

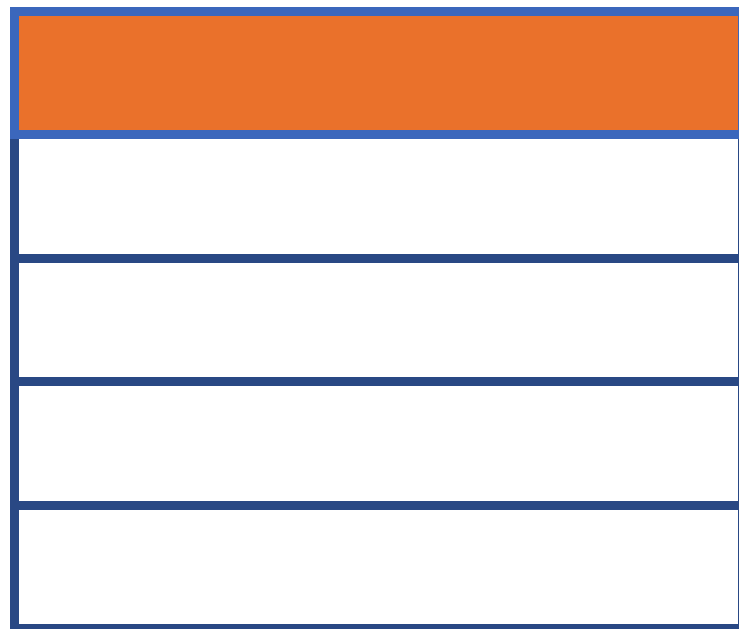
# The problems with holdout sets

MODEL VALIDATION IN PYTHON



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# Transition validation



Model 1

```
X_train, X_val, y_train, y_val =  
    train_test_split(X, y,  
                    test_size=0.2)
```

```
rf = RandomForestRegressor()
```

```
rf.fit(X_train, y_train)
```

```
out_of_sample = rf.predict(X_test)
```

```
print(mae(y_test, out_of_sample))
```

10.24

# Traditional training splits

```
cd = pd.read_csv("candy-data.csv")  
s1 = cd.sample(60, random_state=1111)  
s2 = cd.sample(60, random_state=1112)
```

Overlapping candies:

```
print(len([i for i in s1.index if i in s2.index]))
```

39

# Traditional training splits

Chocolate Candies:

```
print(s1.chocolate.value_counts()[0])  
print(s2.chocolate.value_counts()[0])
```

34

30

# The split matters

## Sample 1 Testing Error

```
print('Testing error: {0:.2f}'.format(mae(s1_y_test, rfr.predict(s1_X_test))))
```

10.32

## Sample 2 Testing Error

```
print('Testing error: {0:.2f}'.format(mae(s2_y_test, rfr.predict(s2_X_test))))
```

11.56

# Train, validation, test

```
X_temp, X_val, y_temp, y_val = train_test_split(..., random_state=1111)
X_train, X_test, y_train, y_test = train_test_split(..., random_state=1111)

rfr = RandomForestRegressor(n_estimators=25, random_state=1111, max_features=4)
rfr.fit(X_train, y_train)
print('Validation error: {0:.2f}'.format(mae(y_test, rfr.predict(X_test))))
```

9.18

```
print('Testing error: {0:.2f}'.format(mae(y_val, rfr.predict(X_val))))
```

8.98

# Round 2

```
X_temp, X_val, y_temp, y_val = train_test_split(..., random_state=1171)
X_train, X_test, y_train, y_test = train_test_split(..., random_state=1171)

rfr = RandomForestRegressor(n_estimators=25, random_state=1111, max_features=4)
rfr.fit(X_train, y_train)
print('Validation error: {0:.2f}'.format(mae(y_test, rfr.predict(X_test))))
```

8.73

```
print('Testing error: {0:.2f}'.format(mae(y_val, rfr.predict(X_val))))
```

