

The strength of “weak” models

ENSEMBLE METHODS IN PYTHON



Román de las Heras

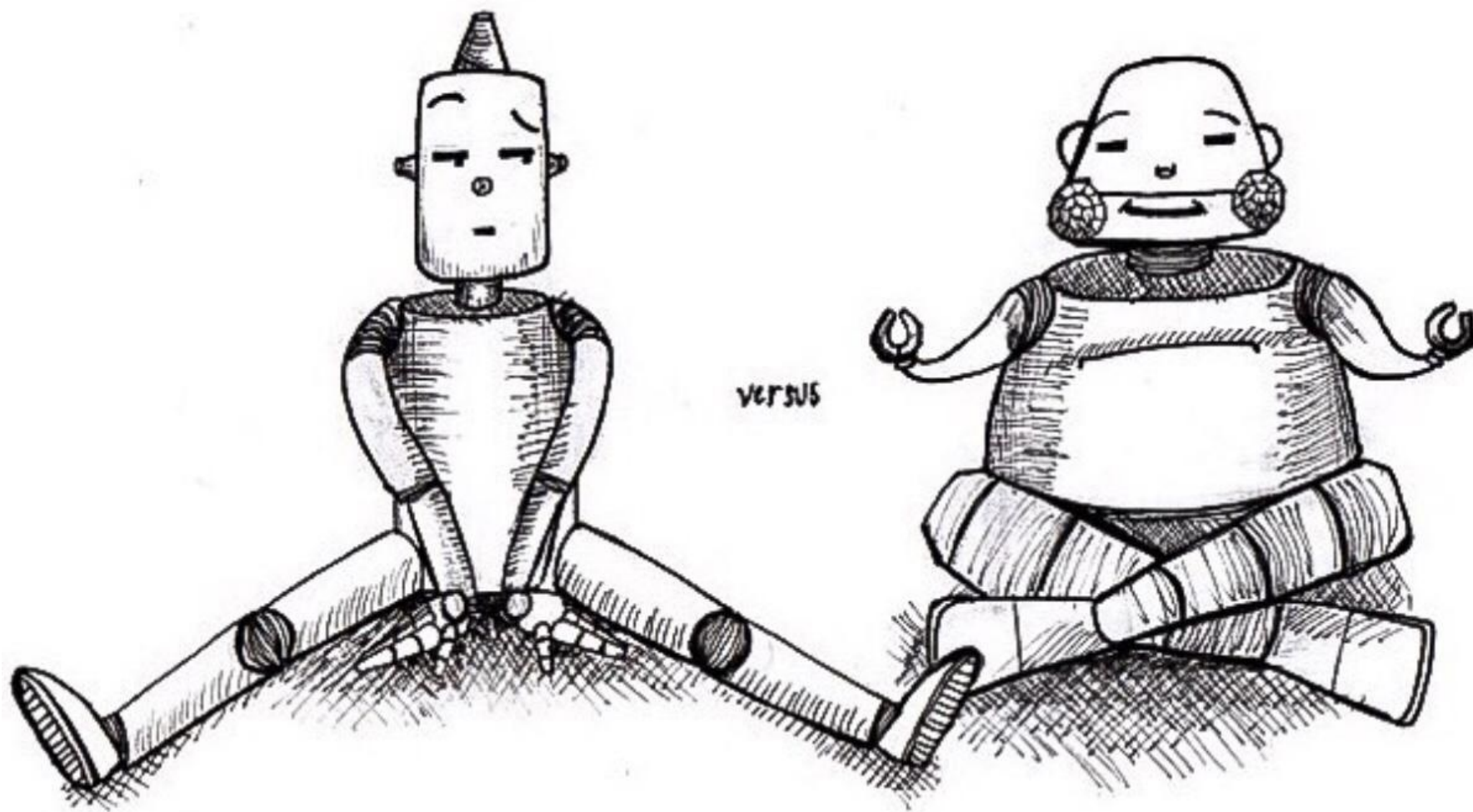
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"Weak" model

Voting and Averaging:

