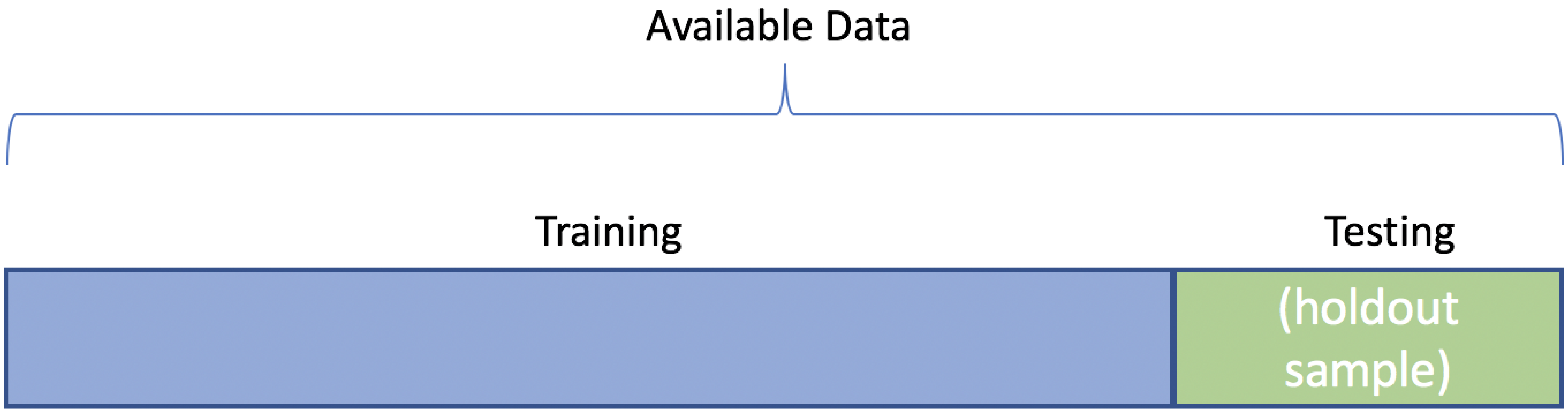
Creating train, test, and validation datasets

MODEL VALIDATION IN PYTHON

Kasey Jones
Data Scientist

Traditional train/test split

- Seen data (used for training)
- Unseen data (unavailable for training)



Dataset definitions and ratios

Dataset	Definition
Train	The sample of data used when fitting models
Test (holdout sample)	The sample of data used to assess model performance

Ratio Examples

- 80:20
- 90:10 (used when we have little data)
- 70:30 (used when model is computationally expensive)

The X and y datasets

```
import pandas as pd

tic_tac_toe = pd.read_csv("tic-tac-toe.csv")
X = pd.get_dummies(tic_tac_toe.iloc[:,0:9])
y = tic_tac_toe.iloc[:, 9]
```

Python courses covering dummy variables:

- **Supervised Learning**
- **Preprocessing for Machine Learning**

Creating holdout samples

```
X_train, X_test, y_train, y_test  =\
    train_test_split(X, y, test_size=0.2, random_state=1111)
```