10.91

random seed

가

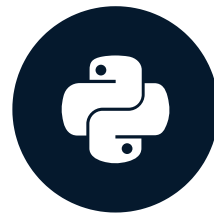
# Holdout set exercises

MODEL VALIDATION IN PYTHON



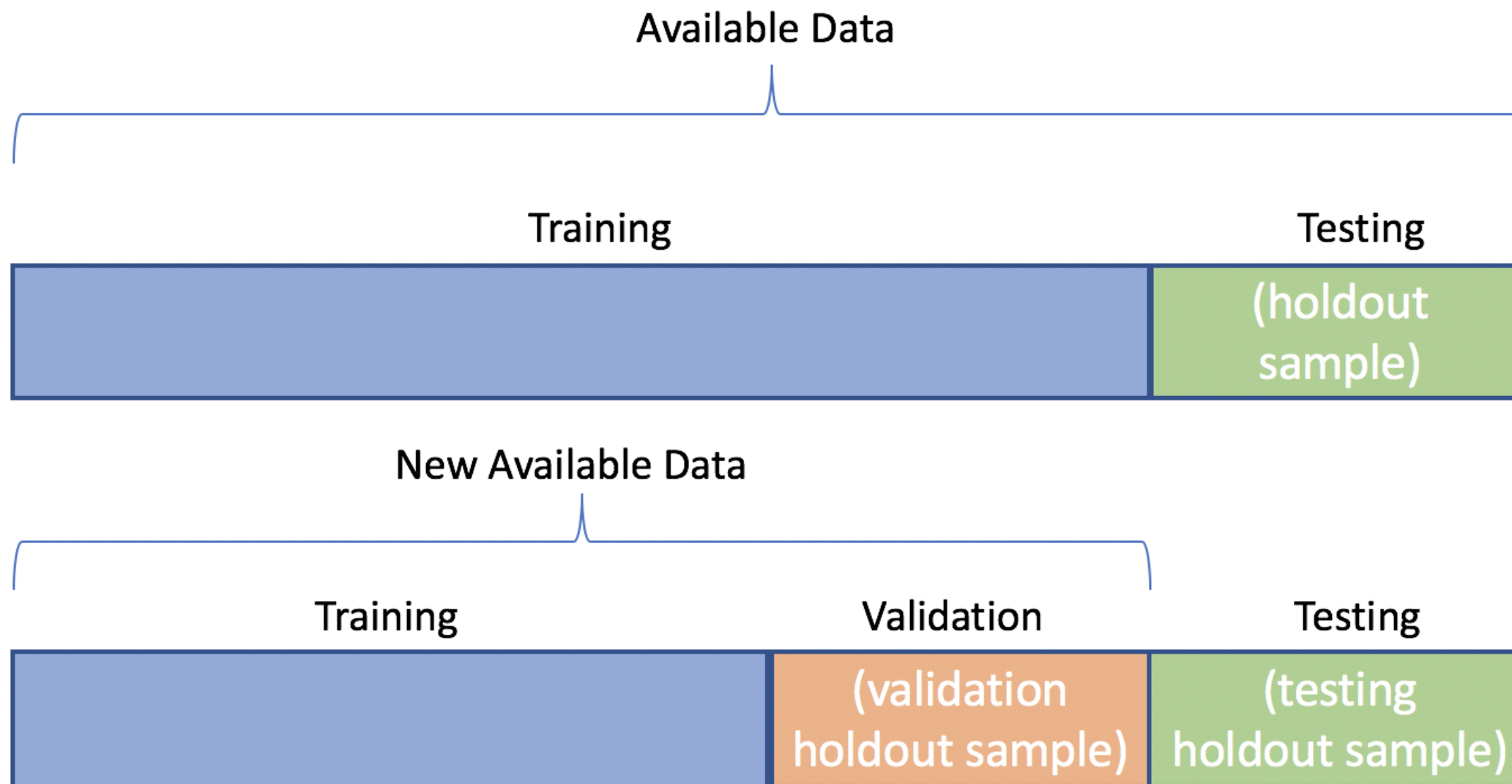
# Cross-validation

MODEL VALIDATION IN PYTHON

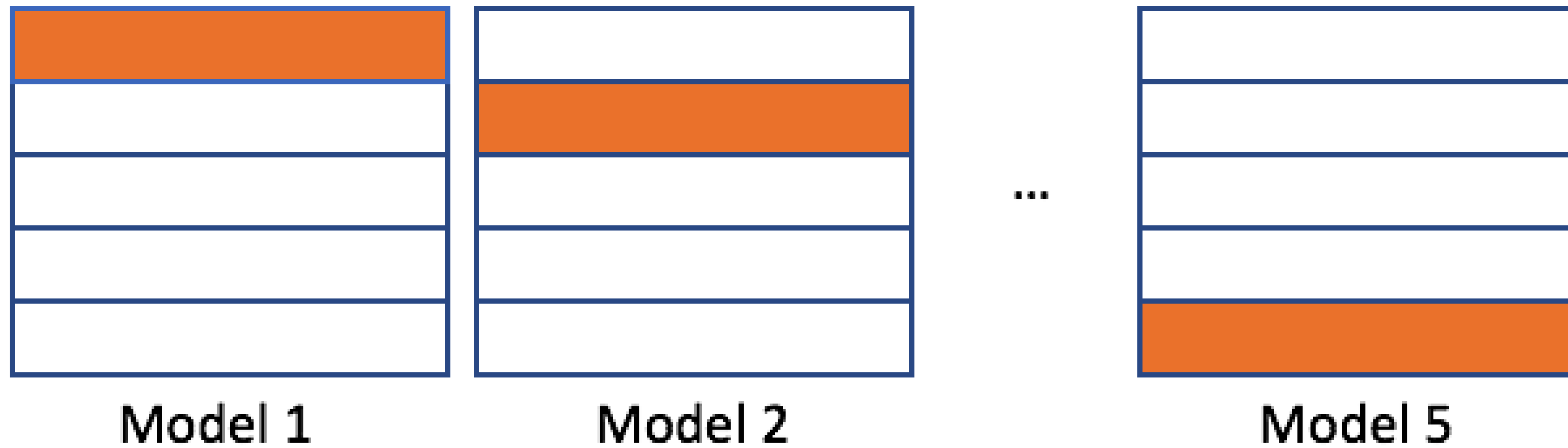
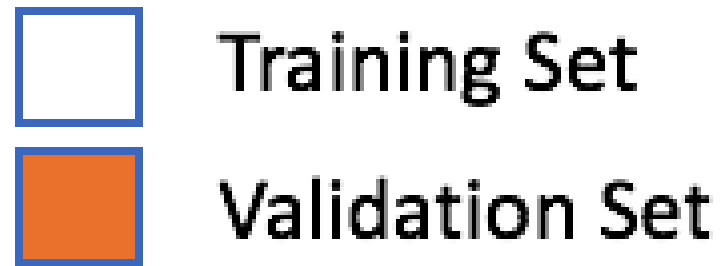


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# Cross-validation



# Cross-validation



`n_splits` : number of cross-validation splits

`shuffle` : boolean indicating to shuffle data before splitting

`random_state` : random seed

```
from sklearn.model_selection import KFold
```

```
X = np.array(range(40))
```

```
y = np.array([0] * 20 + [1] * 20)
```

```
kf = KFold(n_splits=5)
```

```
splits = kf.split(X)
```

```

kf = KFold(n_splits=5)
splits = kf.split(X)
for train_index, test_index in splits:
    print(len(train_index), len(test_index))

```

split X 5가 가

```

32 8 32 8 32 8 32 8 32 8
train_index 32가 , values, test_index 8 가
5

```

```

# Print one of the index sets:
print(train_index, test_index)

```

```

[ 0  1  2  3  4  5  6  7  8  9 10 11 12 13 14 15 16 17 18 19 20 ...]
[32 33 34 35 36 37 38 39]

```

```
rfr = RandomForestRegressor(n_estimators=25, random_state=1111)
errors = []
for train_index, val_index in splits:
    X_train, y_train = X[train_index], y[train_index]
    X_val, y_val = X[val_index], y[val_index]

    rfr.fit(X_train, y_train)
    predictions = rfr.predict(X_val)
    errors.append(<some_accuracy_metric>)
print(np.mean(errors)) 5
```

4.25

# Practice time

MODEL VALIDATION IN PYTHON

# sklearn's `cross_val_score()`

MODEL VALIDATION IN PYTHON



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# cross\_val\_score()

```
from sklearn.model_selection import cross_val_score
from sklearn.ensemble import RandomForestClassifier
rfc = RandomForestClassifier()
```

scikit - learn    cross\_val\_score()  
.

