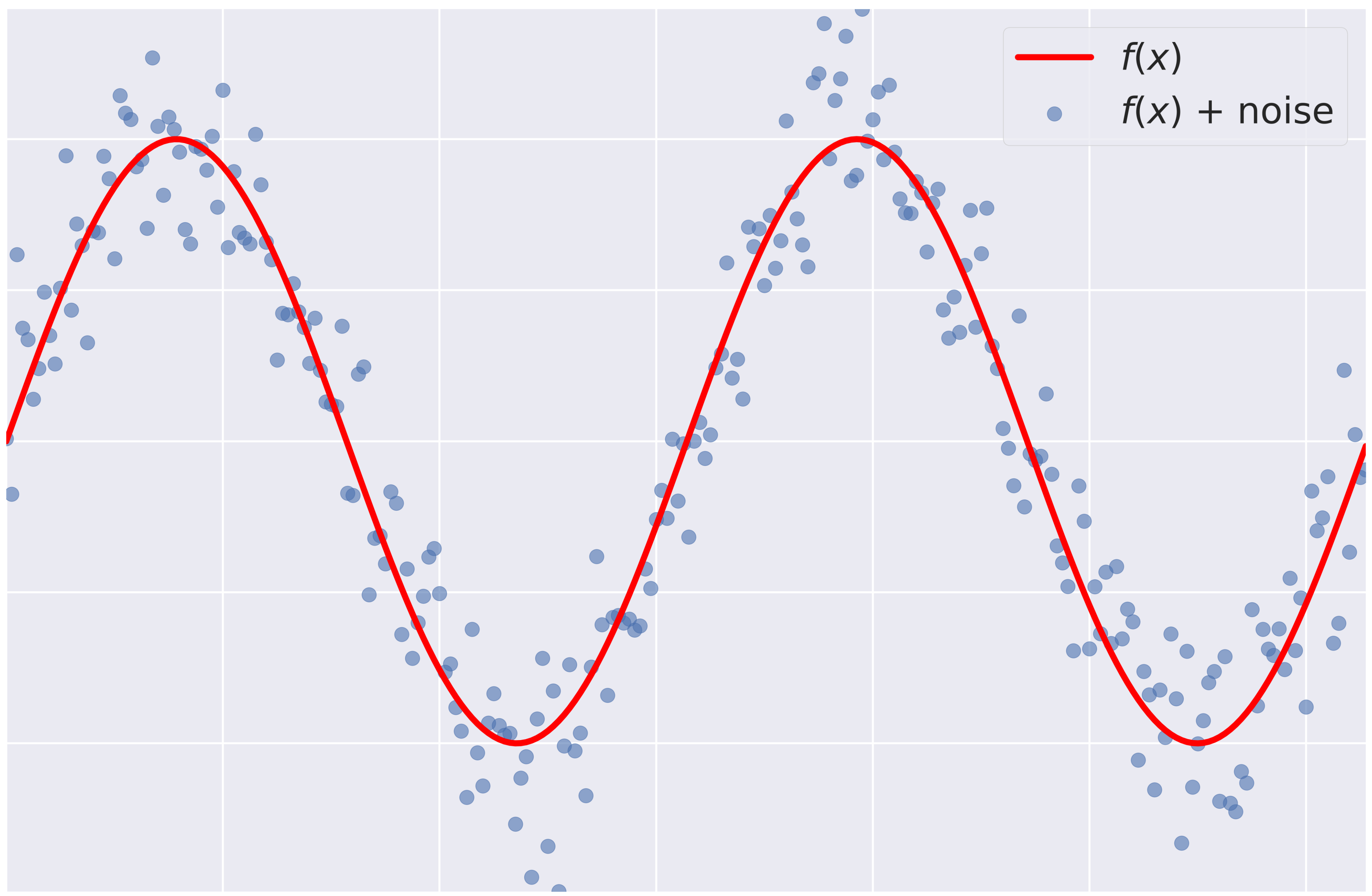
Generalization Error

MACHINE LEARNING WITH TREE-BASED MODELS IN PYTHON

Elie Kawerk
Data Scientist

Supervised Learning - Under the Hood

- Supervised Learning: $y = f(x)$, f is unknown.