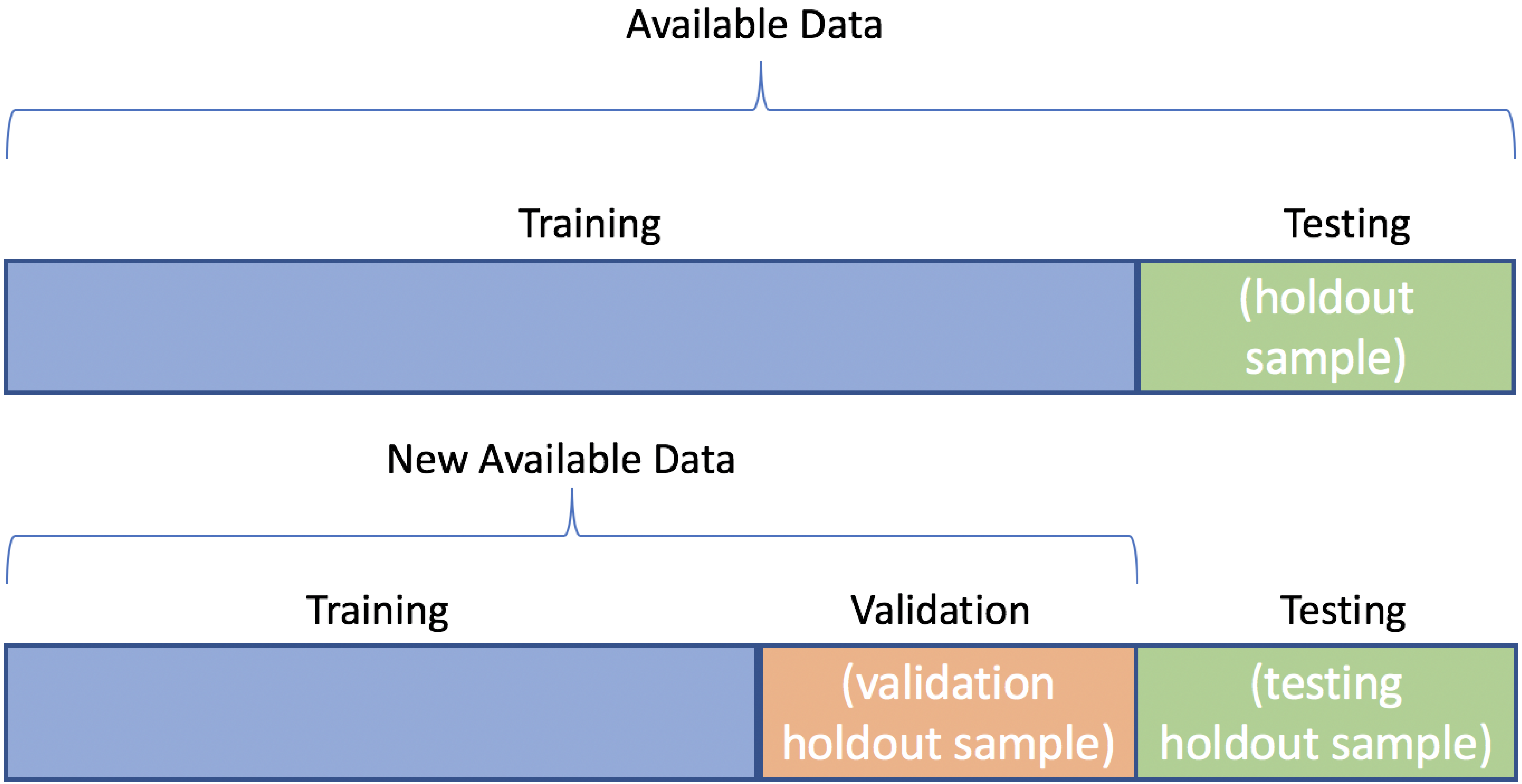
Parameters:

- `test_size`
- `train_size`
- `random_state`

Dataset for preliminary testing?

What do we do when testing different model parameters?

- 100 *versus* 1000 trees


Available Data
Training
Testing
(holdout sample)
New Available Data
Training
Validation
Testing
(validation holdout sample)
(testing holdout sample)

Train, validation, test continued

```
X_temp, X_test, y_temp, y_test  =\
    train_test_split(X, y, test_size=0.2, random_state=1111)
```

```
X_train, X_val, y_train, y_val =\
    train_test_split(X_temp, y_temp, test_size=0.25, random_state=11111)
```

It's holdout time

MODEL VALIDATION IN PYTHON

Accuracy metrics: regression models

MODEL VALIDATION IN PYTHON

Kasey Jones
Data Scientist

Regression models

12.2 points

15 gallons of gas

$1,323,492

6 new puppies

4,320 people

Mean absolute error (MAE)

$$MAE = \frac{\sum_{i=1}^{n} |y_i - \hat{y}_i|}{n}$$

- Simplest and most intuitive metric
- Treats all points equally
- Not sensitive to outliers

Mean squared error (MSE)

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

- Most widely used regression metric
- Allows outlier errors to contribute more to the overall error
- Random family road trips could lead to large errors in predictions

MAE vs. MSE

- Accuracy metrics are always application specific
- MAE and MSE error terms are in different units and should not be compared

