Cross-Validation

Nipun Batra and teaching staff

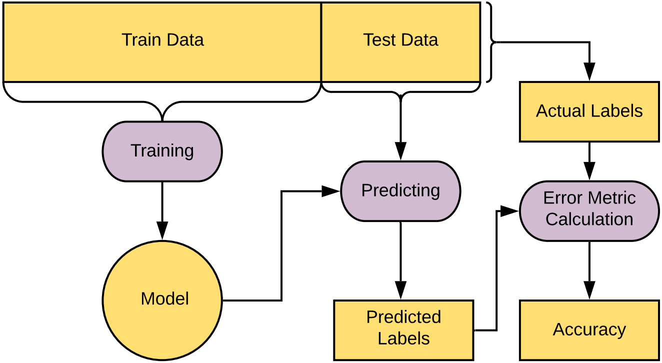
July 26, 2025

IIT Gandhinagar

Introduction to Cross-Validation

Outline

Our General Training Flow



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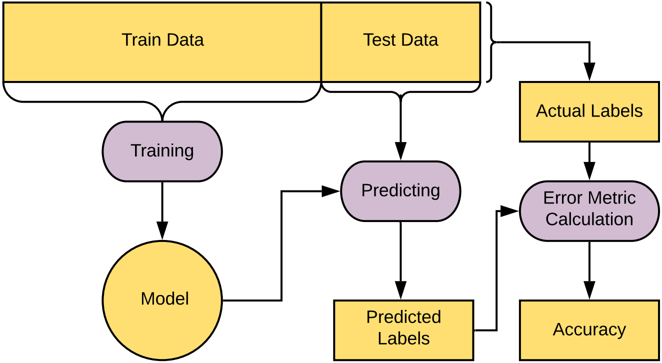

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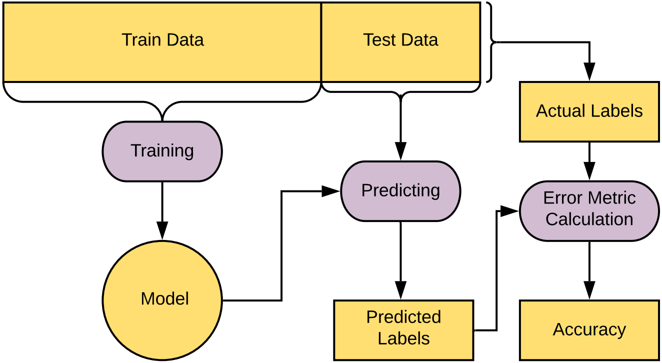

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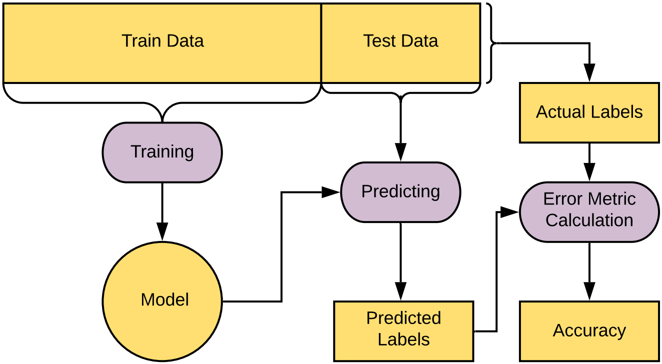

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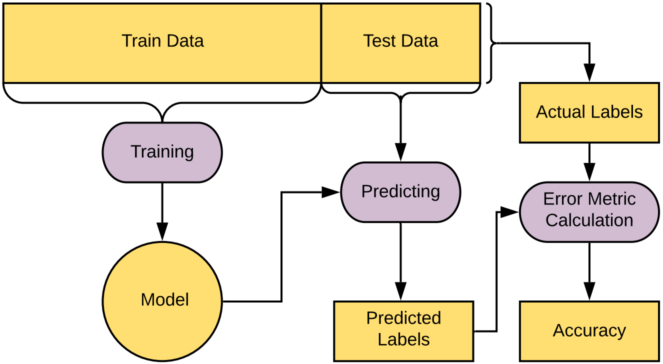