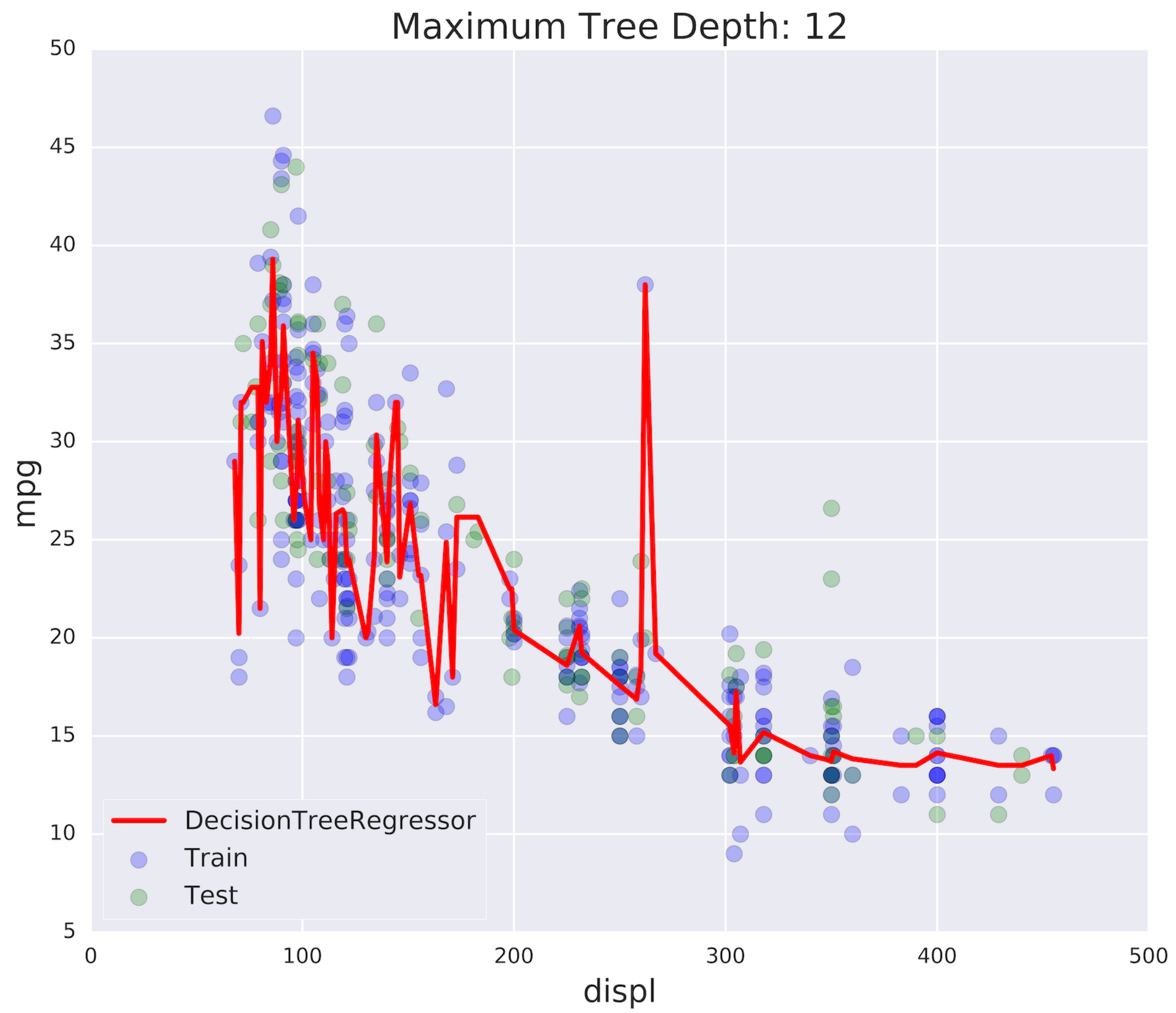
Goals of Supervised Learning

- Find a model $\hat{f}$ that best approximates f: $\hat{f} \approx f$
- $\hat{f}$ can be Logistic Regression, Decision Tree, Neural Network ...
- Discard noise as much as possible.
- **End goal**: $\hat{f}$ should achieve a low predictive error on unseen datasets.

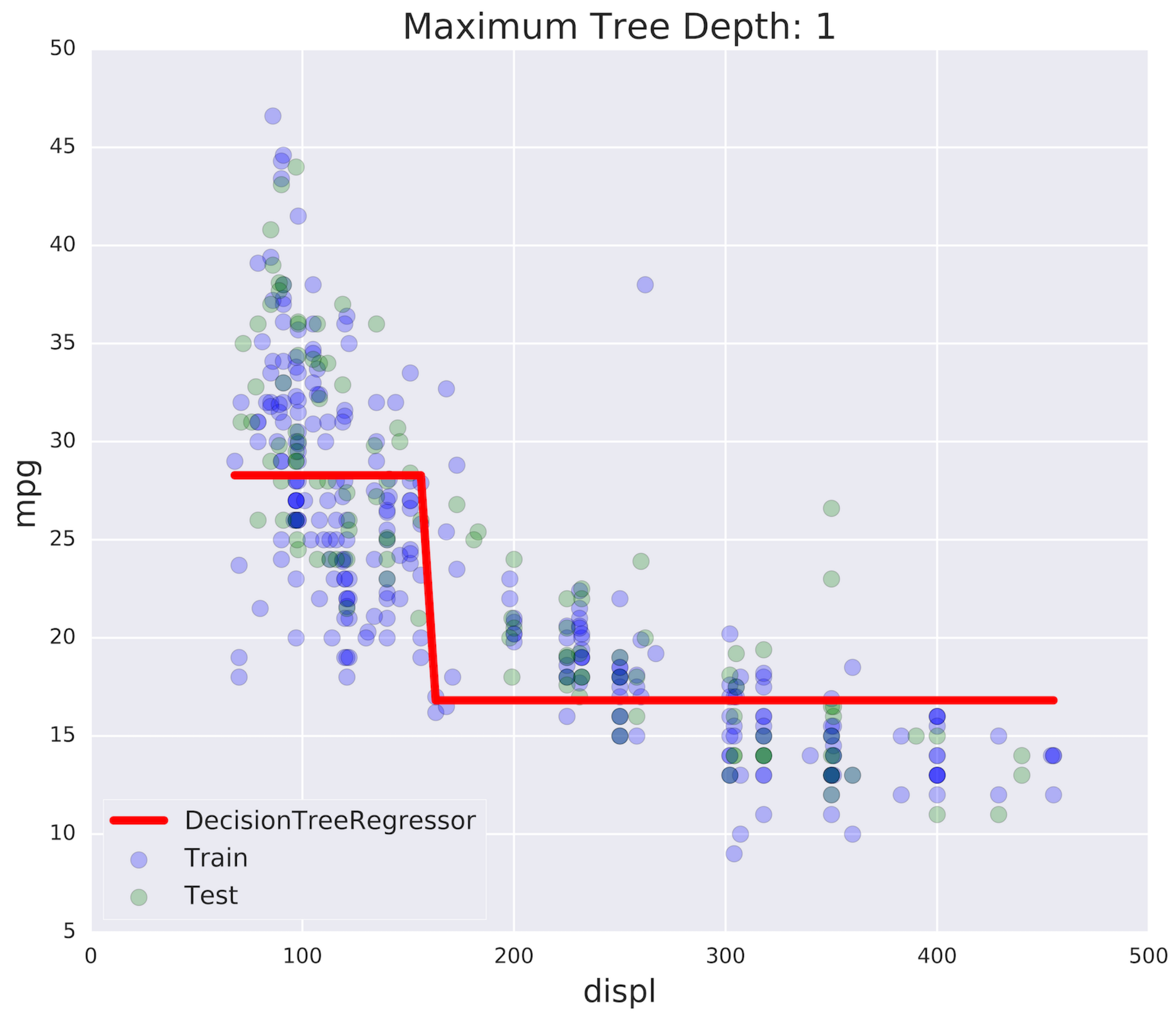
Difficulties in Approximating f

- **Overfitting:** $\hat{f}(x)$ fits the training set noise.
- **Underfitting:** $\hat{f}$ is not flexible enough to approximate f.