Mean absolute error

```
rfr = RandomForestRegressor(n_estimators=500, random_state=1111)
rfr.fit(X_train, y_train)
test_predictions = rfr.predict(X_test)
sum(abs(y_test - test_predictions))/len(test_predictions)
```

```
9.99
```

```
from sklearn.metrics import mean_absolute_error
mean_absolute_error(y_test, test_predictions)
```

```
9.99
```

Mean squared error

```
sum(abs(y_test - test_predictions)**2)/len(test_predictions)
```

```
141.4
```

```
from sklearn.metrics import mean_squared_error
mean_squared_error(y_test, test_predictions)
```

```
141.4
```

Accuracy for a subset of data

```
chocolate_preds = rfr.predict(X_test[X_test[:, 1] == 1])
mean_absolute_error(y_test[X_test[:, 1] == 1], chocolate_preds)
```

```
8.79
```

```
nonchocolate_preds = rfr.predict(X_test[X_test[:, 1] == 0])
mean_absolute_error(y_test[X_test[:, 1] == 0], nonchocolate_preds)
```

```
10.99
```

Let's practice

MODEL VALIDATION IN PYTHON

Classification metrics

MODEL VALIDATION IN PYTHON

Kasey Jones
Data Scientist

Classification metrics

- Precision
- Recall (also called sensitivity)
- Accuracy
- Specificity
- F1-Score, and its variations
- ...

Classification metrics

- **Precision**
- **Recall** (also called sensitivity)
- **Accuracy**
- Specificity
- F1-Score, and its variations
- ...

Confusion matrix

		Predicted Values	
		0	1
Actual Values	0	23 (TN)	7 (FP)
	1	8 (FN)	62 (TP)

True Positive: Predict/Actual are both 1

True Negative: Predict/Actual are both 0

False Positive: Predicted 1, actual 0

False Negative: Predicted 0, actual 1

```python
from sklearn.metrics import confusion_matrix
cm = confusion_matrix(y_test, test_predictions)
print(cm)
```

```
array([[ 23,  7],
       [  8, 62]])
```

```python
cm[<true_category_index>, <predicted_category_index>]
cm[1, 0]
```

```
8
```

Accuracy

		Predicted Values	
		0	1
Actual Values	0	23	7
	1	8	62

$$\frac{23(TN)+62(TP)}{23+7+8+62} = .85$$

Precision

		Predicted Values	
		0	1
Actual Values	0	23	7
	1	8	62

$$\frac{62(\mathrm{TP})}{62(\mathrm{TP})+7(\mathrm{FP})} = .90$$

Recall

Predicted Values

Actual Values	0	1
0	23	7
1	8	62

$$\frac{62(TP)}{62(TP)+8(FN)} = .885$$

Accuracy, precision, recall

```
from sklearn.metrics import accuracy_score, precision_score, recall_score
accuracy_score(y_test, test_predictions)
```

```
.85
```

```
precision_score(y_test, test_predictions)
```

```
.8986
```

```
recall_score(y_test, test_predictions)
```

```
.8857
```

