Evaluating Performance II

Be wary of overall accuracy as sole metric

Case study 1

i	y_i	$\hat{y}_i$
1	**1**	**1**
2	**1**	**1**
3	**1**	**1**
4	**1**	**1**
5	**1**	**1**
6	**1**	**1**
7	**1**	**0**
8	**0**	**1**
9	**0**	**0**
10	**0**	**0**
11	**0**	**0**
12	**0**	**0**
13	**0**	**0**
14	**0**	**0**
15	**0**	**0**

Overall classification accuracy = 13/15 = **0.87**

ROC Curves measure the tradeoff between…

- **A** False positive rate = 1/8 = **0.13**
- **B** True positive rate (Recall) = 6/7 = **0.86**

PR Curves measure the tradeoff between…

- **B** True positive rate (Recall) = 6/7 = **0.86**
- **C** Precision= 6/7 = **0.86**

A

$$\frac{\text{false positive}}{\text{false positive} + \text{true negative}}$$

B

$$\frac{\text{true positive}}{\text{true positive} + \text{false negative}}$$

C

$$\frac{\text{true positive}}{\text{true positive} + \text{false positive}}$$

Case study 2

i	y_i	$\hat{y}_i$
1	**1**	**1**
2	**1**	**1**
3	**1**	**0**
4	**1**	**0**
5	**0**	**0**
6	**0**	**0**
7	**0**	**0**
8	**0**	**0**
9	**0**	**0**
10	**0**	**0**
11	**0**	**0**
12	**0**	**0**
13	**0**	**0**
14	**0**	**0**
15	**0**	**0**

Overall classification accuracy = 13/15 = **0.87**

ROC Curves measure the tradeoff between…

- **A** False positive rate = 0/11 = **0**
- **B** True positive rate (Recall) = 2/4 = **0.5**

PR Curves measure the tradeoff between…

- **B** True positive rate (Recall) = 2/4 = **0.5**
- **C** Precision= 2/2 = **1**

A

$$\frac{\text{false positive}}{\text{false positive} + \text{true negative}}$$

B

$$\frac{\text{true positive}}{\text{true positive} + \text{false negative}}$$

C

$$\frac{\text{true positive}}{\text{true positive} + \text{false positive}}$$

Case study 3

i	y_i	$\hat{y}_i$
1	**1**	**1**
2	**1**	**1**
3	**1**	**1**
4	**1**	**1**
5	**1**	**1**
6	**1**	**1**
7	**1**	**1**
8	**1**	**1**
9	**1**	**1**
10	**1**	**1**
11	**1**	**1**
12	**1**	**1**
13	**1**	**1**
14	**0**	**1**
15	**0**	**1**