Overfitting



Underfitting

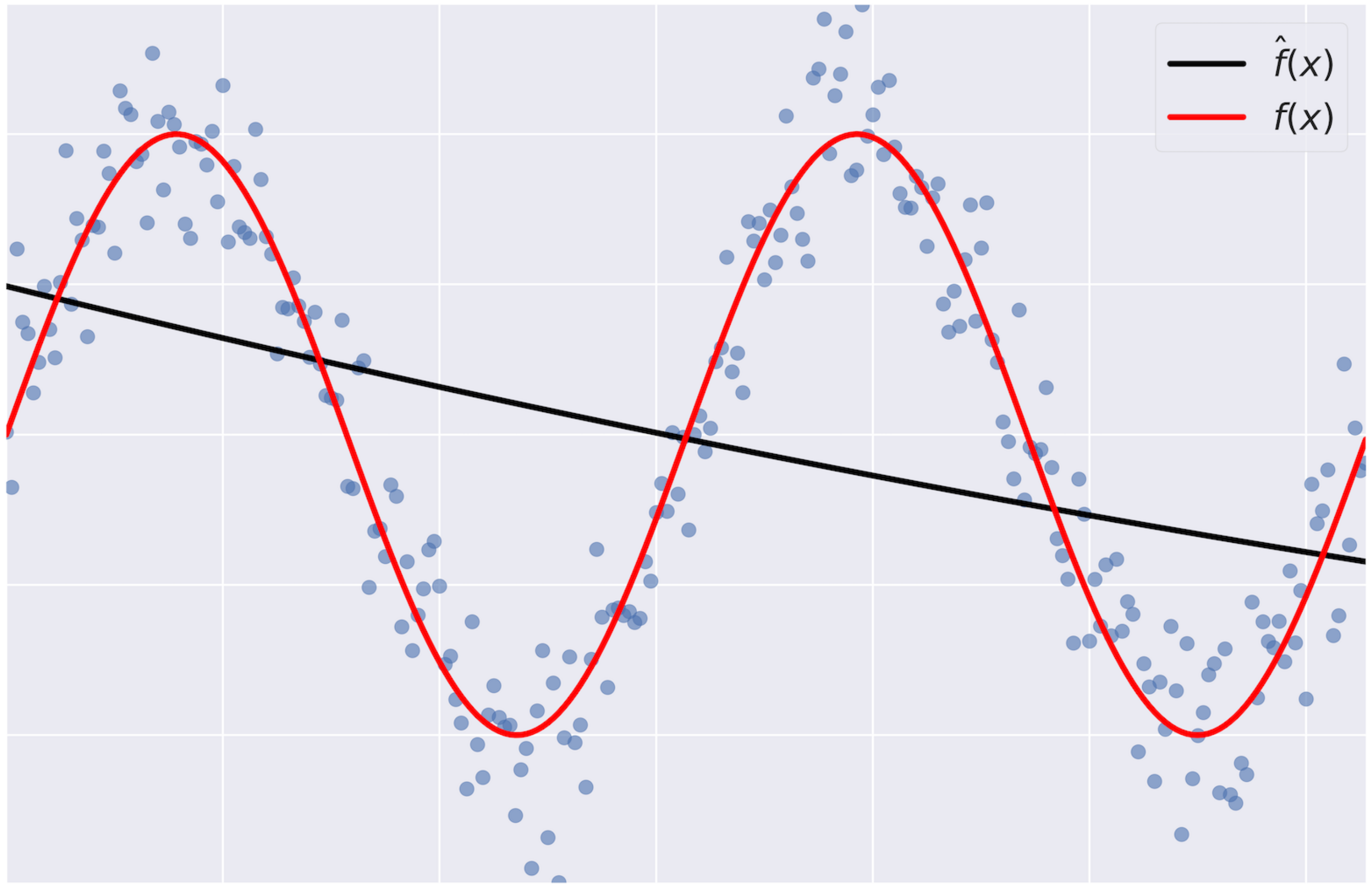


Generalization Error

- **Generalization Error of $\hat{f}$**: Does $\hat{f}$ generalize well on unseen data?
- It can be decomposed as follows: Generalization Error of $\hat{f} = bias^2 + variance + \text{irreducible error}$