Practice time

MODEL VALIDATION IN PYTHON

The bias-variance tradeoff

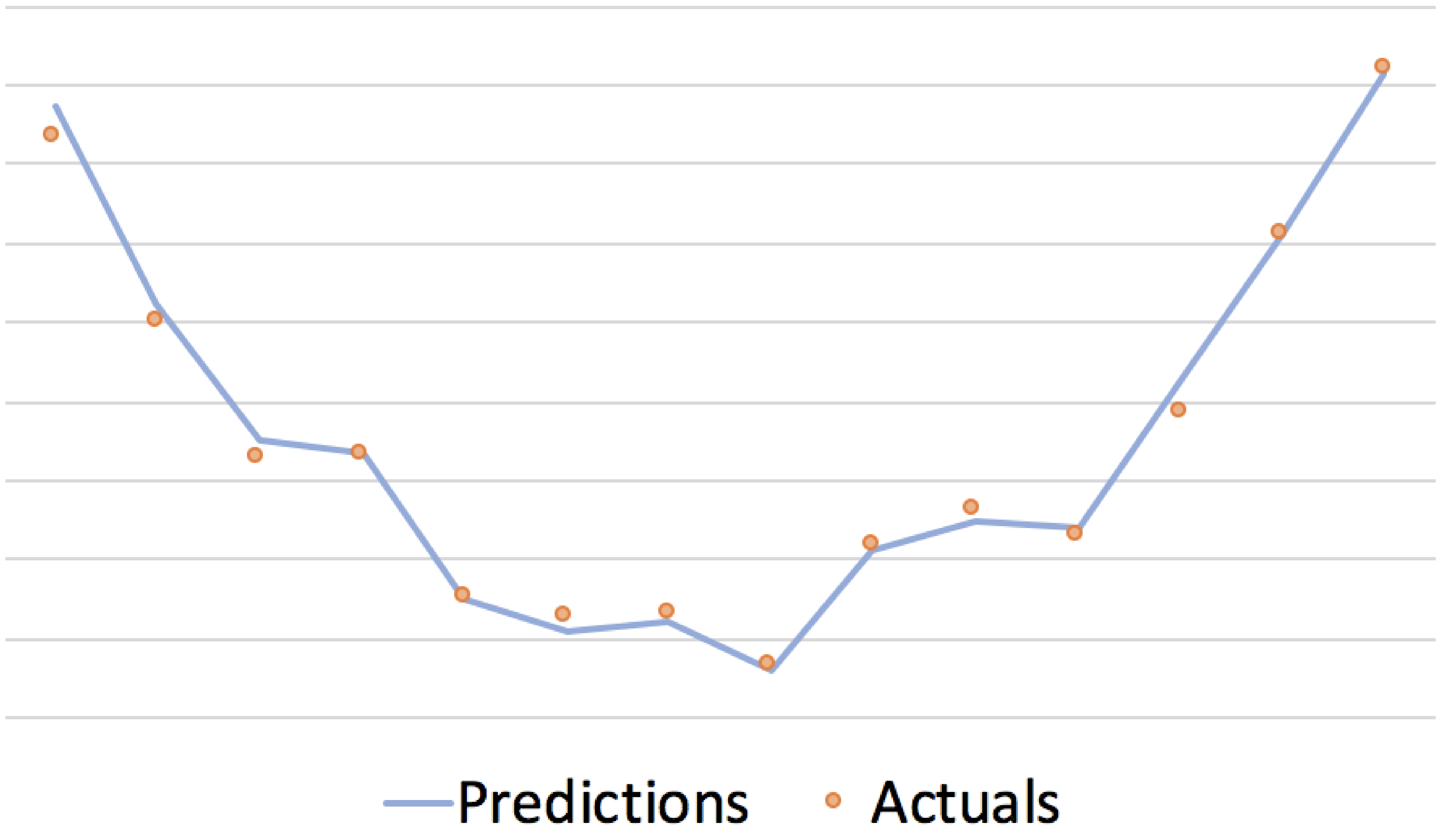
MODEL VALIDATION IN PYTHON

Kasey Jones
Data Scientist

Variance

- Variance: following the training data too closely
  - Fails to generalize to the test data
  - Low training error but high testing error
  - Occurs when models are overfit and have high complexity