**estimator** : the model to use

**X** : the predictor dataset

cross\_val\_score()  
ex) RandomForestClassifier    score  
model    R

**y** : the response array

**cv** : the number of cross-validation splits

```
cross_val_score(estimator=rfc, X=X, y=y, cv=5)
```

# Using scoring and `make_scorer`

The `cross_val_score` `scoring` parameter:

```
# Load the Methods
from sklearn.metrics import mean_absolute_error, make_scorer

# Create a scorer
mae_scorer = make_scorer(mean_absolute_error)

# Use the scorer
cross_val_score(<estimator>, <X>, <y>, cv=5, scoring=mae_scorer)
```

Load all of the `sklearn` methods

```
from sklearn.ensemble import RandomForestRegressor
from sklearn.model_selection import cross_val_score
from sklearn.metrics import mean_squared_error, make_scorer
```

Create a model and a scorer

```
rfc = RandomForestRegressor(n_estimators=20, max_depth=5, random_state=1111)
mse = make_scorer(mean_squared_error)
```

Run `cross_val_score()`

```
cv_results = cross_val_score(rfc, X, y, cv=5, scoring=mse)
```

# Accessing the results

```
print(cv_results)      80/20      86      223
```

```
[196.765, 108.563, 85.963, 222.594, 140.942]
```

Report the mean and standard deviation:

```
print('The mean: {}'.format(cv_results.mean()))  
print('The std: {}'.format(cv_results.std())) =>
```

```
The mean: 150.965
```

```
The std: 51.676
```

가 가

**Let's practice!**  
MODEL VALIDATION IN PYTHON

# Leave-one-out- cross-validation (LOOCV)

MODEL VALIDATION IN PYTHON

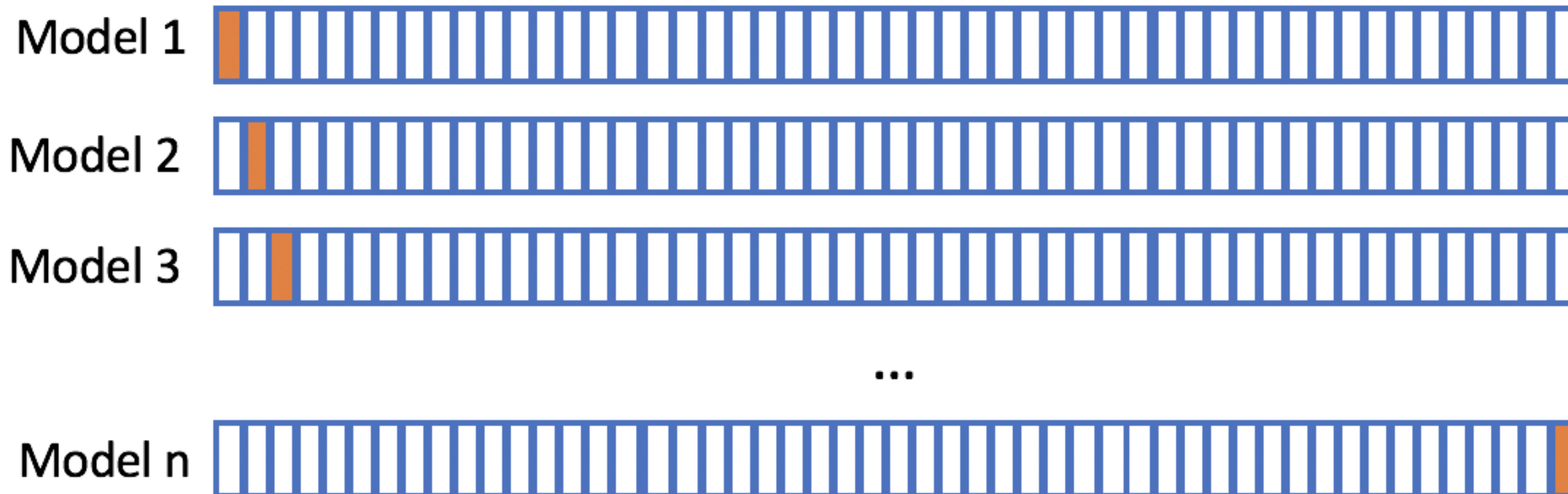


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# LOOCV

ex) 가 n train .

 Training Set  Validation Set



# When to use LOOCV?

## Use when:

- The amount of training data is limited
- You want the absolute best error estimate for new data

## Be cautious when:

- Computational resources are limited
- You have a lot of data
- You have a lot of parameters to test



# LOOCV Example

```
n = X.shape[0]
mse = make_scorer(mean_squared_error)
cv_results = cross_val_score(estimator, X, y, scoring=mse, cv=n)
```

```
print(cv_results) model
```

```
[5.45, 10.52, 6.23, 1.98, 11.27, 9.21, 4.65, ... ]
```

```
print(cv_results.mean())
```

```
6.32
```

# Let's practice

## MODEL VALIDATION IN PYTHON