Lecture 4: Bias-Variance Tradeoff & Cross-Validation

ECE 2410 – Introduction to Machine Learning

Farzad Farnoud

University of Virginia

Spring 2026

Outline

Last Time: Implementing kNN

Key concepts from L03:

- Train/Test split for evaluation
- Images as vectors (flattening)
- Data normalization (Min-Max, Z-score)
- Classification performance metrics: accuracy, precision, recall

What we can do now:

1. Load real datasets (MNIST, NBA)
2. Split into train/test
3. Normalize features
4. Classify with kNN
5. Measure performance

The Big Question

🤔 How do we choose k?

- We've been using $k = 3$ or $k = 5$... why?
- Different k values give different accuracies
- What makes one model "better" than another?

Today's Goals:

1. Understand **why** some models fail (overfitting/underfitting)
2. Learn to **diagnose** issues (bias-variance tradeoff)
3. Know **how** to choose hyperparameters (cross-validation)

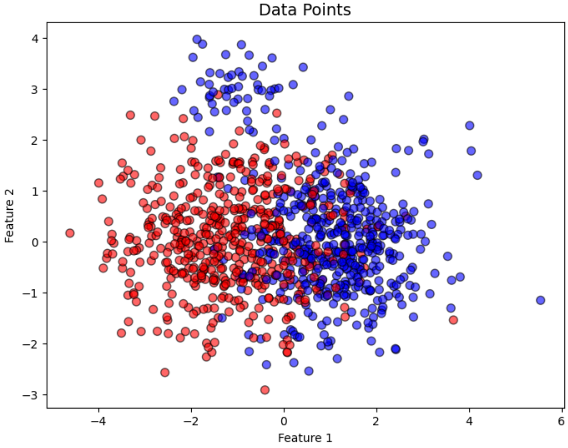
The Setup: Building a Classifier

The Goal:

- We have a dataset (Red vs Blue points).
- We want to separate them.
- The data clearly has some structure (a curved boundary), but also noise.

The Experiment:

- Let's divide this data into **4 disjoint subsets**.
- We will train a kNN model on each subset.
- **Question:** How much does the decision boundary change between subsets?



Possible Outcomes: What are we looking for?

Before we run the models, let's predict what **could** happen:

Scenario A: Variability

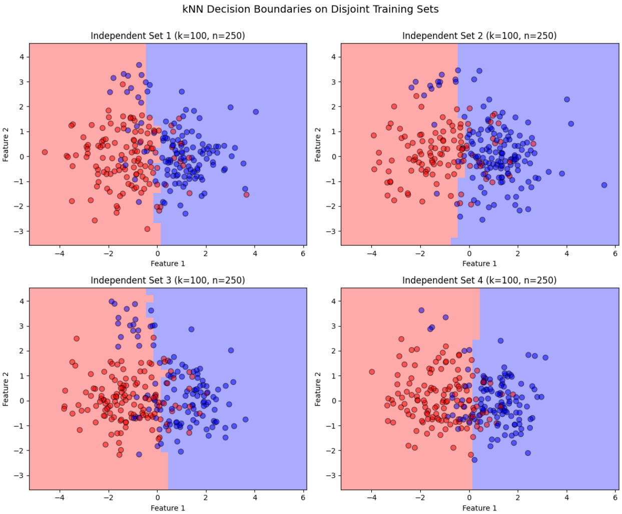
- The 4 models look **quite different**.
- Bad! At least some of them are wrong. Probably all of them (no reason to believe they perform differently).
- This is **High Variance**.

Scenario B: Stability

- The 4 models look **similar**.
- Good? Possibly yes, if they are capturing true patterns.
- Risk: Maybe they are all *wrong in the same way*? This is **High Bias**.

Ideally, training with different datasets from the same population (same underlying patterns) should give **similar** models that **capture the true patterns**.

