 1

Vote: 70 trees say Class 1, 30 say Class 0
Final Prediction: Class 1
```

**Each tree makes different mistakes → Average is better!**

# Random Forest: Key Hyperparameters

| Parameter        | What It Does        | Good Values      |
|------------------|---------------------|------------------|
| n_estimators     | Number of trees     | 100-500          |
| max_depth        | Tree depth          | 10-30 or None    |
| min_samples_leaf | Min samples in leaf | 1-10             |
| max_features     | Features per split  | 'sqrt' or 'log2' |

```
model = RandomForestClassifier(  
    n_estimators=200,  
    max_depth=15,  
    max_features='sqrt',  
    random_state=42  
)
```

# Feature Importance from Random Forest

```
import pandas as pd

# Train model
model.fit(X_train, y_train)

# Get importance
importance = pd.DataFrame({
    'feature': feature_names,
    'importance': model.feature_importances_
}).sort_values('importance', ascending=False)

print(importance.head(10))
```

|     | feature      | importance |
|-----|--------------|------------|
| 0   | income       | 0.25       |
| 1   | age          | 0.18       |
| 2   | credit_score | 0.15       |
| ... |              |            |

# Boosting: Learning from Mistakes

**Key Idea:** Each model focuses on what previous models got wrong.

Round 1: Train model on all data  
Some examples misclassified (X)

Round 2: Train new model, weight misclassified X higher  
Fixes some errors, might make new ones

Round 3: Focus even more on remaining errors  
...

Final: Combine all models (weighted vote)

# Gradient Boosting

```
from sklearn.ensemble import GradientBoostingClassifier

model = GradientBoostingClassifier(
    n_estimators=100,      # Number of boosting rounds
    learning_rate=0.1,     # Step size (smaller = slower but better)
    max_depth=3,          # Shallow trees work best
    random_state=42
)
model.fit(X_train, y_train)
```

# XGBoost: The Competition Winner

```
# pip install xgboost
from xgboost import XGBClassifier

model = XGBClassifier(
    n_estimators=100,
    learning_rate=0.1,
    max_depth=5,
    random_state=42
)
model.fit(X_train, y_train)

# Often wins Kaggle competitions!
```

**XGBoost = Extreme Gradient Boosting**

Faster, more regularized, handles missing values.

# Bagging vs Boosting

| Aspect           | Bagging             | Boosting            |
|------------------|---------------------|---------------------|
| Goal             | Reduce variance     | Reduce bias         |
| Training         | Parallel (fast)     | Sequential (slower) |
| Trees            | Independent         | Build on each other |
| Overfitting risk | Low                 | Higher              |
| Example          | Random Forest       | XGBoost, LightGBM   |
| When to use      | High variance model | High bias model     |

# Ensemble Comparison

| Model         | Speed  | Accuracy  | Interpretable? |
|---------------|--------|-----------|----------------|
| Decision Tree | Fast   | Medium    | Yes            |
| Random Forest | Medium | High      | Somewhat       |
| XGBoost       | Slow   | Very High | No             |
| LightGBM      | Fast   | Very High | No             |

**Start with Random Forest** - great out of the box.

**Use XGBoost/LightGBM** when you need maximum accuracy.



# Practical Example

```
from sklearn.ensemble import RandomForestClassifier, GradientBoostingClassifier
from xgboost import XGBClassifier

models = {
    'Random Forest': RandomForestClassifier(n_estimators=100),
    'Gradient Boosting': GradientBoostingClassifier(n_estimators=100),
    'XGBoost': XGBClassifier(n_estimators=100)
}

for name, model in models.items():
    scores = cross_val_score(model, X, y, cv=5)
    print(f"{name}: {scores.mean():.3f} ± {scores.std():.3f}")
```