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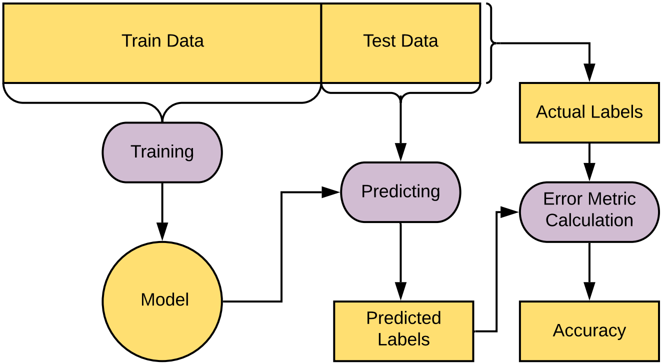

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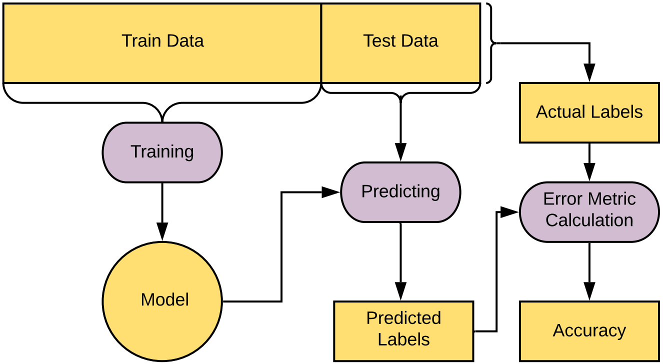

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Pop Quiz #1

Question

What are the main limitations of using only a single train/test split?

Pop Quiz #2

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Pop Quiz #3

Question

What are the main limitations of using only a single train/test split?

Answer

Pop Quiz #4

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Answer

- Does not utilize the full dataset for training

Pop Quiz #5

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Answer

- Does not utilize the full dataset for training
- Cannot optimize hyperparameters systematically

Pop Quiz #6

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Answer

- Does not utilize the full dataset for training
- Cannot optimize hyperparameters systematically
- Results depend on the particular split chosen

Pop Quiz #7

Question

What are the main limitations of using only a single train/test split?

Answer

- Does not utilize the full dataset for training
- Cannot optimize hyperparameters systematically
- Results depend on the particular split chosen
- May not get reliable performance estimates

Full Dataset Utilization

How to use the full dataset for training?

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- Over multiple iterations, use different parts of the dataset for training and testing

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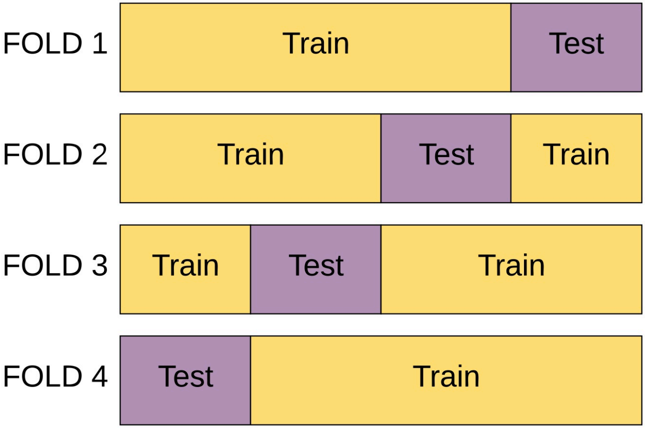
- Typically done via different random splits of the dataset
- **Challenge:** How to ensure systematic evaluation?
- May not use every data point for training or testing with random splits
- May be computationally expensive