Result 1: kNN with Large k ($k = 100$)



Result 1: Underfitting ($k = 100$)

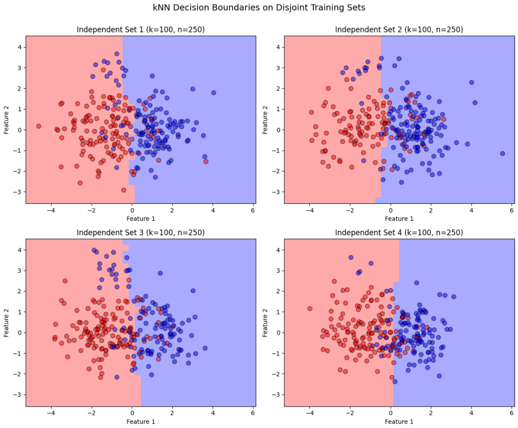
Observations:

- Boundaries are very smooth and nearly identical across subsets
- Low Variance (Stable)
- But wrong in the same way (systematic/consistent error): High Bias

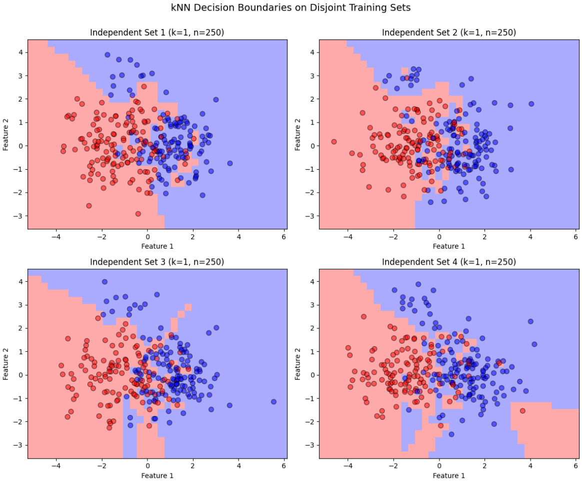
What happens:

- Model is too simple
- Fails to capture complex patterns

In kNN: $k = N$ always predicts majority class



Result 2: kNN with Small k ($k = 1$)



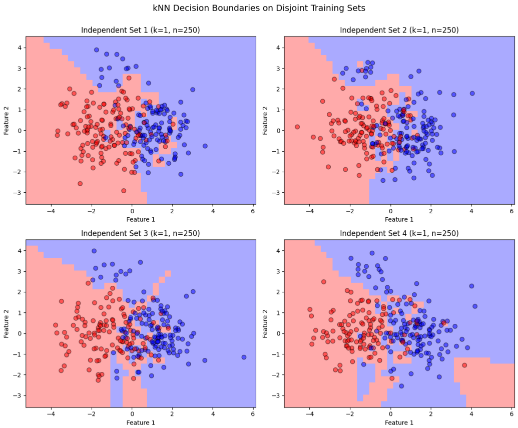
Observations:

- Boundaries are jagged
- Change wildly between subsets: High Variance
- There is no systematic or consistent error pattern: Low Bias

What happens:

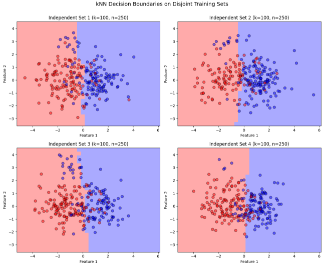
- Model is too complex
- Too sensitive to any noise or overlap
- Memorizes training data including noise

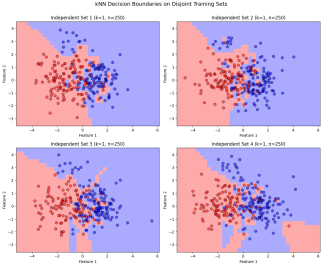
In kNN: $k = 1$ means training accuracy $= 100\%$!



High Bias vs High Variance: Comparison

High Bias	High Variance
Low ability to represent complex patterns	High ability to represent complex patterns
Low model complexity (Few parameters)	High model complexity (Many parameters)
Less sensative to training data	More sensative to training data
Bias: Same error for different datasets	**Variance:** Different errors for different datasets
Underfitting — High training error High test error	**Overfitting** — Low training error High test error





Disclaimer 1: These are general trends and not all of them hold for all models.
Disclaimer 2: Some terms (e.g. Bias, Variance) have precise technical meanings.

Is there a sweet spot?

🤔 The Central Question

Is there a model that is **sensitive** enough to training data to capture the **underlying pattern**, but not so sensitive that it memorizes the **noise**?

The Ideal Balance:

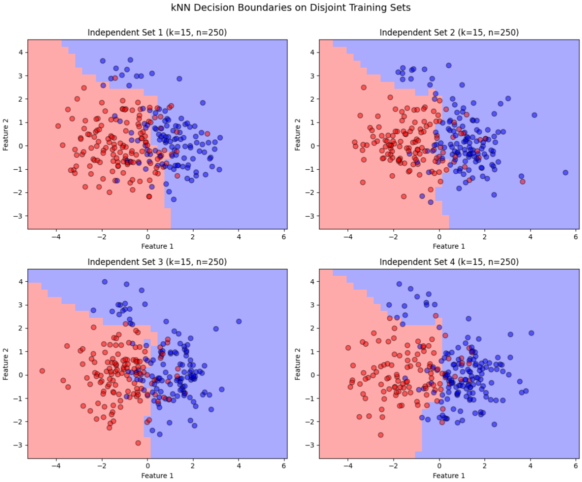
- **Signal (Strong Patterns):** Captured by the model.
- **Noise (Weak Fluctuations):** Filtered out.