```
Random Forest:      0.925 ± 0.015
Gradient Boosting:  0.932 ± 0.012
XGBoost:            0.938 ± 0.010 ← Best
```

# **Part 5: Unsupervised Learning**

## **Learning Without Labels**

# The Unsupervised Problem

**Supervised:** You have  $X$  (features) and  $y$  (labels)

**Unsupervised:** You only have  $X$  (no labels!)

| Supervised                 | Unsupervised        |
|----------------------------|---------------------|
| Email → Spam/Not Spam      | Email → ???         |
| Image → Cat/Dog            | Customers → ???     |
| Price history → Next price | Similar items → ??? |

# Why Unsupervised?

| Use Case              | What You Want              |
|-----------------------|----------------------------|
| Customer Segmentation | Group similar customers    |
| Anomaly Detection     | Find unusual patterns      |
| Data Compression      | Reduce dimensions          |
| Visualization         | Plot high-dimensional data |
| Feature Learning      | Discover useful features   |

# Clustering: Finding Groups

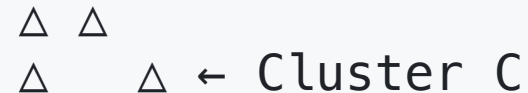
**Goal:** Group similar items together automatically.

Before Clustering:



→

After Clustering:



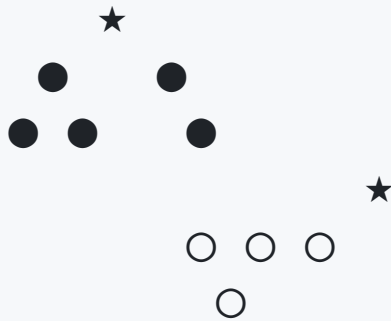
# K-Means: The Most Popular

Algorithm:

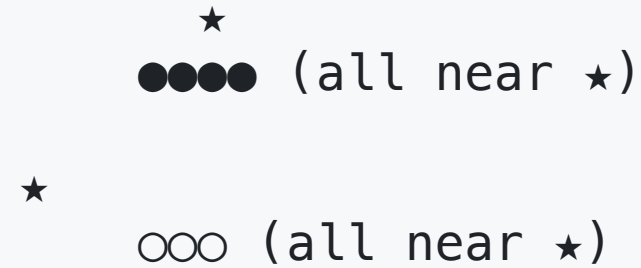
| Step          | What Happens                   |
|---------------|--------------------------------|
| 1. Initialize | Place K random centroids       |
| 2. Assign     | Each point → nearest centroid  |
| 3. Update     | Move centroids to cluster mean |
| 4. Repeat     | Until centroids stop moving    |

# K-Means Visualization

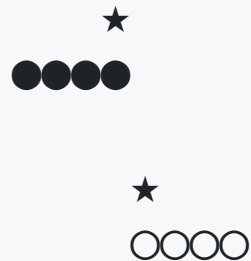
Step 1: Random centroids



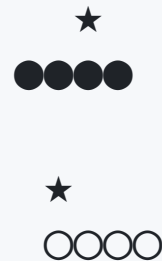
Step 2: Assign points



Step 3: Move centroids



Step 4: Converged!



# K-Means in sklearn

```
from sklearn.cluster import KMeans

# Create and fit
model = KMeans(
    n_clusters=3,          # How many clusters?
    random_state=42
)
model.fit(X)

# Get results
labels = model.labels_      # Which cluster is each point in?
centers = model.cluster_centers_ # Where are the centers?

# Assign new points
new_labels = model.predict(X_new)
```



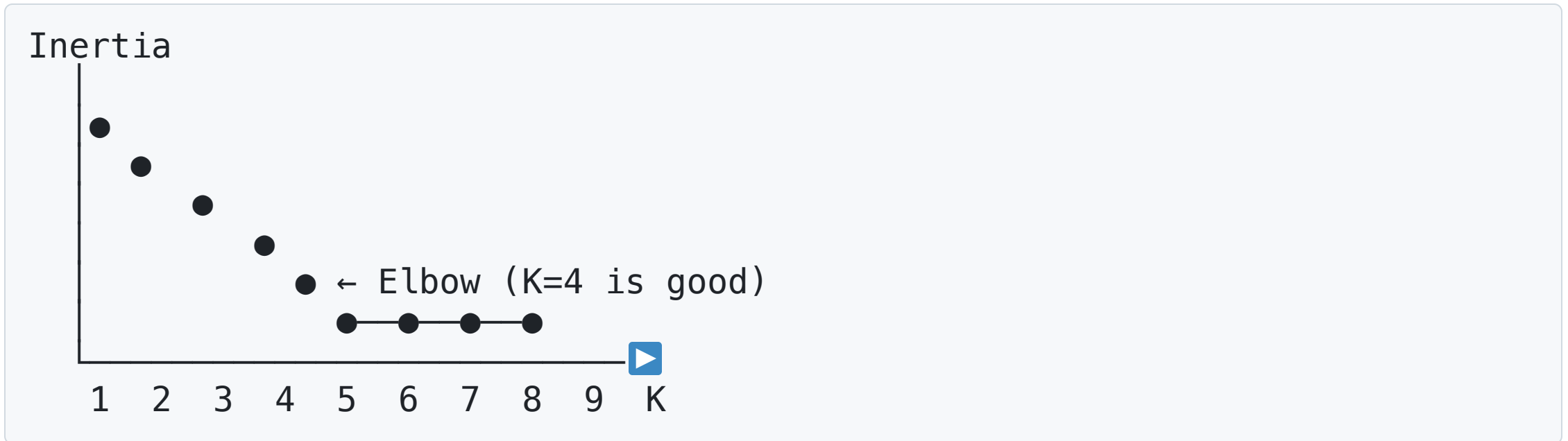
# Choosing K: The Elbow Method

Plot "inertia" (within-cluster sum of squares) vs K:

```
inertias = []  
for k in range(1, 11):  
    model = KMeans(n_clusters=k, random_state=42)  
    model.fit(X)  
    inertias.append(model.inertia_)  
  
plt.plot(range(1, 11), inertias, marker='o')  
plt.xlabel('K (number of clusters)')  
plt.ylabel('Inertia')
```

Look for the "elbow" - where improvement slows down

# Elbow Plot



After the elbow, adding more clusters doesn't help much.

# Dimensionality Reduction

**Problem:** Can't visualize 100 features!

**Solution:** Reduce to 2-3 dimensions while preserving structure.

| Method | Type       | Best For                  |
|--------|------------|---------------------------|
| PCA    | Linear     | General use, fast         |
| t-SNE  | Non-linear | Visualization             |
| UMAP   | Non-linear | Visualization + structure |

# PCA: Principal Component Analysis

**Idea:** Find directions of maximum variance.

```
from sklearn.decomposition import PCA

# Reduce 100 dimensions → 2 dimensions
pca = PCA(n_components=2)
X_2d = pca.fit_transform(X) # X was 100D, now 2D

# Visualize
plt.scatter(X_2d[:, 0], X_2d[:, 1], c=labels)
plt.xlabel('PC1')
plt.ylabel('PC2')
```

# How Much Variance Explained?

```
pca = PCA(n_components=10)
pca.fit(X)

# How much does each component explain?
print(pca.explained_variance_ratio_)
# [0.35, 0.20, 0.12, 0.08, 0.06, 0.05, 0.04, 0.03, 0.02, 0.02]

# Cumulative
import numpy as np
print(np.cumsum(pca.explained_variance_ratio_))
# [0.35, 0.55, 0.67, 0.75, 0.81, 0.86, 0.90, 0.93, 0.95, 0.97]

# 10 components explain 97% of the variance!
```

# t-SNE: Better Visualization

```
from sklearn.manifold import TSNE

# Better for visualization (preserves local structure)
tsne = TSNE(
    n_components=2,
    perplexity=30,          # Balance local/global
    random_state=42
)
X_2d = tsne.fit_transform(X)

plt.scatter(X_2d[:, 0], X_2d[:, 1], c=labels)
```

**t-SNE often reveals clusters that PCA misses!**

# PCA vs t-SNE

| Aspect        | PCA                      | t-SNE         |
|---------------|--------------------------|---------------|
| Type          | Linear                   | Non-linear    |
| Speed         | Fast                     | Slow          |
| Interpretable | Yes (axes have meaning)  | No            |
| Best for      | Preprocessing, reduction | Visualization |
| New data      | Can transform            | Need to refit |

# Anomaly Detection

**Goal:** Find the "odd ones out"

```
from sklearn.ensemble import IsolationForest

# Detect anomalies
model = IsolationForest(
    contamination=0.05, # Expect 5% anomalies
    random_state=42
)
model.fit(X)

# Predict: 1 = normal, -1 = anomaly
predictions = model.predict(X)
anomalies = X[predictions == -1]
```



# Summary Table

| Task              | No Labels        | With Labels            |
|-------------------|------------------|------------------------|
| Grouping          | K-Means, DBSCAN  | -                      |
| Visualization     | PCA, t-SNE       | -                      |
| Outlier detection | Isolation Forest | -                      |
| Prediction        | -                | All supervised methods |

# Putting It All Together

| Step | What to Do                     | Tools                            |
|------|--------------------------------|----------------------------------|
| 1    | Start with simple baseline     | LogisticRegression, DecisionTree |
| 2    | Evaluate with cross-validation | cross_val_score                  |
| 3    | Tune hyperparameters           | GridSearchCV, RandomizedSearchCV |
| 4    | Try ensembles                  | RandomForest, XGBoost            |
| 5    | Final evaluation on test set   | accuracy_score, etc.             |

# Key Takeaways

1. **Bias-Variance Tradeoff:** Can't minimize both - find the balance
2. **Cross-Validation:** Always use it - single split is unreliable
3. **Hyperparameter Tuning:** Grid search for small spaces, random for large
4. **Ensembles:** Combine models for better performance
  - Bagging (Random Forest) reduces variance
  - Boosting (XGBoost) reduces bias
5. **Unsupervised:** Clustering and dimensionality reduction when no labels

# You Can Now Select & Tune Models!

## Next: Neural Networks - Deep Learning Begins

**Lab:** Cross-validation, hyperparameter tuning, Random Forest

*"Ensemble methods: Because two heads are better than one!"*

**Questions?**