K-Fold Cross-Validation

K-Fold Cross-Validation: Utilize Full Dataset for Testing



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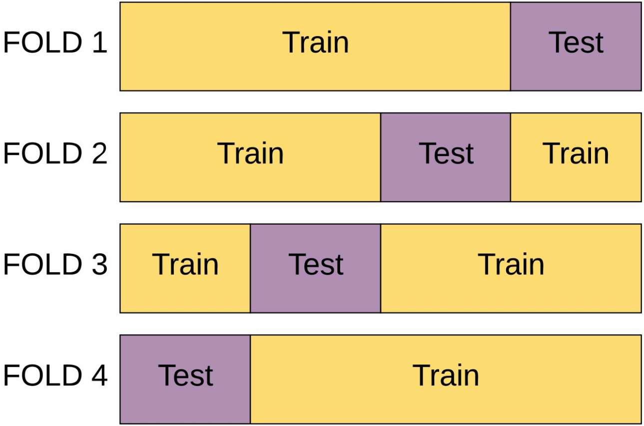

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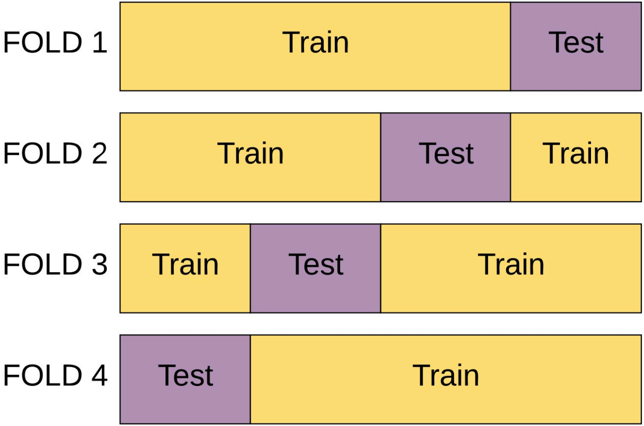

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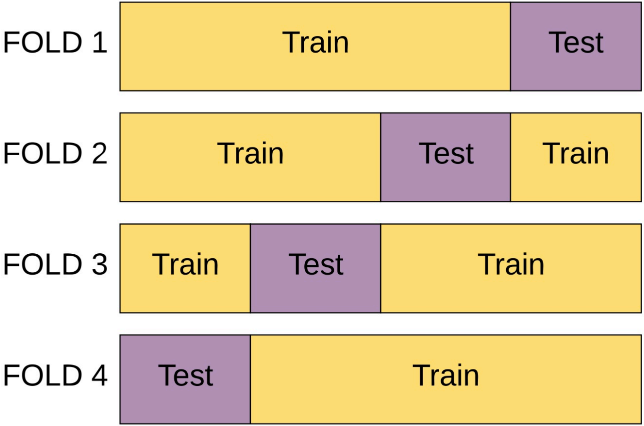

Pop Quiz #8

Question

If you have 100 data points and use 5-fold cross-validation, how many data points are used for training in each fold?

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Pop Quiz #10

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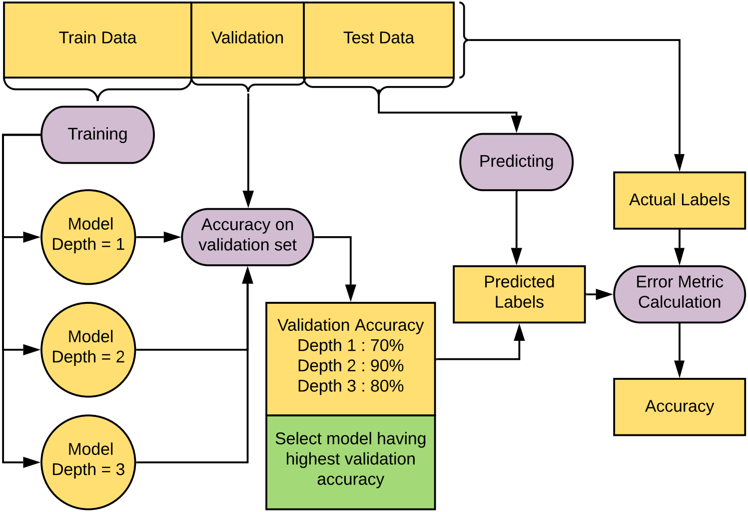
Answer

80 data points (4 out of 5 folds $= 4/5 \times 100 = 80$)