📝 What is "Noise"?

Noise isn't just random errors! It includes:

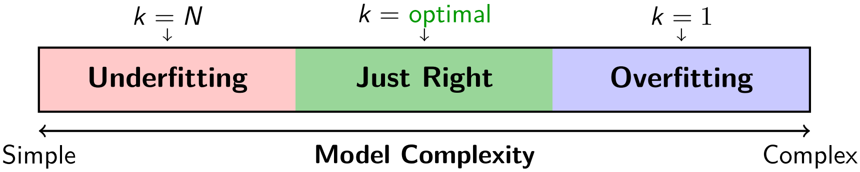
- Mislabeled data points.
- Outliers that don't follow the general rule (e.g., a basketball player in an atypical role).

Result 3: The Sweet Spot ($k = 15$)



Result 3: The Sweet Spot ($k = 15$)

Observation: Boundaries capture the curve, but are relatively stable.
Diagnosis: Good balance between Bias and Variance $\rightarrow$ **Generalization!**

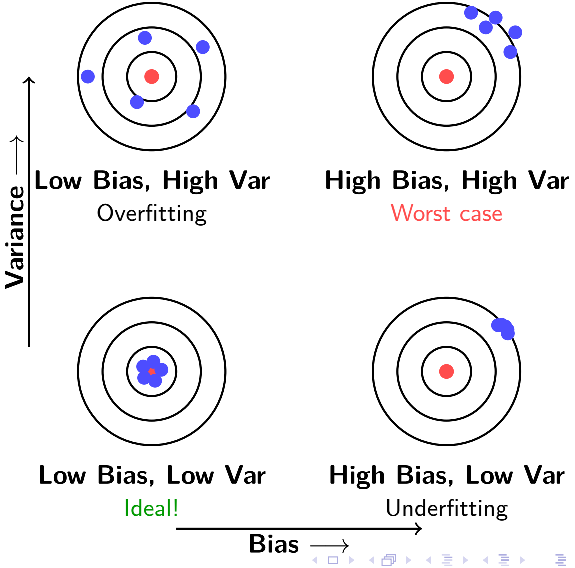


🎯 **Goal:** Find a model complex enough to learn patterns, but simple enough to generalize

🚨 Where the sweet spot is depends on the data!
Usually, with more data, overfitting is less of a problem, so we can use more complex models.

The Bullseye Analogy

- Each blue dot represents a model trained on a different dataset (different sample from the same population)
- The **spread** of dots shows **variance**
- The **distance from center** shows **bias**



The Three-Way Split

Problem with Two-Way Split

- We need to choose k using *some* data
- But we can't use test data (that's cheating!)
- Solution: Split into **three** parts

Data

Training (60%) | **Val (20%)** | **Test (20%)**

Learn patterns (fit model)

Tune hyperparams (choose k)

Final evaluation (report accuracy)

Why Not Just Use Test Data?

The "Golden Rule" of ML Evaluation

The test set is for **final evaluation only**!
Never use it to make any decisions about your model.

Why this matters:

- If you pick k based on test performance, you're "overfitting to the test set"
- Your reported accuracy will be **overoptimistic**
- This is called **data snooping** or **data leakage**

Proper Workflow

1. Try different k values on validation set
2. Pick k^* with lowest validation error
3. Report final accuracy on test set (only once!)

Problem: Validation Set Wastes Data

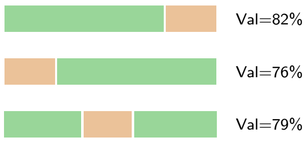
Issue with fixed validation split:

1. We "lose" 20% of training data
2. With small datasets, this is a big problem!
3. With small datasets, validation results depend on which samples end up where

Solution: Cross-Validation

- Use *all* data for both training and validation
- Rotate which part is validation
- Average results over all rotations

Fixed Split Problem



Which one is right?