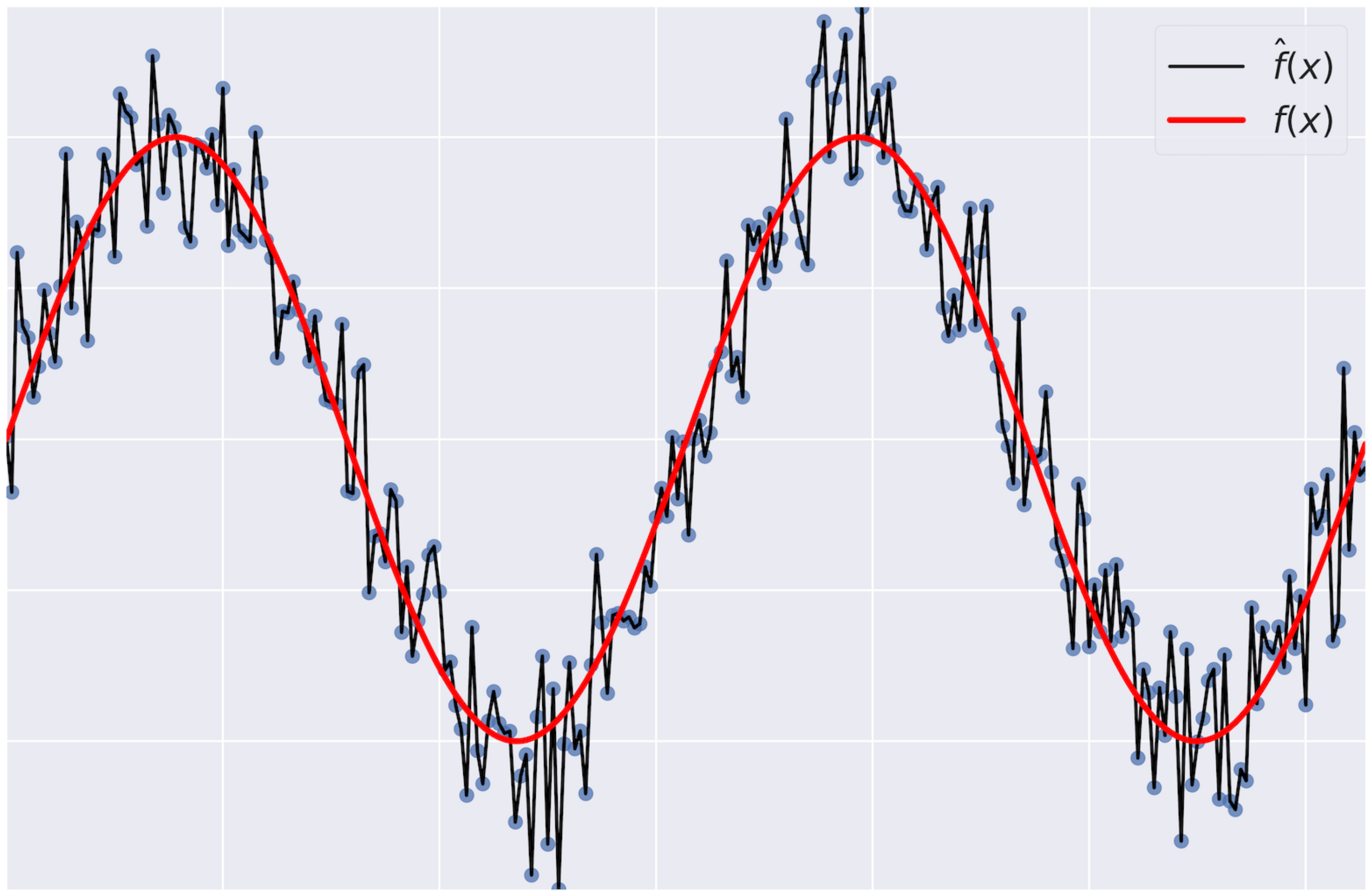
Bias

- **Bias:** error term that tells you, on average, how much $\hat{f} \neq f$.



Variance

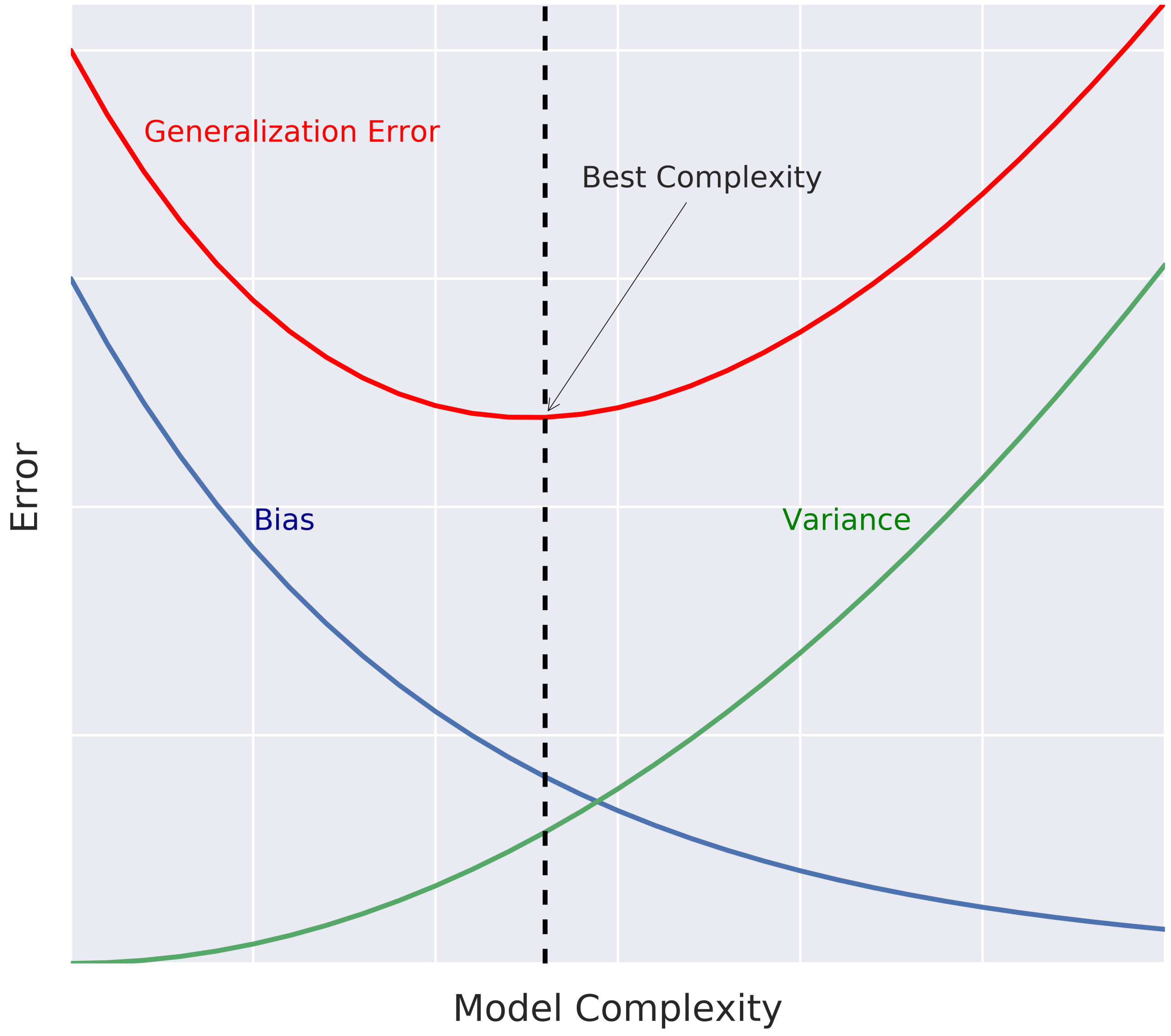
- **Variance:** tells you how much $\hat{f}$ is inconsistent over different training sets.