Overall classification accuracy = 13/15 = **0.87**

ROC Curves measure the tradeoff between…

A False positive rate = 2/2 = **1**

B True positive rate (Recall) = 13/13 = **1**

PR Curves measure the tradeoff between…

B True positive rate (Recall) = 13/13 = **1**

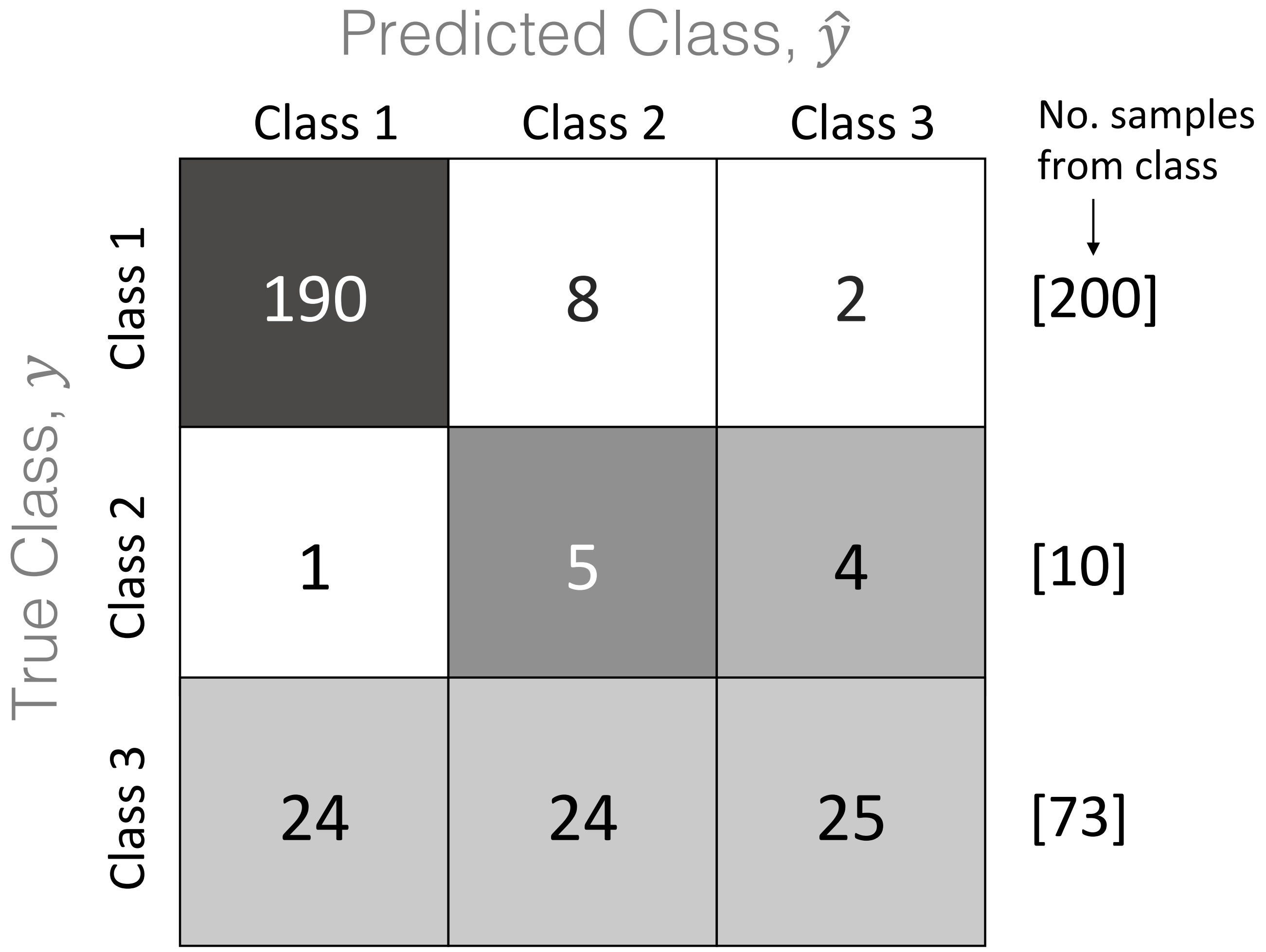
C Precision= 13/15 = **0.87**

A $\dfrac{\text{false positive}}{\text{false positive} + \text{true negative}}$

B $\dfrac{\text{true positive}}{\text{true positive} + \text{false negative}}$

C $\dfrac{\text{true positive}}{\text{true positive} + \text{false positive}}$

Multiclass Classification: Confusion Matrix



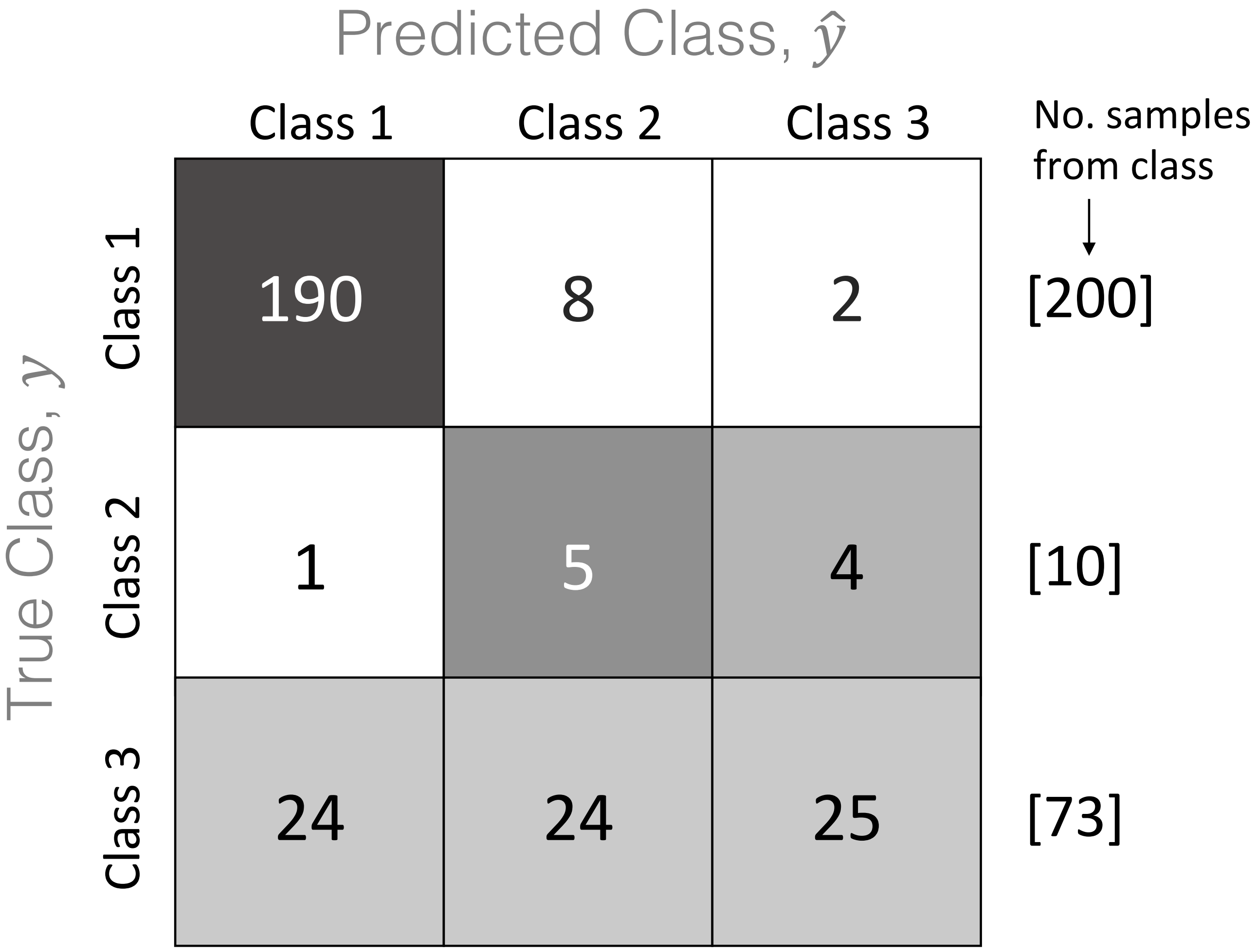
Predicted Class, $\hat{y}$

True Class, y

	Class 1	Class 2	Class 3	No. samples from class
Class 1	190	8	2	[200]
Class 2	1	5	4	[10]
Class 3	24	24	25	[73]