Hyperparameter Optimization

Optimizing Hyperparameters via the Validation Set



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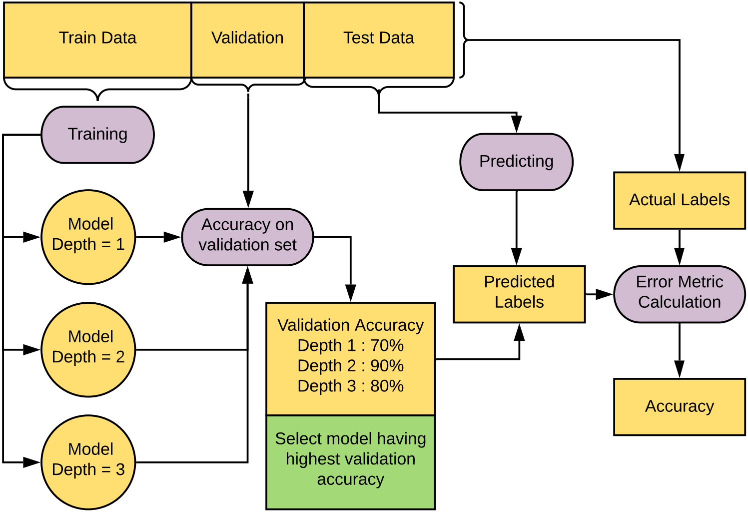

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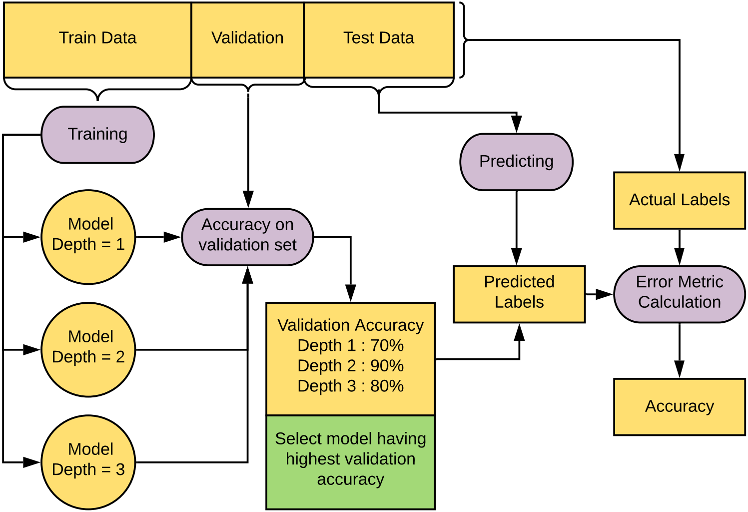

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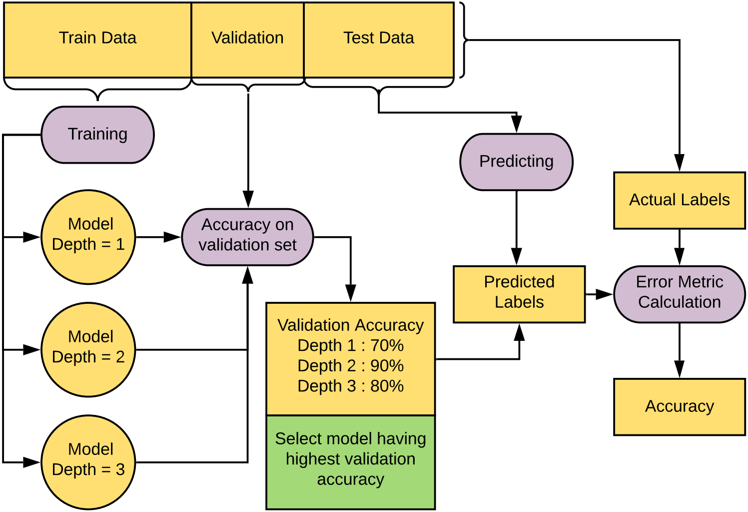