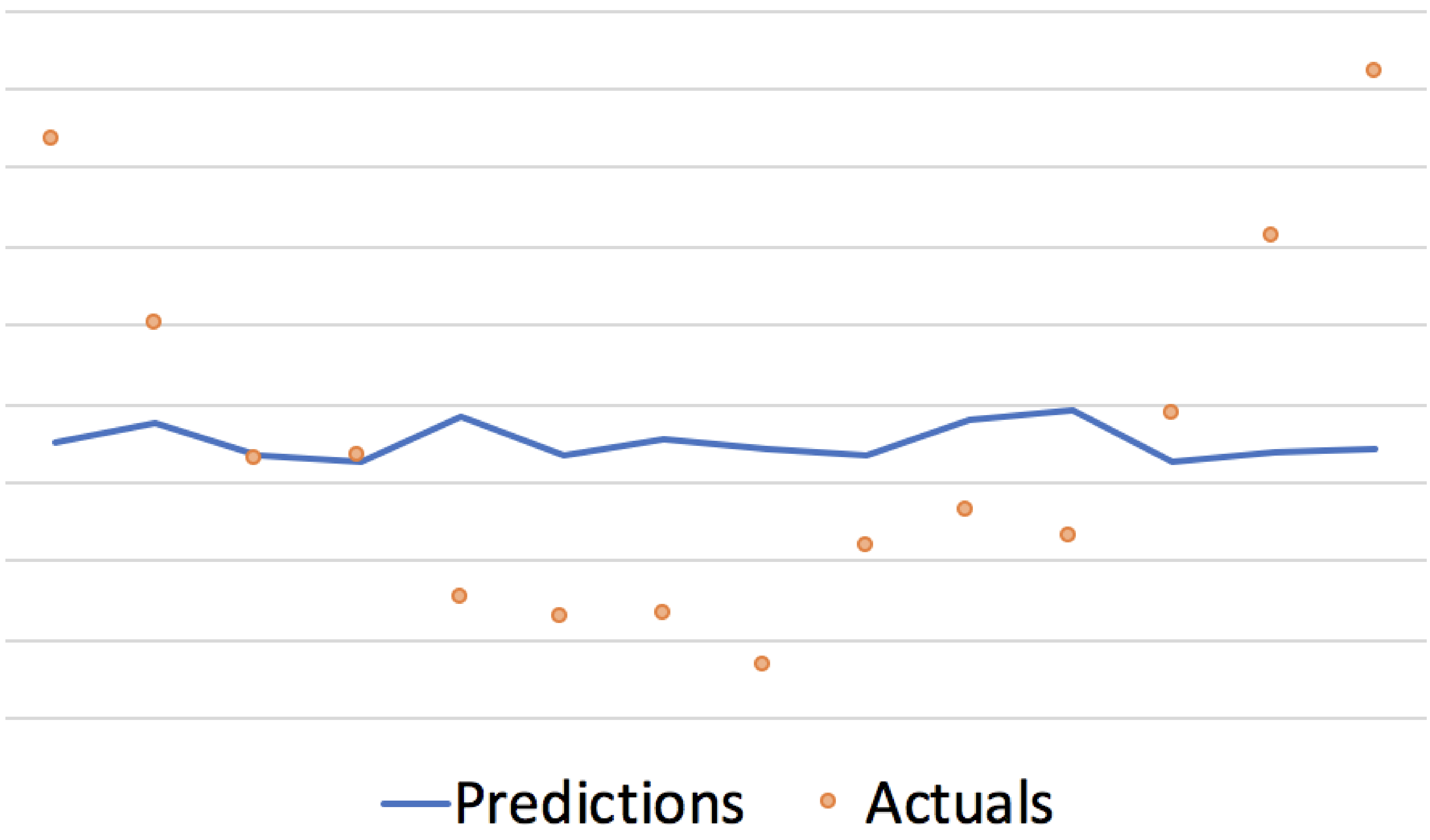
Overfitting models (high variance)