K-Fold Cross-Validation

5-Fold Cross-Validation

Val	Train	Train	Train	Train	$\rightarrow$ Error$_1$
Train	Val	Train	Train	Train	$\rightarrow$ Error$_2$
Train	Train	Val	Train	Train	$\rightarrow$ Error$_3$
Train	Train	Train	Val	Train	$\rightarrow$ Error$_4$
Train	Train	Train	Train	Val	$\rightarrow$ Error$_5$

$\longrightarrow$ **CV Error** $= \frac{1}{5}\sum_{i=1}^{5}$ Error$_i$

- Split data into K equal "folds" (common: $K = 5$ or $K = 10$)
- Each fold takes a turn as the validation set
- Average the K error estimates

Benefits of Cross-Validation

Advantages:

1. **Uses all data**: Every point is used for both training and validation
2. **More stable estimate**: Averaging reduces variance
3. **Better for small datasets**: Don't waste data on fixed validation set

Common choices:

- $K = 5$: Fast, works well in practice
- $K = 10$: Standard choice, good balance
- $K = N$ (LOOCV): "Leave-one-out" — most expensive but uses maximum data

Leave-One-Out CV (LOOCV)

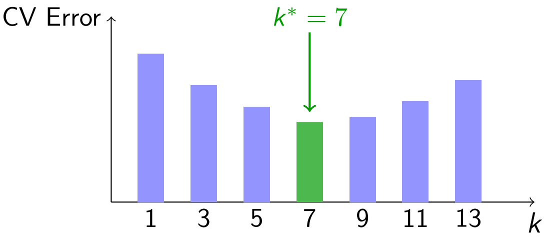
$K = N$ (number of samples): Each sample is its own validation fold.

⚠️ Very expensive for large datasets! (N training runs)

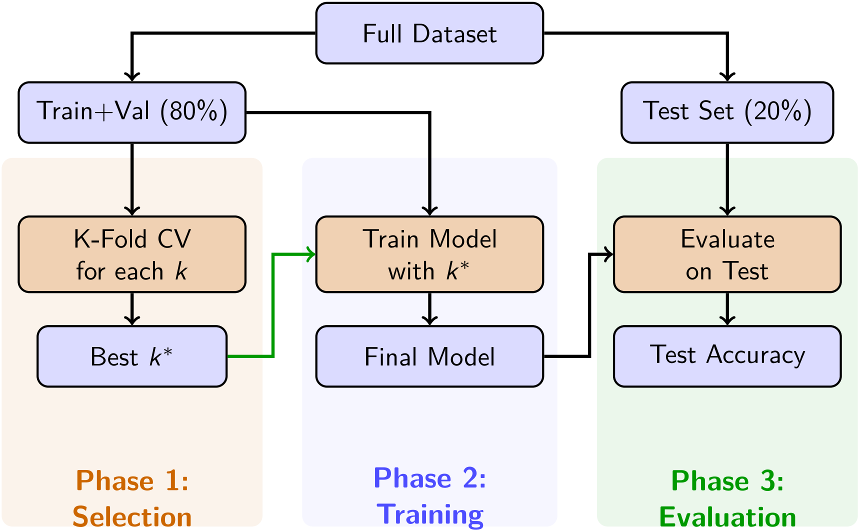
Grid Search: Finding the Best k

Algorithm: Grid Search with Cross-Validation

1. Define a grid of k values to try: $\{1, 3, 5, 7, 9, ...\}$
2. For each k:
   - Compute K-fold CV error
3. Pick $k^* = \text{argmin(CV error)}$
4. Evaluate final model (k^*) on test set



Complete Workflow



Key Takeaways

1. **Overfitting vs Underfitting**:
   - Overfitting: Too complex, memorizes noise (kNN: small k)
   - Underfitting: Too simple, misses patterns (kNN: large k)
2. **Bias-Variance Tradeoff**:
   - Bias = systematic error (underfitting)
   - Variance = sensitivity to training data (overfitting)
   - Goal: minimize total error ($=$ Bias^2 $+$ Variance)
3. **Cross-Validation**:
   - Use all data for training and validation
   - K-fold: rotate validation set, average results
4. **Hyperparameter Selection**:
   - Grid search: try many values, pick best by CV error
   - Only use test set for final evaluation!

Notebook Activities

Today's Hands-On Work

1. **Visualize Variance**: See how decision boundaries change with training data
2. **Implement K-Fold CV**: Write cross-validation from scratch
3. **Grid Search**: Find optimal k for kNN on real data
4. **Plot**: Training error vs CV error as k changes

📓 Open `L04-2026-01-26-Bias-Variance.ipynb`