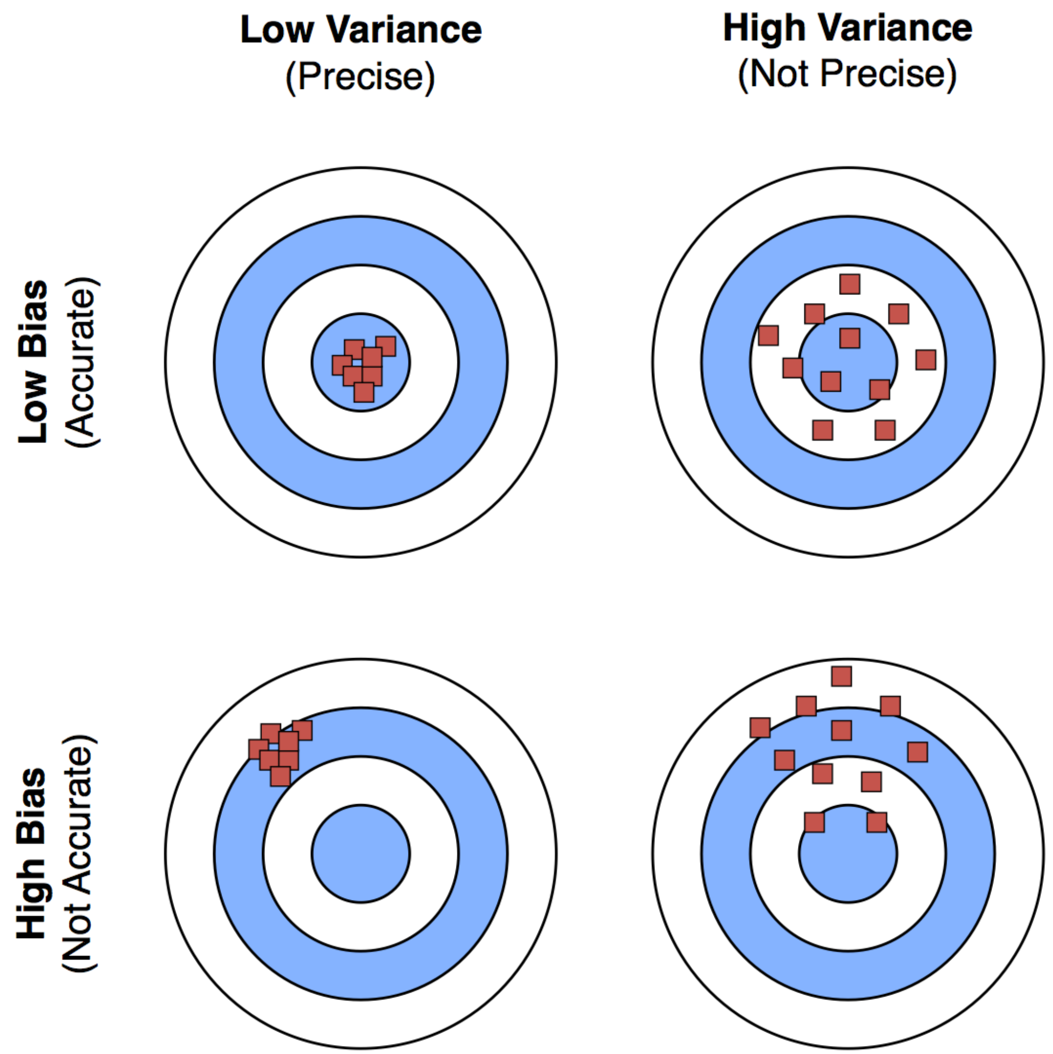
Model Complexity

- **Model Complexity:** sets the flexibility of $\hat{f}$.
- Example: Maximum tree depth, Minimum samples per leaf, ...

Bias-Variance Tradeoff



Bias-Variance Tradeoff: A Visual Explanation



Let's practice!

MACHINE LEARNING WITH TREE-BASED MODELS IN PYTHON

Diagnosing Bias and Variance Problems

MACHINE LEARNING WITH TREE-BASED MODELS IN PYTHON

Elie Kawerk
Data Scientist

Estimating the Generalization Error

- How do we estimate the generalization error of a model?
- Cannot be done directly because:
  - f is unknown,
  - usually you only have one dataset,
  - noise is unpredictable.