- Small number of estimators
- **Fine-tuned** estimators
- Individually trained

New concept: "*weak*" estimator



"Weak" model

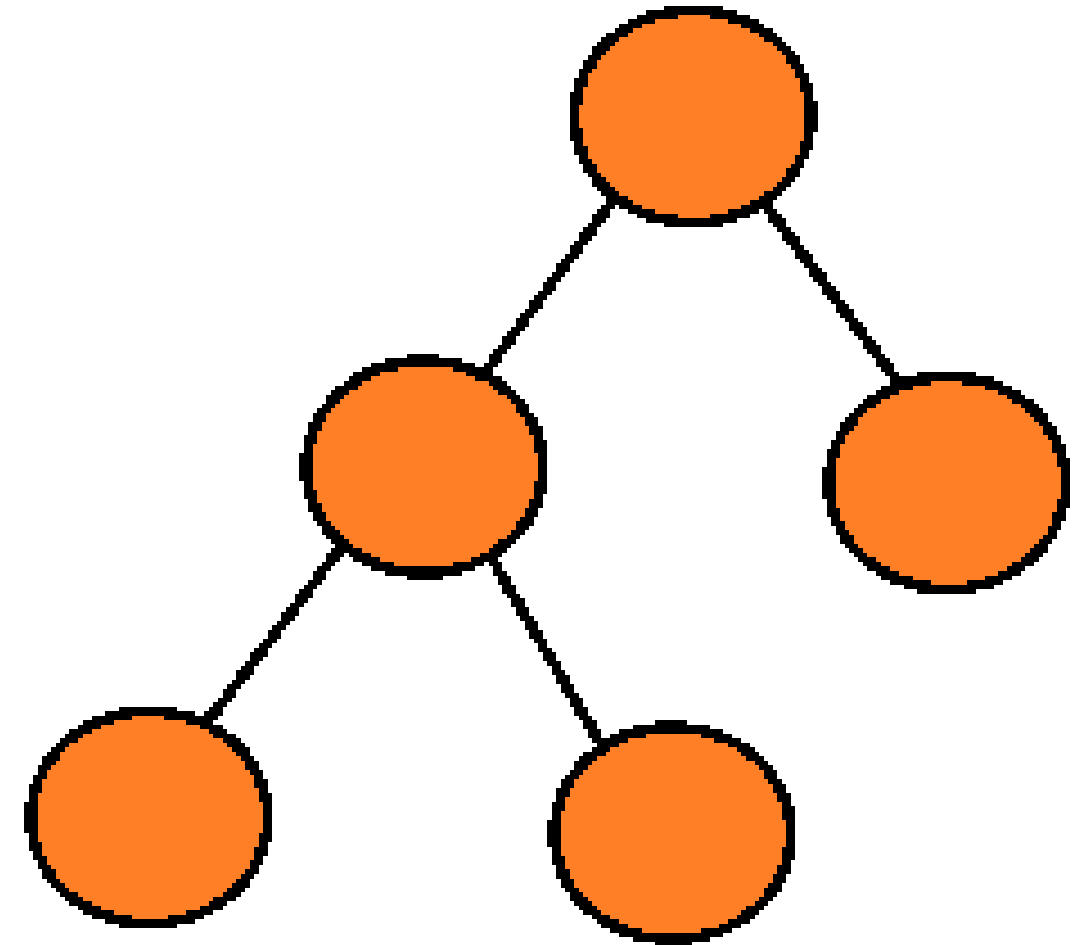
Fine-tuned model

Properties of "weak" models

Weak estimator

- Performance better than random guessing
- Light model
- Low training and evaluation time

Example: Decision Tree



Examples of "weak" models

Some "weak" models:

- Decision tree: small depth
- Logistic Regression
- Linear Regression
- Other restricted models

Sample code:

```
model = DecisionTreeClassifier(  
    max_depth=3  
)  
  
model = LogisticRegression(  
    max_iter=50, C=100.0  
)  
  
model = LinearRegression(  
    normalize=False  
)
```

Let's practice!