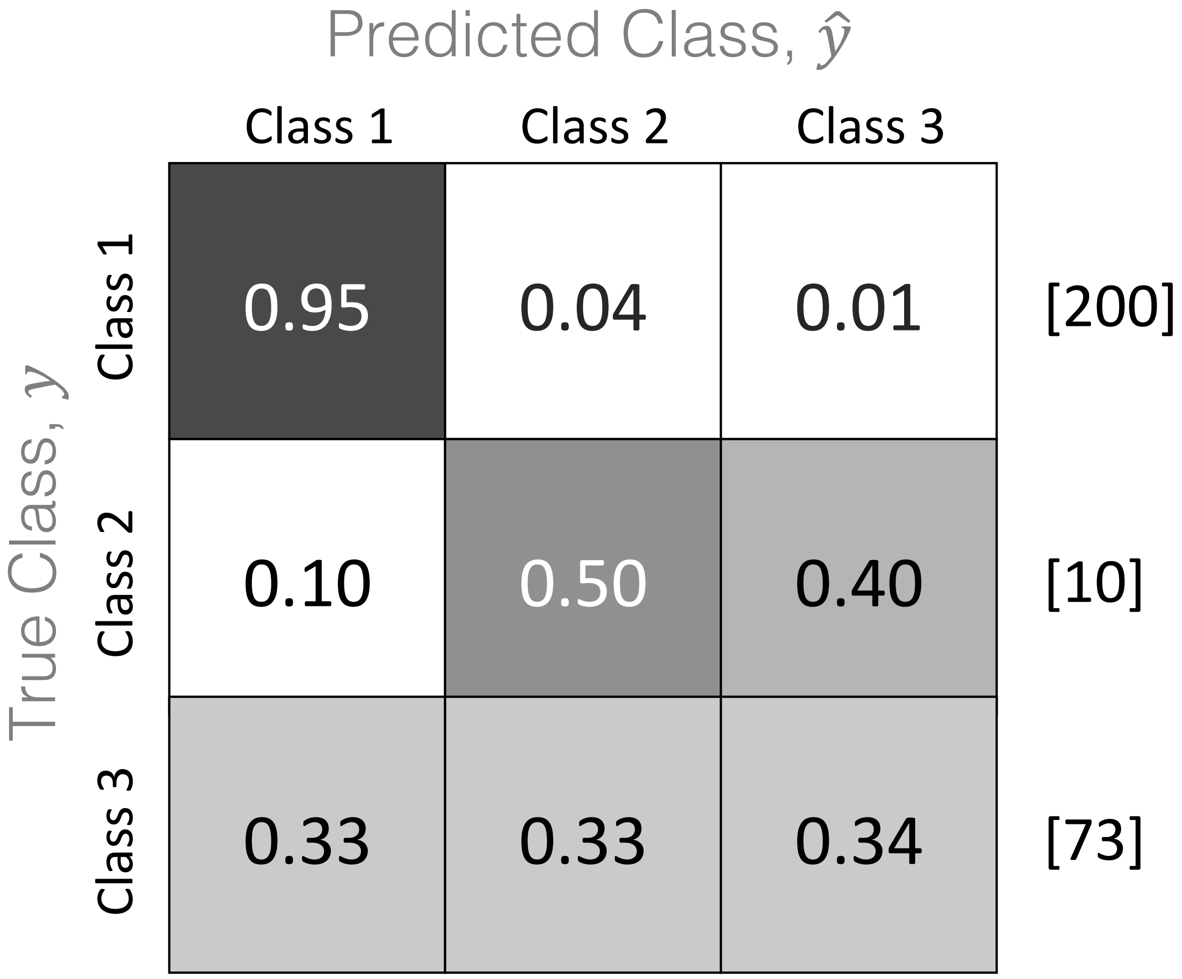
confusion matrix with number of samples

Multiclass Classification: Confusion Matrix



		Predicted Class, $\hat{y}$			
		Class 1	Class 2	Class 3	No. samples from class
True Class, y	Class 1	190	8	2	[200]
	Class 2	1	5	4	[10]
	Class 3	24	24	25	[73]

confusion matrix with number of samples



		Predicted Class, $\hat{y}$			
		Class 1	Class 2	Class 3	
True Class, y	Class 1	0.95	0.04	0.01	[200]
	Class 2	0.10	0.50	0.40	[10]
	Class 3	0.33	0.33	0.34	[73]

confusion matrix with probabilities

F_1-score

$$F_1 = 2\frac{1}{\frac{1}{\text{recall}} + \frac{1}{\text{precision}}}$$

Harmonic mean of precision and recall

$$= 2\frac{\text{precision} \cdot \text{recall}}{\text{precision} + \text{recall}}$$

Generally:

$$F_\beta = (1+\beta^2)\frac{\text{precision} \cdot \text{recall}}{\beta^2 \cdot \text{precision} + \text{recall}}$$

β controls the relative weight of precision/recall

Multiclass F_1

Micro-average: Calculate precision and recall metrics globally by counting the total true positives, false negatives, and false positives

(average for the whole dataset)

Macro-average: Use the average precision and recall for each class label

(average of class-averages)

Modeling Considerations

Accuracy

Computational Efficiency

Interpretability

Accuracy

Supervised Learning Performance Evaluation

Regression

Classification

Binary

Multiclass

Cost / Loss Functions

Regression

- Mean squared error (MSE)
- Mean absolute error (MAE)
- Huber loss

Classification

- Cross entropy / log loss

Performance Evaluation Metrics and Tools

Regression

- Root mean squared error (RMSE)
- R^2, coefficient of determination

Binary

- Classification accuracy
- True positive rate (Recall)
- False positive rate
- Precision
- F_1 Score
- Area under the ROC curve (AUC)
- Receiver Operating Characteristic (ROC) curves

Multiclass

- Classification accuracy
- Micro-averaged F_1 Score
- Macro-averaged F_1 Score
- Confusion matrices
- Per class metrics (recall, precision, etc.)

We can always compute our accuracy metrics of a trained model on our test set…

…BUT, they may not be valid (i.e. may not reflect generalization performance) if:

1. The underlying data are NOT representative of what we will encounter in practice
2. The test data set DOES NOT remain separate from our model training process

Goal: estimate generalization performance

Spot the misstep

1

1. Your train a logistic regression algorithm on training data
2. You evaluate the generalization performance of your trained algorithm on the training data
3. Your estimated performance is exceptional!

NEVER USE THE SAME DATA USED FOR TRAINING FOR ESTIMATING GENERALIZATION PERFORMANCE

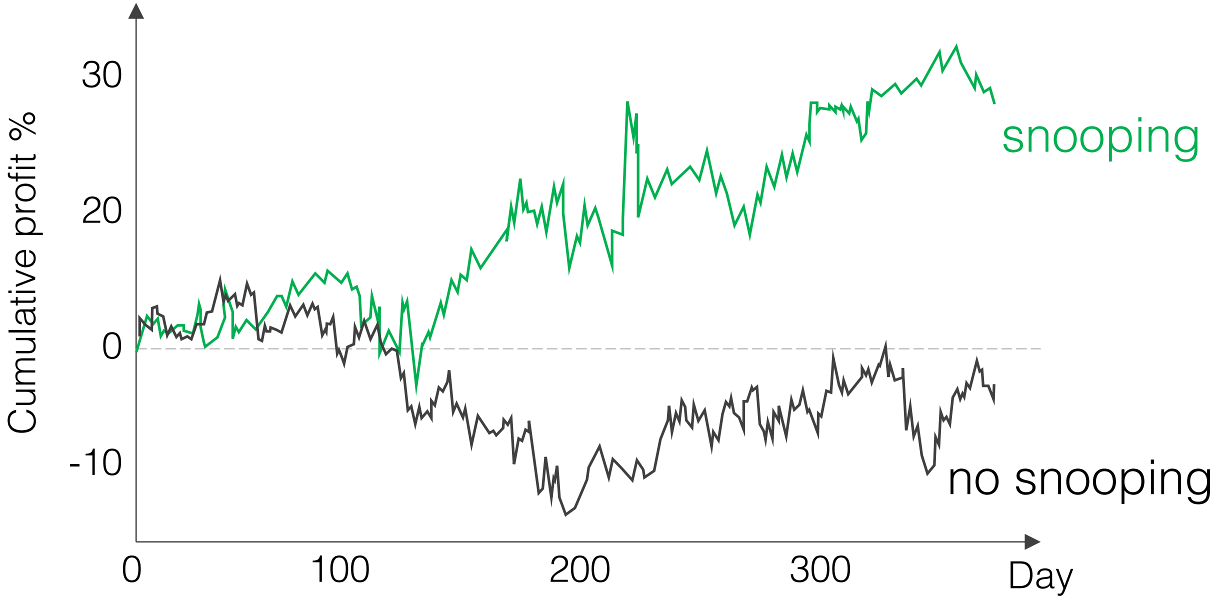
2

1. Goal: predict the exchange rate for the U.S. Dollar vs British Pound (using 20 past observations)
2. You take your historical data, normalize it, then split it randomly into a training and test set

   DATA SNOOPING!
3. You train on the training data, test on the test data

Results:
Your predictions are correct 56% of the time

Estimate your profits…



All preprocessing should be based on the training data alone

Abu-Mostafa, Learning From Data

3

1. Goal: predict the Dow Jones Industrial average

2. You randomly split your data into a training and test dataset

3. Choose a model with lots of flexibility

4. You iterate on the following process hundreds of times:
    1. Train your model on the training data
    2. Test your model on the test data
    3. Evaluate performance on the test data

DATA SNOOPING!

5. Report that you were able to achieve 75% accuracy on your test set!

4

1. Goal: predict long-term performance of a “buy and hold” strategy in stocks
2. You collect 50 years of historical data and include all companies that are currently traded in the S&P500

   SAMPLING BIAS!
3. You randomly split your data into a training and test dataset.
4. You assume you will strictly follow the “buy and hold” strategy
5. You then use apply your model on the current portfolio and predict that you will be rich in retirement!