Estimating the Generalization Error

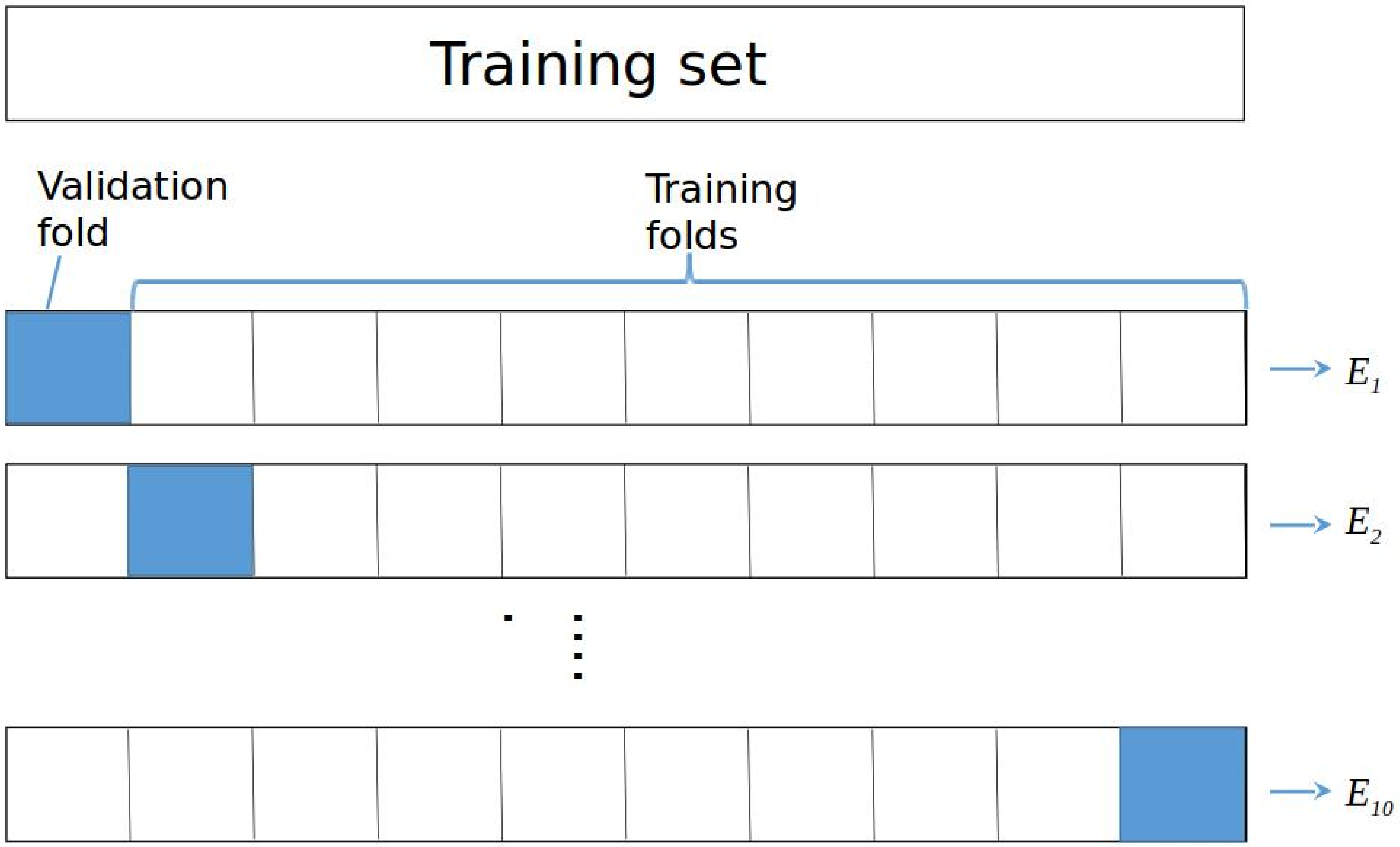
Solution:

- split the data to training and test sets,
- fit $\hat{f}$ to the training set,
- evaluate the error of $\hat{f}$ on the **unseen** test set.
- generalization error of $\hat{f} \approx$ test set error of $\hat{f}$.

Better Model Evaluation with Cross-Validation

- Test set should not be touched until we are confident about $\hat{f}$'s performance.
- Evaluating $\hat{f}$ on training set: biased estimate, $\hat{f}$ has already seen all training points.
- Solution $\rightarrow$ Cross-Validation (CV):
  - K-Fold CV,
  - Hold-Out CV.

K-Fold CV



K-Fold CV

$$\text{CV error} = \frac{E_1 + \ldots + E_{10}}{10}$$

Diagnose Variance Problems

- If $\hat{f}$ suffers from **high variance**: CV error of $\hat{f}$ > training set error of $\hat{f}$.
- $\hat{f}$ is said to overfit the training set. To remedy overfitting:
  - decrease model complexity,
  - for ex: decrease max depth, increase min samples per leaf, ...
  - gather more data, ..

Diagnose Bias Problems

- if $\hat{f}$ suffers from high bias: CV error of $\hat{f}$ $\approx$ training set error of $\hat{f}$ $>>$ desired error.
- $\hat{f}$ is said to underfit the training set. To remedy underfitting:
  - increase model complexity
  - for ex: increase max depth, decrease min samples per leaf, ...
  - gather more relevant features

K-Fold CV in sklearn on the Auto Dataset

```
from sklearn.tree import DecisionTreeRegressor
from sklearn.model_selection import train_test_split
from sklearn.metrics import mean_squared_error as MSE
from sklearn.model_selection import cross_val_score
# Set seed for reproducibility
SEED = 123
# Split data into 70% train and 30% test
X_train, X_test, y_train, y_test = train_test_split(X,y,
                                                    test_size=0.3,
                                                    random_state=SEED)
# Instantiate decision tree regressor and assign it to 'dt'
dt = DecisionTreeRegressor(max_depth=4,
                           min_samples_leaf=0.14,
                           random_state=SEED)
```

K-Fold CV in sklearn on the Auto Dataset

```
# Evaluate the list of MSE ontained by 10-fold CV
# Set n_jobs to -1 in order to exploit all CPU cores in computation
MSE_CV = - cross_val_score(dt, X_train, y_train, cv= 10,
                           scoring='neg_mean_squared_error',
                           n_jobs = -1)
# Fit 'dt' to the training set
dt.fit(X_train, y_train)
# Predict the labels of training set
y_predict_train = dt.predict(X_train)
# Predict the labels of test set
y_predict_test = dt.predict(X_test)
```

```python
# CV MSE
print('CV MSE: {:.2f}'.format(MSE_CV.mean()))
```

```
CV MSE: 20.51
```

```python
# Training set MSE
print('Train MSE: {:.2f}'.format(MSE(y_train, y_predict_train)))
```

```
Train MSE: 15.30
```

```python
# Test set MSE
print('Test MSE: {:.2f}'.format(MSE(y_test, y_predict_test)))
```

```
Test MSE: 20.92
```

Let's practice!