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Bootstrap aggregating

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Heterogeneous vs Homogeneous Ensembles

Heterogeneous:

- Different algorithms (fine-tuned)
- Small amount of estimators
- Voting, Averaging, and Stacking

Homogeneous:

- The same algorithm ("weak" model)
- Large amount of estimators
- Bagging and Boosting

Condorcet's Jury Theorem

Requirements:

- Models are independent
- Each model performs better than random guessing
- All individual models have similar performance

Conclusion: Adding more models improves the performance of the ensemble (*Voting* or *Averaging*), and this approaches 1 (100%)



Marquis de Condorcet, French philosopher and mathematician

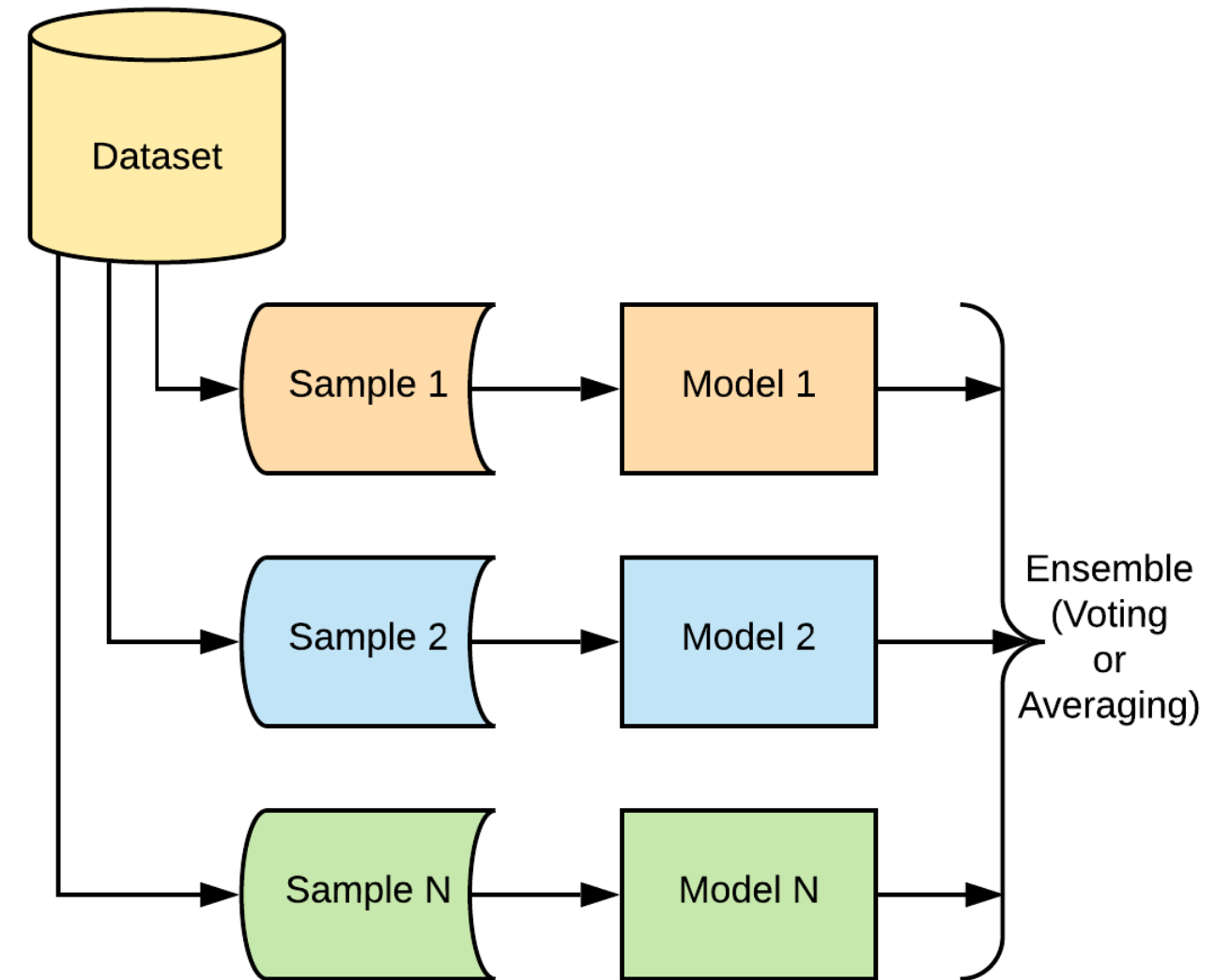
Bootstrapping

Bootstrapping requires:

- Random subsamples
- Using replacement

Bootstrapping guarantees:

- **Diverse crowd:** different datasets
- **Independent:** separately sampled



Pros and cons of bagging

Pros

- Bagging usually reduces variance
- Overfitting can be avoided by the ensemble itself
- More stability and robustness

Cons

- It is computationally expensive

It's time to practice!

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BaggingClassifier: nuts and bolts

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Heterogeneous vs Homogeneous Functions

Heterogeneous Ensemble Function

```
het_est = HeterogeneousEnsemble(  
    estimators=[('est1', est1), ('est2', est2), ...],  
    # additional parameters  
)
```

Homogeneous Ensemble Function

```
hom_est = HomogeneousEnsemble(  
    base_estimator=est_base,  
    n_estimators=chosen_number,  
    # additional parameters  
)
```

BaggingClassifier

Bagging Classifier example:

```
# Instantiate the base estimator ("weak" model)
clf_dt = DecisionTreeClassifier(max_depth=3)
```

```
# Build the Bagging classifier with 5 estimators
clf_bag = BaggingClassifier(
    base_estimator=clf_dt,
    n_estimators=5
)
```

```
# Fit the Bagging model to the training set
clf_bag.fit(X_train, y_train)
```

```
# Make predictions on the test set
y_pred = clf_bag.predict(X_test)
```

BaggingRegressor

Bagging Regressor example:

```
# Instantiate the base estimator ("weak" model)
reg_lr = LinearRegression(normalize=False)
```

```
# Build the Bagging regressor with 10 estimators
reg_bag = BaggingRegressor(
    base_estimator=reg_lr
)
```

```
# Fit the Bagging model to the training set
reg_bag.fit(X_train, y_train)
```

```
# Make predictions on the test set
y_pred = reg_bag.predict(X_test)
```


Out-of-bag score

- Calculate the individual predictions using all estimators for which an instance was out of the sample
- Combine the individual predictions
- Evaluate the metric on those predictions:
 - **Classification:** accuracy
 - **Regression:** R^2

```
clf_bag = BaggingClassifier(  
    base_estimator=clf_dt,  
    oob_score=True  
)  
clf_bag.fit(X_train, y_train)
```

```
print(clf_bag.oob_score_)
```

```
0.9328125
```

```
pred = clf_bag.predict(X_test)  
print(accuracy_score(y_test, pred))
```

```
0.9625
```

Now it's your turn!

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Bagging parameters: tips and tricks

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Basic parameters for bagging

BASIC PARAMETERS

- `base_estimator`
- `n_estimators`
- `oob_score`
 - `est_bag.oob_score_`

Additional parameters for bagging

ADDITIONAL PARAMETERS

- `max_samples` : the number of samples to draw for each estimator.
- `max_features` : the number of features to draw for each estimator.
 - Classification $\sim \sqrt{\text{number_of_features}}$
 - Regression $\sim \text{number_of_features} / 3$
- `bootstrap` : whether samples are drawn with replacement.
 - True --> `max_samples = 1.0`
 - False --> `max_samples < 1.0`

Random forest

Classification

```
from sklearn.ensemble import RandomForestClassifier

clf_rf = RandomForestClassifier(
    # parameters...
)
```

Regression

```
from sklearn.ensemble import RandomForestRegressor

reg_rf = RandomForestRegressor(
    # parameters...
)
```