Abu-Mostafa, Learning From Data

Data snooping / leakage

If a test data set has affected **any step** in the learning process, its ability to assess the generalization performance has been **compromised**.

Abu-Mostafa, Learning From Data

Sampling bias

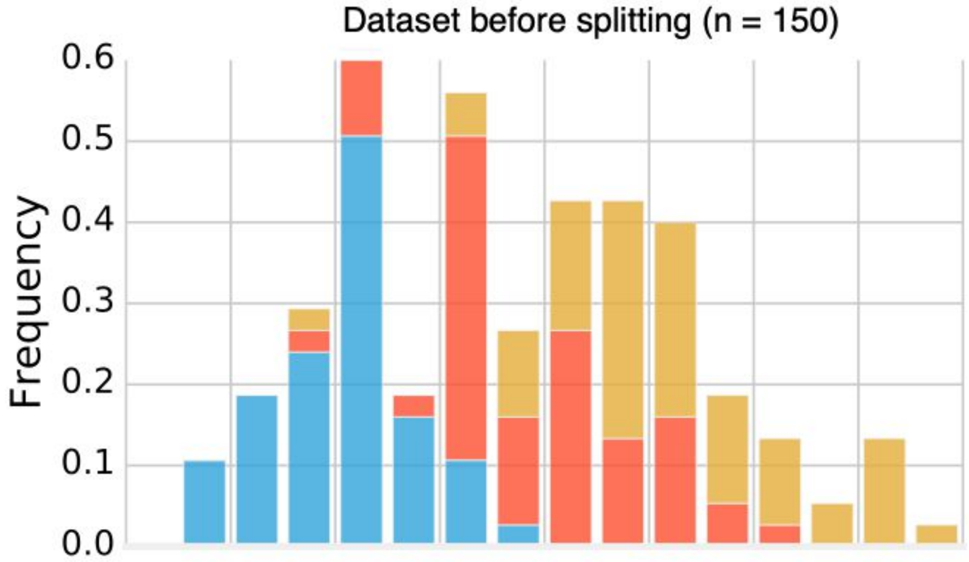
Are the data we’re using for machine learning **representative of the population you will apply on in practice**?

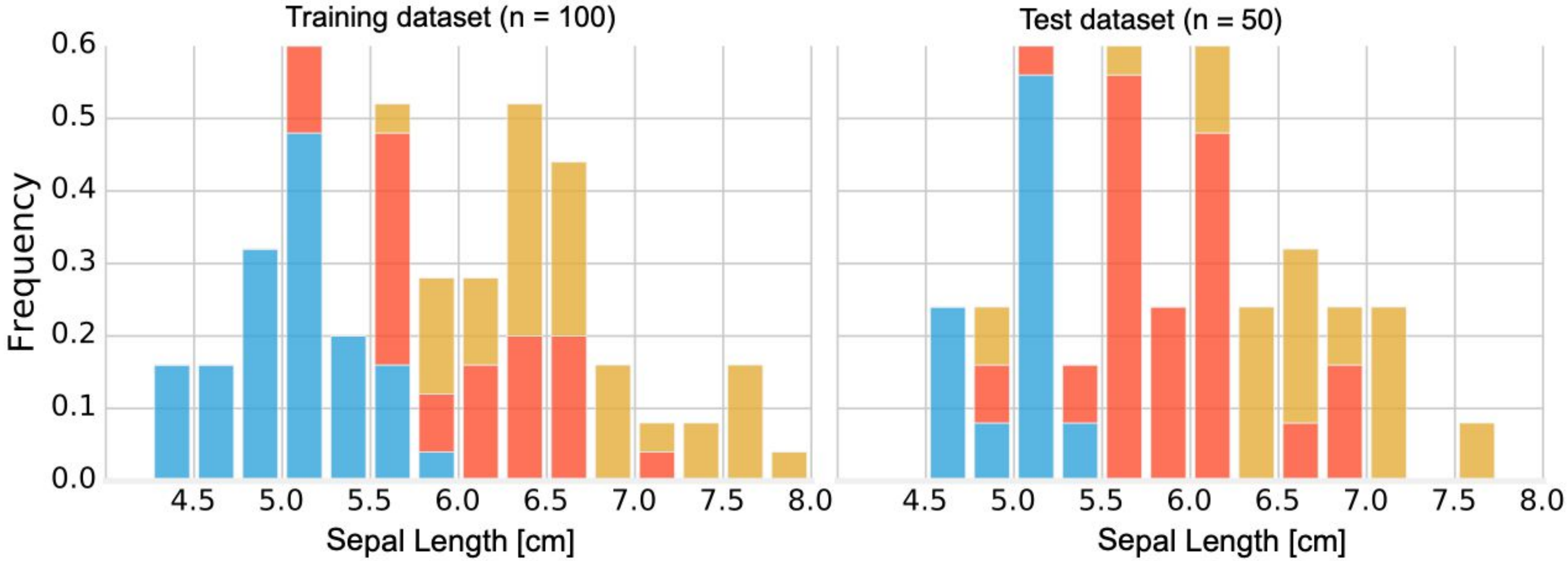
One form of sampling bias

All: 50 Setosa, 50 Versicolor, 50 Virginica

Train: 38 Setosa, 28 Versicolor, 34 Virginica

Test: 12 Setosa, 22 Versicolor, 16 Virginica





Ideally training and test sets are independent and statistically representative of the population

Dividing up your dataset we violate independence assumptions

Reduce this bias with **stratified sampling**

Images from Sebastian Raschka (https://sebastianraschka.com/blog/2016/model-evaluation-selection-part1.html)

Sample Size

Ideally, we would use infinite samples in our training set representing the population