MACHINE LEARNING WITH TREE-BASED MODELS IN PYTHON

Ensemble Learning

MACHINE LEARNING WITH TREE-BASED MODELS IN PYTHON

Elie Kawerk
Data Scientist

Advantages of CARTs

- Simple to understand.
- Simple to interpret.
- Easy to use.
- Flexibility: ability to describe non-linear dependencies.
- Preprocessing: no need to standardize or normalize features, ...

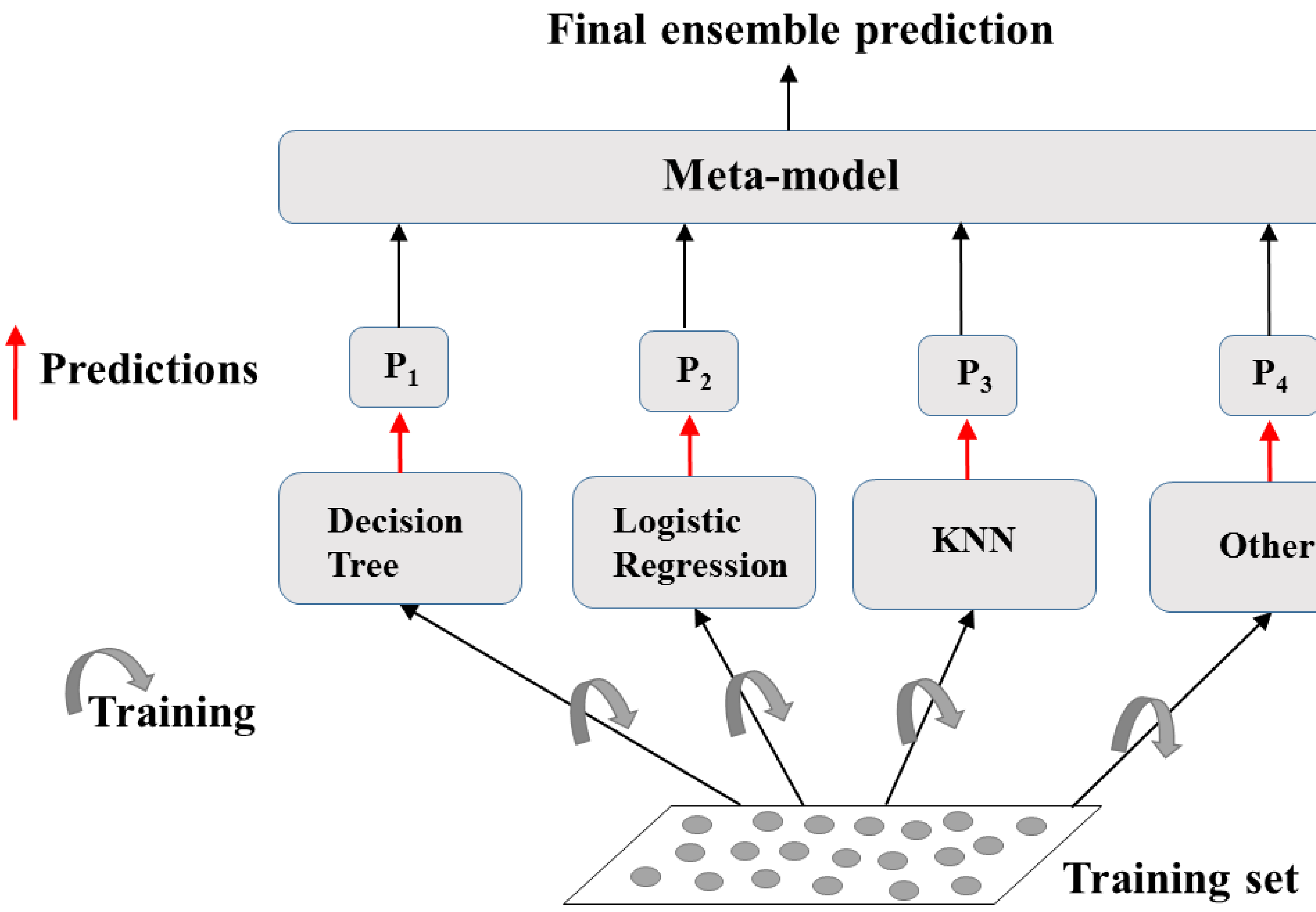
Limitations of CARTs

- Classification: can only produce orthogonal decision boundaries.
- Sensitive to small variations in the training set.
- High variance: unconstrained CARTs may overfit the training set.
- Solution: ensemble learning.

Ensemble Learning

- Train different models on the same dataset.
- Let each model make its predictions.
- Meta-model: aggregates predictions of individual models.
- Final prediction: more robust and less prone to errors.
- Best results: models are skillful in different ways.