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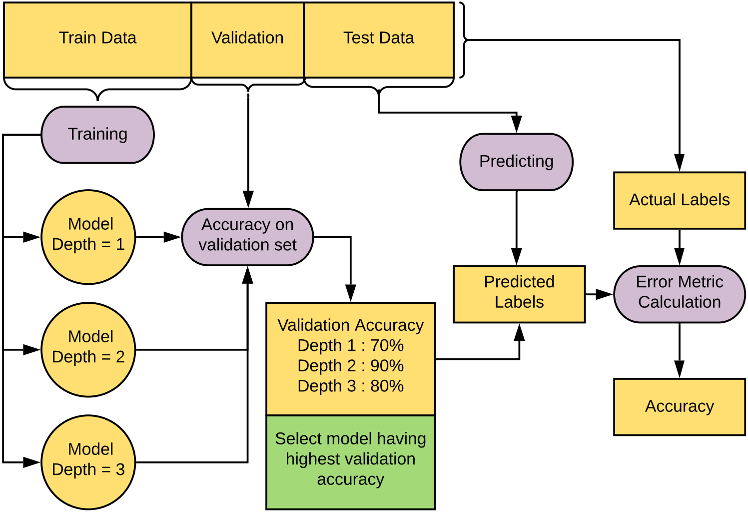

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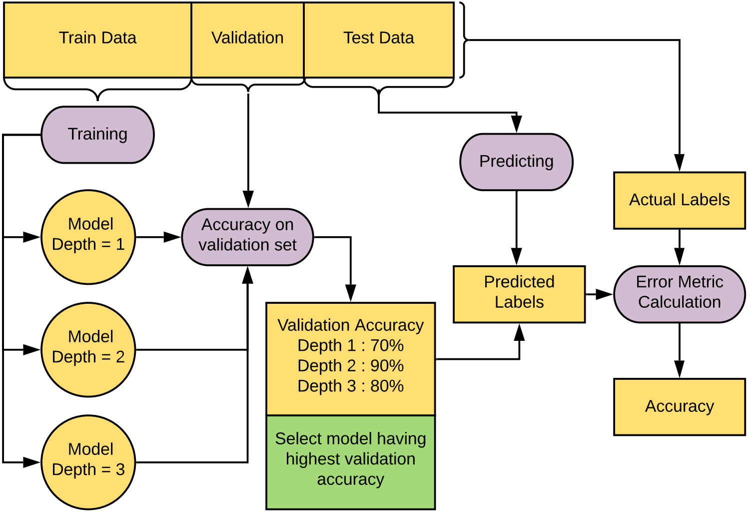

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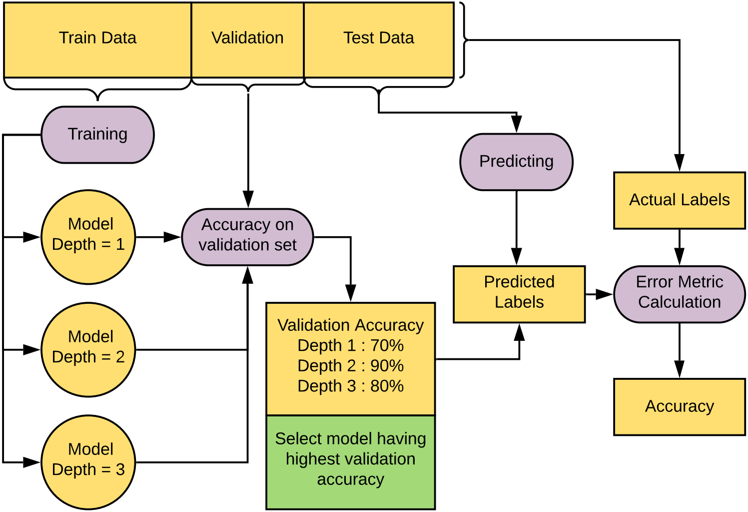


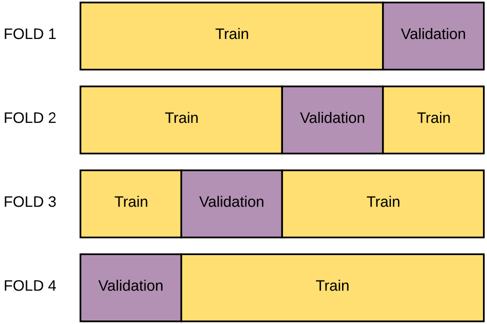
Nested Cross-Validation

Nested Cross-Validation Process

Divide your training set into k equal parts.