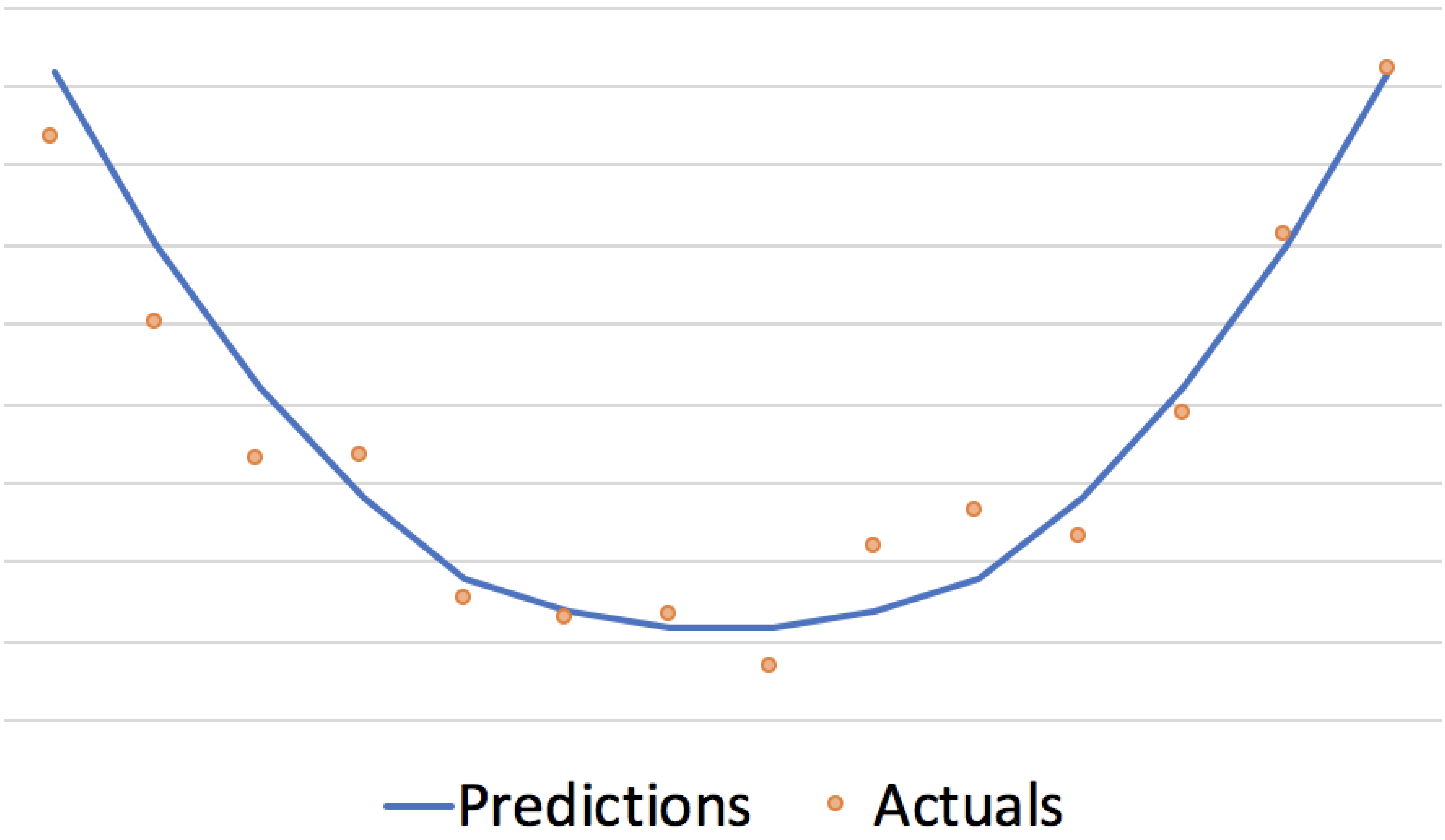
Bias

- Bias: failing to find the relationship between the data and the response
  - High training/testing error
  - Occurs when models are underfit

Underfitting models (high bias)



Optimal performance



- Bias-Variance Tradeoff

Parameters causing over/under fitting

```
rfc = RandomForestClassifier(n_estimators=100, max_depth=4)
rfc.fit(X_train, y_train)

print("Training: {0:.2f}".format(accuracy_score(y_train, train_predictions)))
```

```
Training: .84
```

```
print("Testing: {0:.2f}".format(accuracy_score(y_test, test_predictions)))
```

```
Testing: .77
```

```python
rfc = RandomForestClassifier(n_estimators=100, max_depth=14)
rfc.fit(X_train, y_train)

print("Training: {0:.2f}".format(accuracy_score(y_train, train_predictions)))
```

```
Training: 1.0
```

```python
print("Testing: {0:.2f}".format(accuracy_score(y_test, test_predictions)))
```

```
Testing: .83
```

```
rfc = RandomForestClassifier(n_estimators=100, max_depth=10)
rfc.fit(X_train, y_train)

print("Training: {0:.2f}".format(accuracy_score(y_train, train_predictions)))
```

```
Training: .89
```

```
print("Testing: {0:.2f}".format(accuracy_score(y_test, test_predictions)))
```

```
Testing: .86
```

Remember, only you can prevent overfitting!

MODEL VALIDATION IN PYTHON