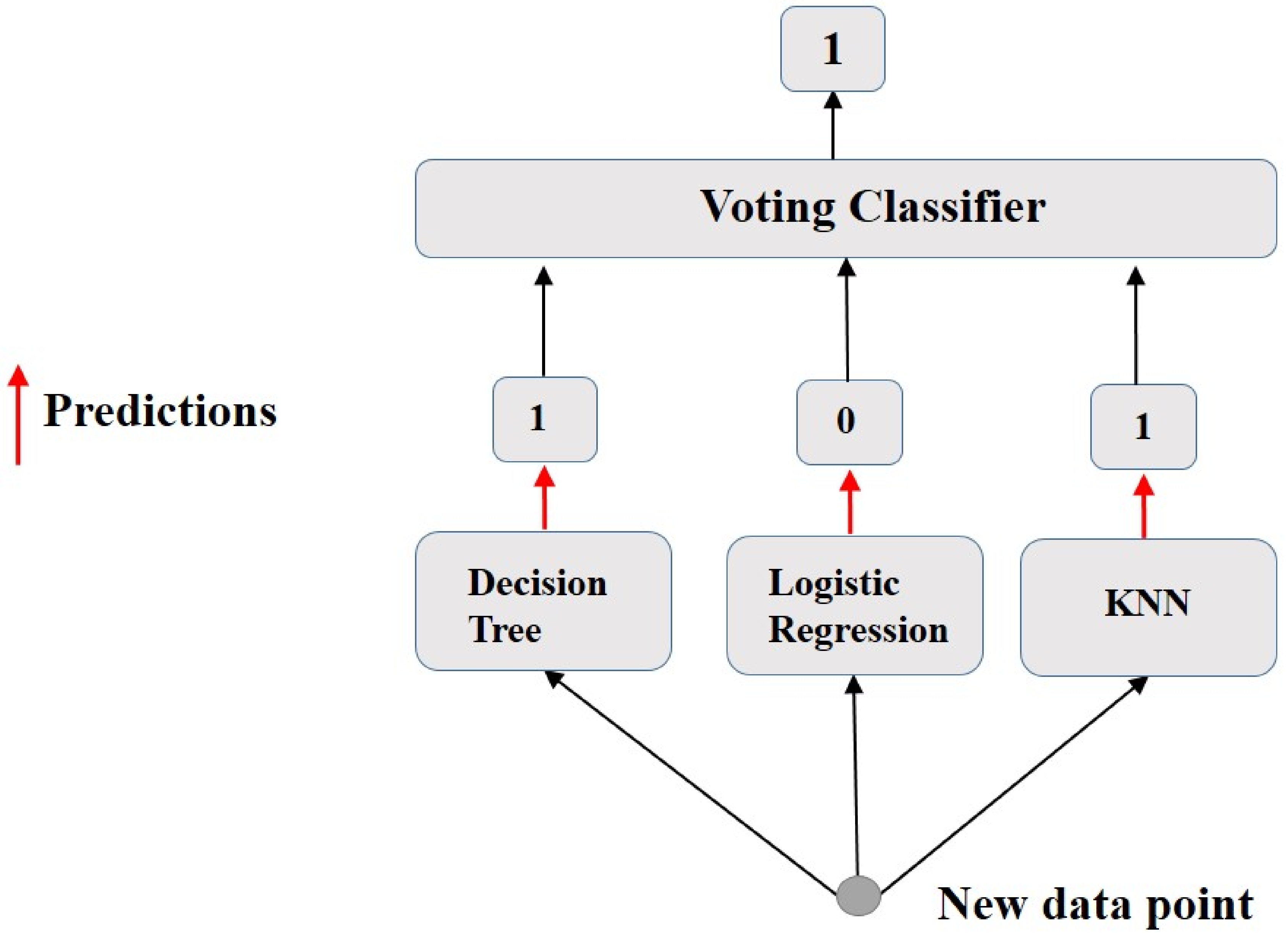
Ensemble Learning: A Visual Explanation



Ensemble Learning in Practice: Voting Classifier

- Binary classification task.
- N classifiers make predictions: P_1, P_2, ..., P_N with P_i = 0 or 1.
- Meta-model prediction: hard voting.

Hard Voting



1
Voting Classifier
Predictions
1
0
1
Decision Tree
Logistic Regression
KNN
New data point

Voting Classifier in sklearn (Breast-Cancer dataset)

```
# Import functions to compute accuracy and split data
from sklearn.metrics import accuracy_score
from sklearn.model_selection import train_test_split

# Import models, including VotingClassifier meta-model
from sklearn.linear_model import LogisticRegression
from sklearn.tree import DecisionTreeClassifier
from sklearn.neighbors import KNeighborsClassifier as KNN
from sklearn.ensemble import VotingClassifier

# Set seed for reproducibility
SEED = 1
```

Voting Classifier in sklearn (Breast-Cancer dataset)

```
# Split data into 70% train and 30% test
X_train, X_test, y_train, y_test = train_test_split(X, y,
                                                    test_size= 0.3,
                                                    random_state= SEED)
# Instantiate individual classifiers
lr = LogisticRegression(random_state=SEED)
knn = KNN()
dt = DecisionTreeClassifier(random_state=SEED)
# Define a list called classifier that contains the tuples (classifier_name, classifier)
classifiers = [('Logistic Regression', lr),
               ('K Nearest Neighbours', knn),
               ('Classification Tree', dt)]
```

```python
# Iterate over the defined list of tuples containing the classifiers
for clf_name, clf in classifiers:
    #fit clf to the training set
    clf.fit(X_train, y_train)

    # Predict the labels of the test set
    y_pred = clf.predict(X_test)

    # Evaluate the accuracy of clf on the test set
    print('{:s} : {:.3f}'.format(clf_name, accuracy_score(y_test, y_pred)))
```

```
Logistic Regression: 0.947
K Nearest Neighbours: 0.930
Classification Tree: 0.930
```

Voting Classifier in sklearn (Breast-Cancer dataset)

```
# Instantiate a VotingClassifier 'vc'
vc = VotingClassifier(estimators=classifiers)

# Fit 'vc' to the traing set and predict test set labels
vc.fit(X_train, y_train)
y_pred = vc.predict(X_test)

# Evaluate the test-set accuracy of 'vc'
print('Voting Classifier: {.3f}'.format(accuracy_score(y_test, y_pred)))
```

```
Voting Classifier: 0.953
```

Let's practice!