Cyclically use 1 part as "validation set" and the rest for training.

Here $k = 4$



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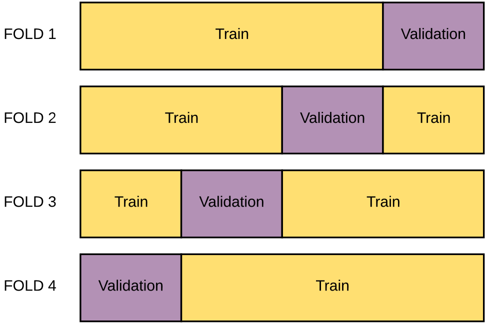

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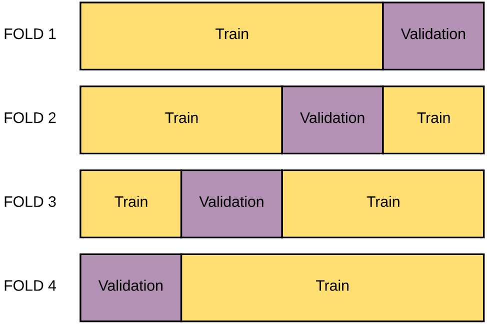

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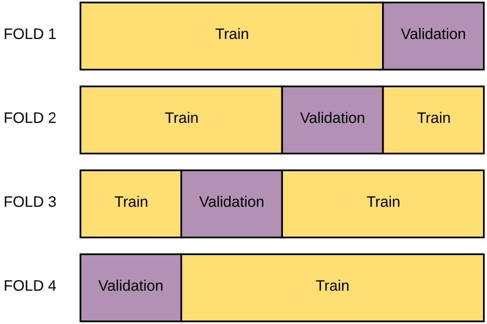

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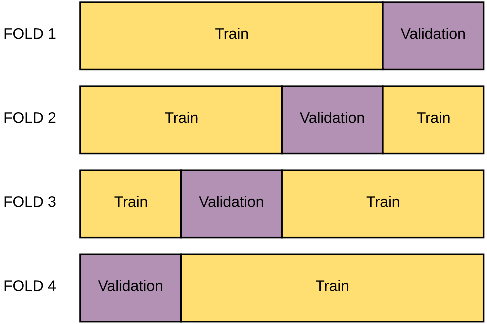

- Each fold provides one validation score
- Process is systematic and exhaustive

Pop Quiz #11

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Pop Quiz #13

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Pop Quiz #16

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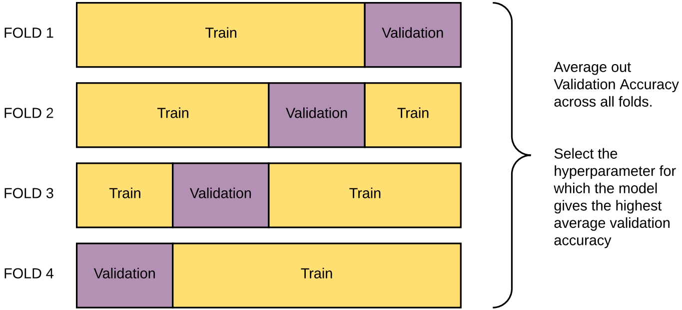
Answer

- Simple CV: Used for model evaluation only
- Nested CV: Outer loop for model evaluation, inner loop for hyperparameter tuning
- Nested CV provides unbiased estimates when doing hyperparameter search

Cross-Validation Results

Average out the validation accuracy across all the folds

Use the hyperparameters with highest average validation accuracy



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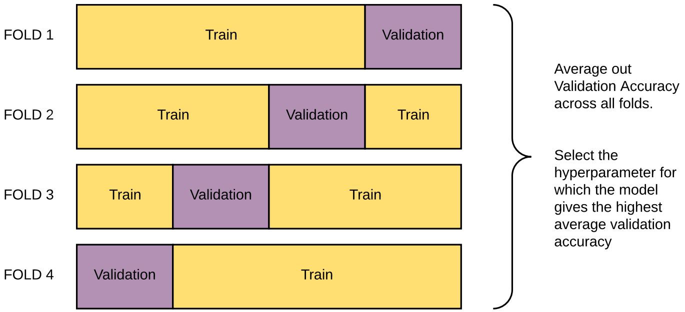