In practice, we try to use as much data as possible

Larger datasets may also reduce overfit

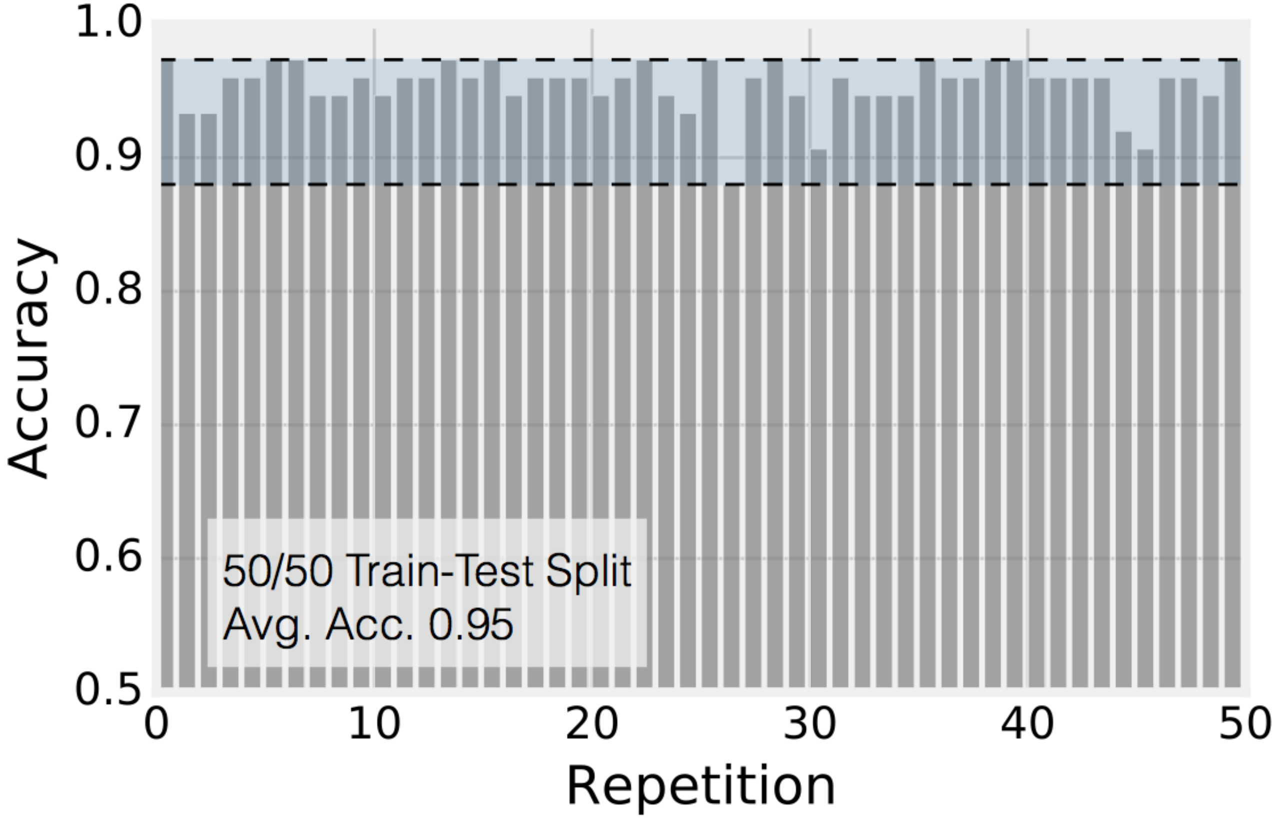
Images from Sebastian Raschka (https://sebastianraschka.com/blog/2016/model-evaluation-selection-part2.html)

Size of test set for train/test splits

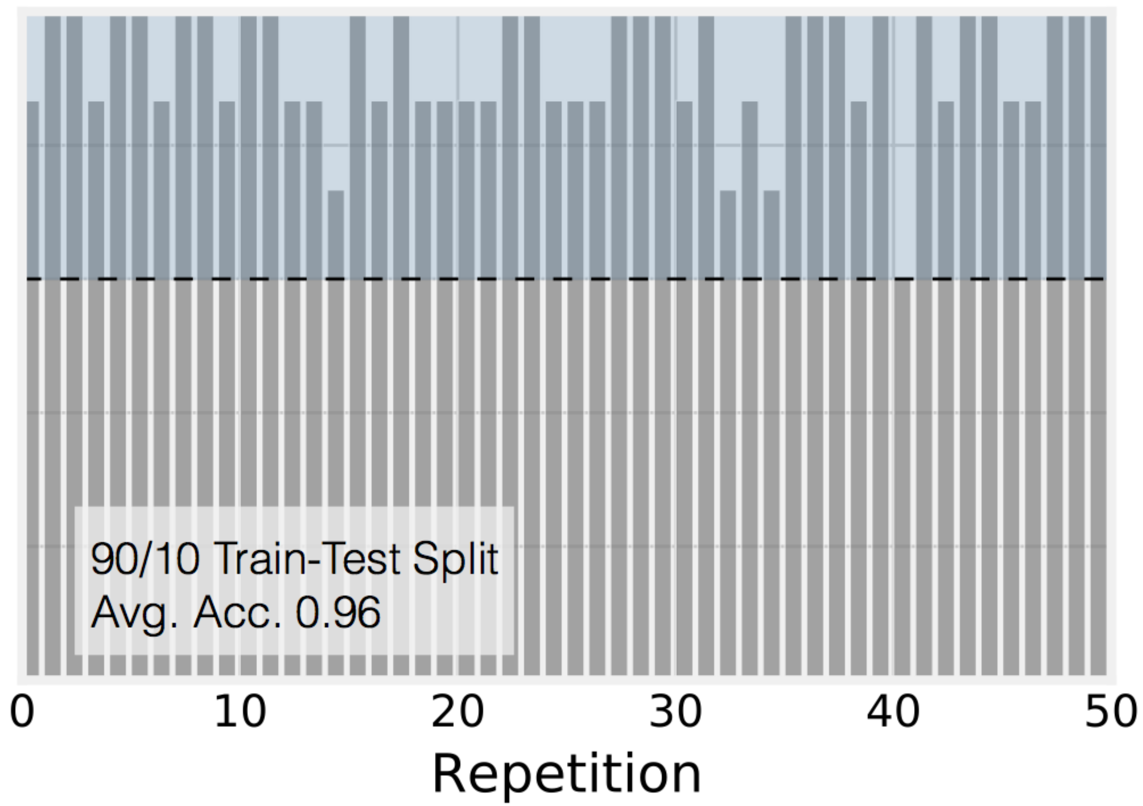
Each bar represents test performance for model trained on different random splits of data

Smaller test datasets lead to greater variance in the estimate of generalization performance

50% Test Data



10% Test Data



Images from Sebastian Raschka (https://sebastianraschka.com/blog/2016/model-evaluation-selection-part2.html)

How do we use the metrics to evaluate performance?

Train-Test Split

Learning model parameters and evaluating performance

Commonly ~80/20

Used for model training: select model parameters

Evaluate generalization performance

1. If our test split is too small, our estimate of generalization performance will have high variance
2. Not using all data for training produces an algorithm that is pessimistically biased
3. For small datasets, this reduction in dataset size may be detrimental

What are Hyperparameters?

Parameters: Configuration variable that control model predictions that are adjusted during the training process based on data

Hyperparameters: parameters set prior to model training; they are not modified during the training procedure, but often impact the training procedure.

Hyperparameter Examples

- k in KNN
- Learning rates for gradient descent of your model fitting procedure
- Model architectures (configuration of neural networks)
- You could consider the choice of model itself a hyperparameter (e.g. linear regression vs polynomial regression vs neural networks)

Training, Validation, Test Split

Learning model parameters AND **hyperparameters** and evaluating performance

Used for model training / fitting

Used to optimize hyperparameters

Used to evaluate generalization performance of the final model(s)