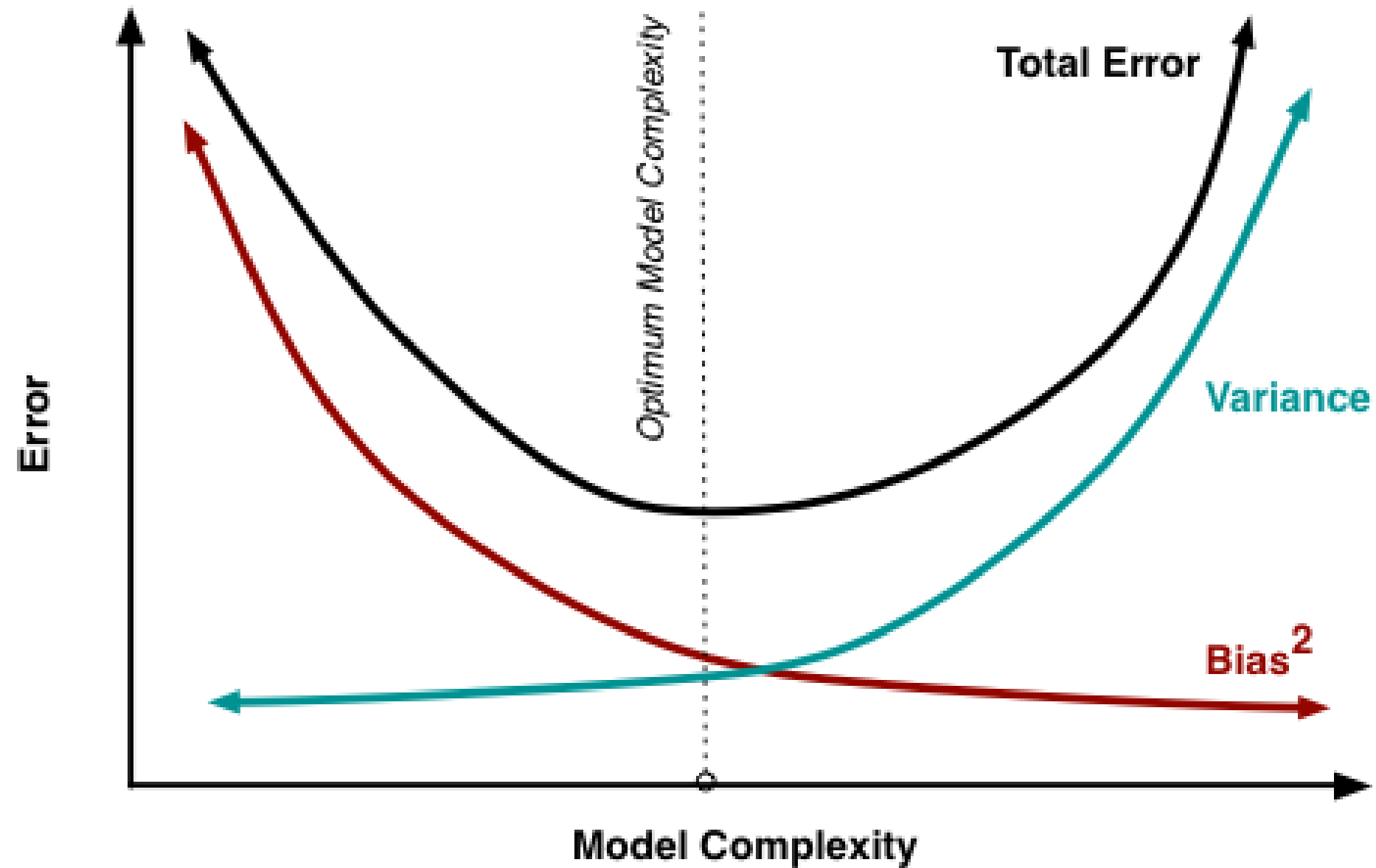
Bagging parameters:

- `n_estimators`
- `max_features`
- `oob_score`

Tree-specific parameters:

- `max_depth`
- `min_samples_split`
- `min_samples_leaf`
- `class_weight` (`"balanced"`)

Bias-variance tradeoff



Let's practice!

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