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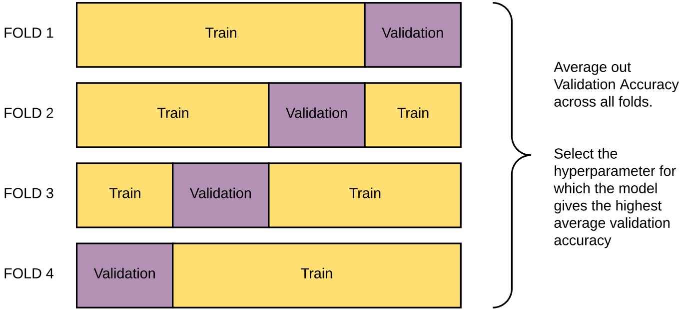

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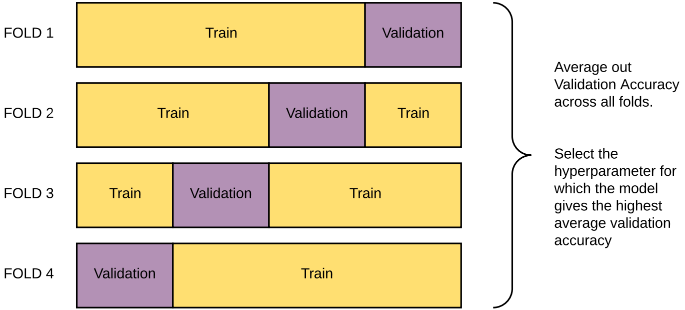

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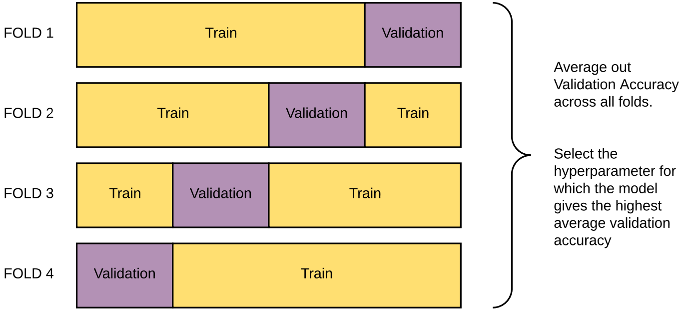

- Final model is trained on entire training set
- Standard deviation gives confidence in results

Pop Quiz #17

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Pop Quiz #18

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Pop Quiz #19

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Answer

Pop Quiz #20

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- Reduces impact of lucky/unlucky splits

Pop Quiz #23

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- Averaging provides more robust performance estimates
- Reduces impact of lucky/unlucky splits
- Standard deviation indicates reliability of the estimate

Cross-Validation Variants

Leave-One-Out Cross-Validation (LOOCV)

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Stratified Cross-Validation

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Pop Quiz #24

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You have a binary classification dataset with 90% negative and 10% positive examples. Why is stratified cross-validation important here?

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Answer

- Regular CV might create folds with very few (or zero) positive examples
- This would give misleading performance estimates
- Stratified CV ensures each fold has $\sim$10% positive examples
- Results in more reliable and consistent evaluation

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- **Expanding Window:** Growing training set over time
- Never use future data to predict past!

Common Pitfalls and Best Practices

Common Cross-Validation Mistakes

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- **Wrong Preprocessing:** Scaling on entire dataset before splitting
- **Ignoring Class Imbalance:** Not using stratified CV when needed

Pop Quiz #31

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- Test fold statistics influence the training preprocessing
- Should compute statistics only on training folds
- Apply same transformation to corresponding test fold
- This gives more realistic performance estimates

Summary and Key Takeaways

Cross-Validation: Key Benefits

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- **Better Data Utilization:** Every point used for both training and testing

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Cross-Validation: Key Benefits

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