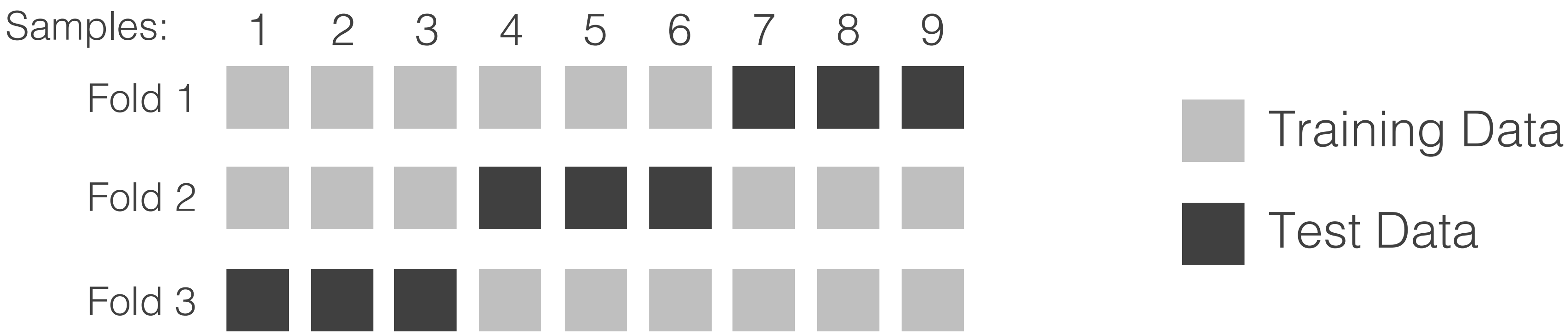
Hyperparameters: parameters that control how your algorithm learns; typically set before training begins (e.g. k in KNN, learning rate, etc.)

What if you have a small dataset?

K-folds cross-validation

K-fold cross validation K = 3

❶ **Performance evaluation**: Train your model K times, once for each fold



Samples:	1	2	3	4	5	6	7	8	9
Fold 1	▨	▨	▨	▨	▨	▨	■	■	■
Fold 2	▨	▨	▨	■	■	■	▨	▨	▨
Fold 3	■	■	■	▨	▨	▨	▨	▨	▨

▨ Training Data

■ Test Data

Typical choices for k are 5 or 10

Average performance metrics across the splits

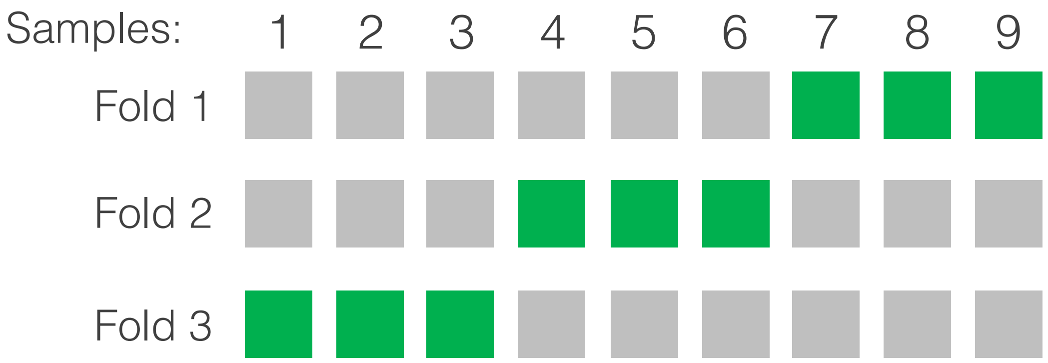
If k = N (number of samples): Leave-one-out cross validation

The number of splits impacts the bias-variance tradeoff of your performance estimates
(larger k means lower bias on the performance estimate, but with higher variance)

What if you need to select hyperparameters for a small dataset?

Cross-validation with hyperparameters

❶ Repeatedly fit your model to your K folds. Each iteration try different hyperparameters

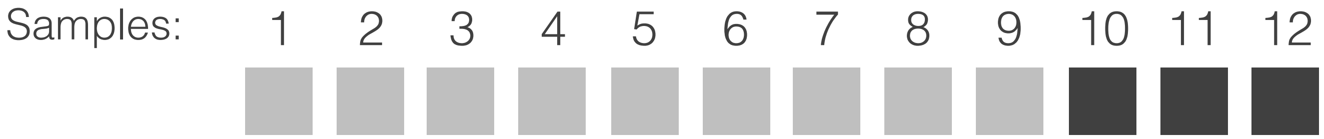


⬜ Training Data

🟩 Validation Data

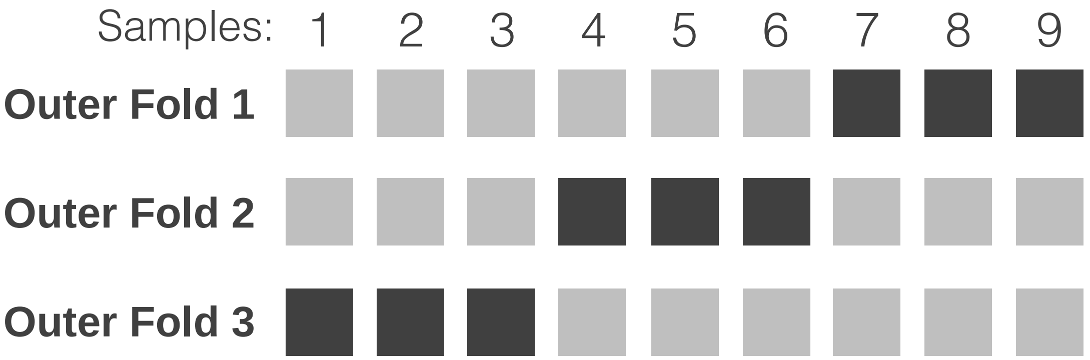
⬛ Test Data

❷ Using the best-performing hyperparameters from (a), train on all training data and evaluate performance on the test data



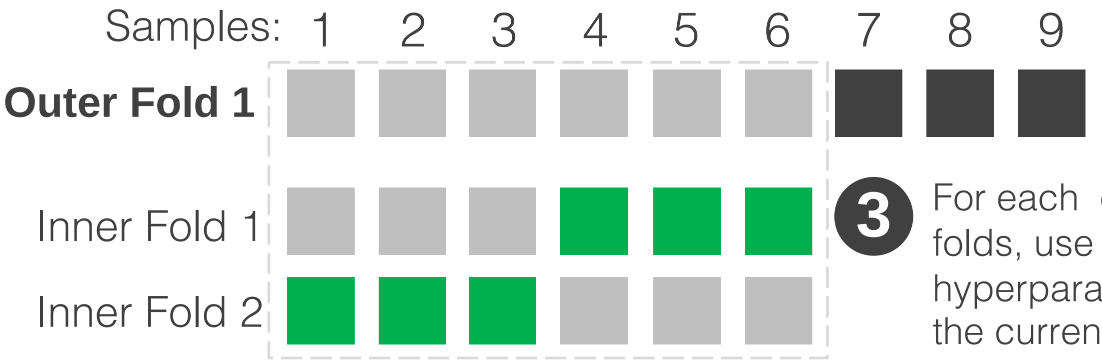
But this uses a small test set…
Variance will be high…

Nested cross-validation with hyperparameters



Samples:	1	2	3	4	5	6	7	8	9
Outer Fold 1	⬜	⬜	⬜	⬜	⬜	⬜	⬛	⬛	⬛
Outer Fold 2	⬜	⬜	⬜	⬛	⬛	⬛	⬜	⬜	⬜
Outer Fold 3	⬛	⬛	⬛	⬜	⬜	⬜	⬜	⬜	⬜

① For each outer fold, train your model with the best-performing hyperparameters from the inner folds



Samples:	1	2	3	4	5	6	7	8	9
Outer Fold 1	⬜	⬜	⬜	⬜	⬜	⬜	⬛	⬛	⬛
Inner Fold 1	⬜	⬜	⬜	🟩	🟩	🟩			
Inner Fold 2	🟩	🟩	🟩	⬜	⬜	⬜			

② For the inner folds, repeatedly run K-folds, each time with a different set of hyperparameters

③ For each of the K inner folds, use the hyperparameters from the current iteration to train the model, then evaluate performance on validation data

	1	2	3	4	5	6	7	8	9
Outer Fold 2	⬜	⬜	⬜	⬛	⬛	⬛	⬜	⬜	⬜
Inner Fold 1	⬜	⬜	⬜				🟩	🟩	🟩
Inner Fold 2	🟩	🟩	🟩				⬜	⬜	⬜
Outer Fold 3	⬛	⬛	⬛	⬜	⬜	⬜	⬜	⬜	⬜
Inner Fold 1				⬜	⬜	⬜	🟩	🟩	🟩
Inner Fold 2				🟩	🟩	🟩	⬜	⬜	⬜

④ Repeat steps (2) and (3) for the remaining outer folds

⬜ Training Data

🟩 Validation Data

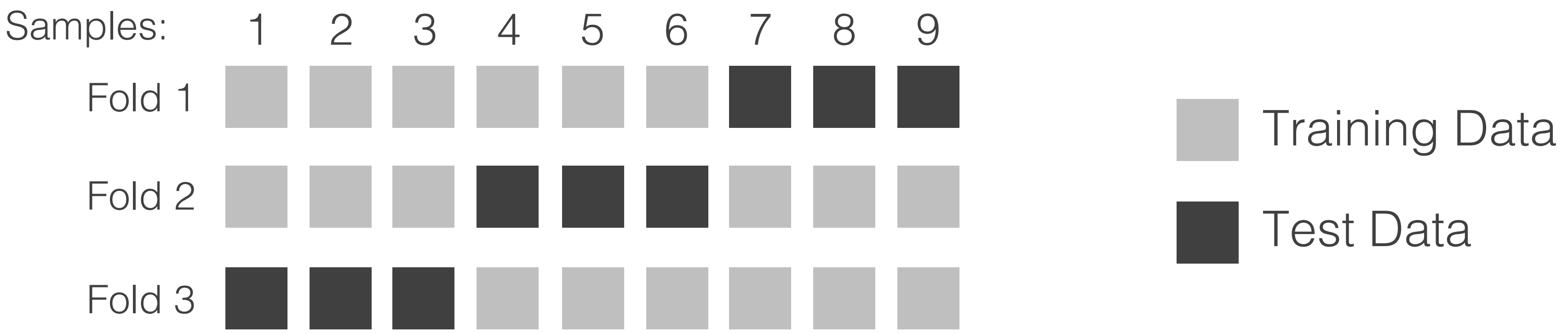
⬛ Test Data

K-folds cross validation results in **k models**

How do we pick which to use?

After performance has been validated, train on all the data you have before you apply the model in practice

1 **Performance evaluation**: Train your model K times, once for each fold



2 **Model application**: Once you've evaluated model performance and are ready apply the model then retrain the model on ALL of your data to prepare it for unseen data

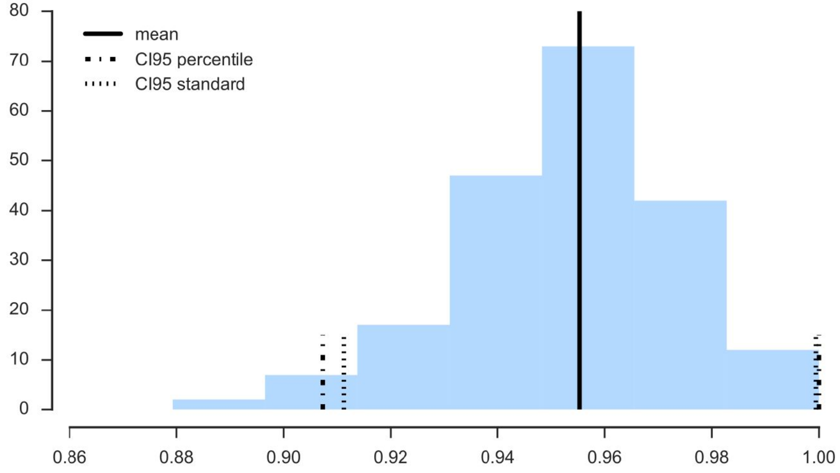
(this is not a model evaluation step, but only when you're ready to apply in practice)

Bootstrap sampling

Sampling **with replacement**

Often used to estimate standard errors and confidence intervals

Integral part of model ensembles (i.e. bagging in random forests)



Images from Sebastian Raschka

When to use each technique for performance evaluation?

	Performance estimation (without hyperparameter optimization) OR Hyperparameter optimization (without performance estimation)	Performance estimation AND hyperparameter optimization
Large Dataset	**Train-test split**	**Train-validation-test split**
Small Dataset	**Cross-validation**	**Nested Cross-validation**

Note: hyperparameter optimization can be considered a form of model comparison

Summary / best practices

- **Resampling techniques are techniques to estimate generalization performance**
    - Resampling techniques = train/test split, train/val/test split, cross validation, nested cross validation, bootstrap

- When **comparing models** biased performance estimates are acceptable if they affect all models equally
    - CV, train/test splits, etc., need to be the same for each model that you need to compare (same splits and random seeds)

- If you use the performance estimate of a dataset for adjusting the model – there must be a separate held out dataset if you want a true estimate of generalization performance

But how do I get ROC's out of CV?

Each of the K folds will produce a set of confidence scores for the test / validation data of that fold.

Fold 1

y_i	confidence
1	0.98
0	0.87
1	0.43
0	0.02

Fold 2

y_i	confidence
1	0.99
1	0.65
0	0.22
0	0.14

Fold 3

y_i	confidence
1	0.58
0	0.87
0	0.33
0	0.82

① Merge the outputs from the K folds into a single set of confidence scores for making one ROC curve

Note: The confidence scores need to be on the same scale for this merging method to work properly

y_i	confidence
1	0.98
0	0.87
1	0.43
0	0.02
1	0.99
1	0.65
0	0.22
0	0.14
1	0.58
0	0.87
0	0.33
0	0.82

② Average the individual ROC curves from each fold

(This also enables measures of variation across the folds)

Note: you only have point data for changes in the ROC curve value, to compute the average you must interpolate between the points on the curve and evaluate the average across all the curves

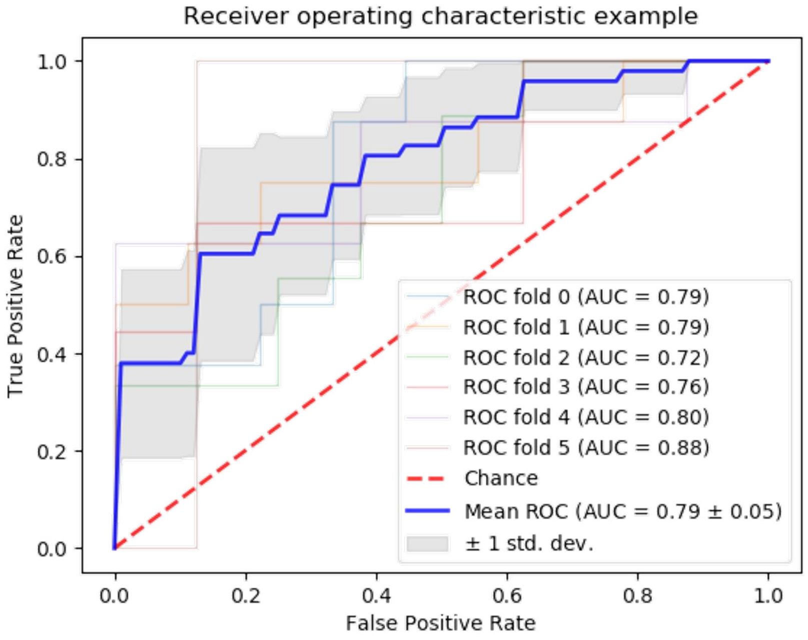


Image from: https://scikit-learn.org/

Modeling Considerations

Accuracy (and techniques to measure it)

Computational Efficiency

Interpretability

Computational Efficiency

Measure of how an algorithm's run time (or space requirements) grow as the input size grows

Complexity of making predictions with kNN

(compare an unseen sample to the training samples)

Assume we have n = 10,000, p = 2

The Euclidean distance between $\begin{bmatrix} x_{1,1} \\ x_{1,2} \end{bmatrix}$ and $\begin{bmatrix} x_{2,1} \\ x_{2,2} \end{bmatrix}$ can be measured as:

$$\sqrt{\left(x_{2,1} - x_{1,1}\right)^2 + \left(x_{2,1} - x_{1,1}\right)^2}$$

That's two (p) distinct sets of operations dependent on the data

We repeat that n times – once for each sample in the training dataset

$$O(np)$$

Computational Efficiency

Training time efficiency?

Test time efficiency?

How do each change with the size of our data?

Interpretability

Transparency (can I tell how the model works)

- **Simulatability**: can I contemplate the whole model at once?
- **Decomposability**: is there an intuitive explanation for each part of the model? (e.g. all patients with diastolic blood pressure over 150)

Explainability (post-hoc explanations)

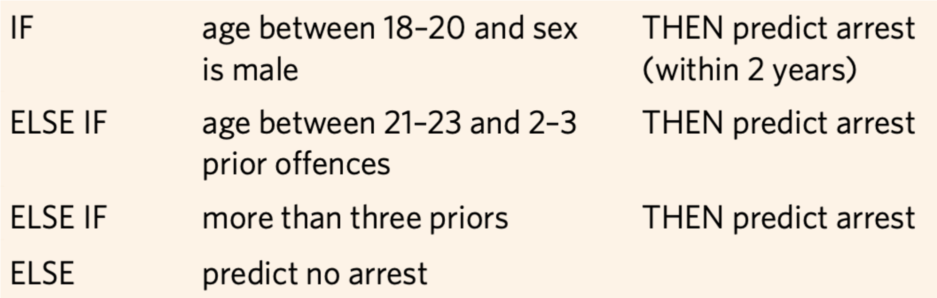
Visualization, local explanations, explanations by example

(e.g. this tumor is classified as malignant because to the model it looks a lot like these other tumors)

Lipton, Zachary C. "The Mythos of Model Interpretability: In Machine Learning, the Concept of Interpretability Is Both Important and Slippery." Queue 16, no. 3 (2018): 31–57.

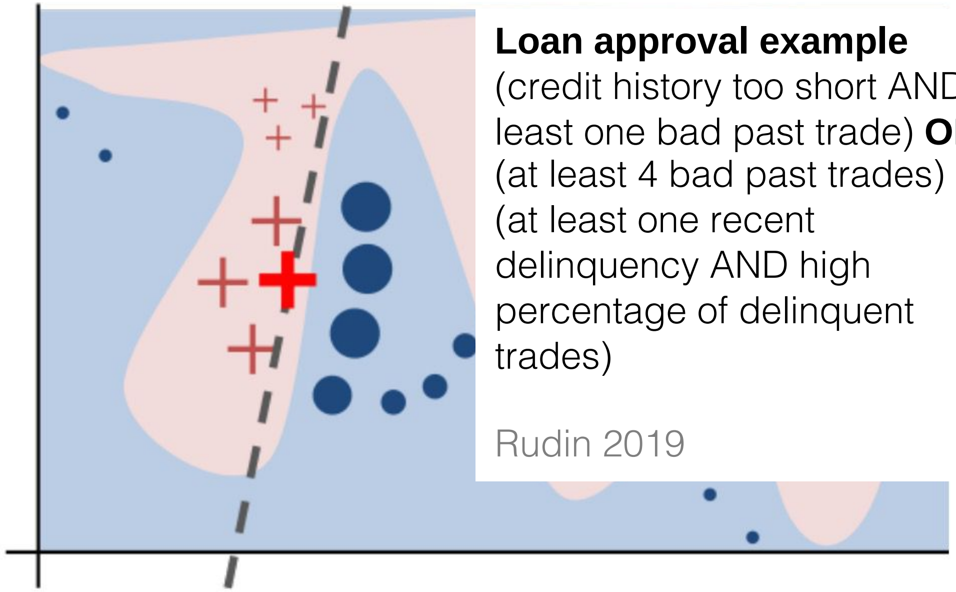
Recidivism prediction algorithm

Performance as good as a black box model with 130+ factors; might include socio-economic info; expensive (software license); within software used in US justice system



IF	age between 18-20 and sex is male	THEN predict arrest (within 2 years)
ELSE IF	age between 21-23 and 2-3 prior offences	THEN predict arrest
ELSE IF	more than three priors	THEN predict arrest
ELSE	predict no arrest	

Rudin, Cynthia. "Stop Explaining Black Box Machine Learning Models for High Stakes Decisions and Use Interpretable Models Instead." Nature Machine Intelligence 1, no. 5 (2019): 206–15.



Loan approval example (credit history too short AND at least one bad past trade) **OR** (at least 4 bad past trades) **OR** (at least one recent delinquency AND high percentage of delinquent trades)

Rudin 2019

Ribeiro, Marco Tulio, Sameer Singh, and Carlos Guestrin. "Model-Agnostic Interpretability of Machine Learning." ArXiv Preprint ArXiv:1606.05386, 2016.

For further reading…

Raschka, Sebastian. “Model Evaluation, Model Selection, and Algorithm Selection in Machine Learning.” *ArXiv:1811.12808 [Cs, Stat]*, November 10, 2020. http://arxiv.org/abs/1811.12808.

Kohavi, Ron. “A Study of Cross-Validation and Bootstrap for Accuracy Estimation and Model Selection.” In *IJCAI*, 14:1137–45. Montreal, Canada, 1995. (link)