

Getting started with Isolation Forests

ANOMALY DETECTION IN PYTHON



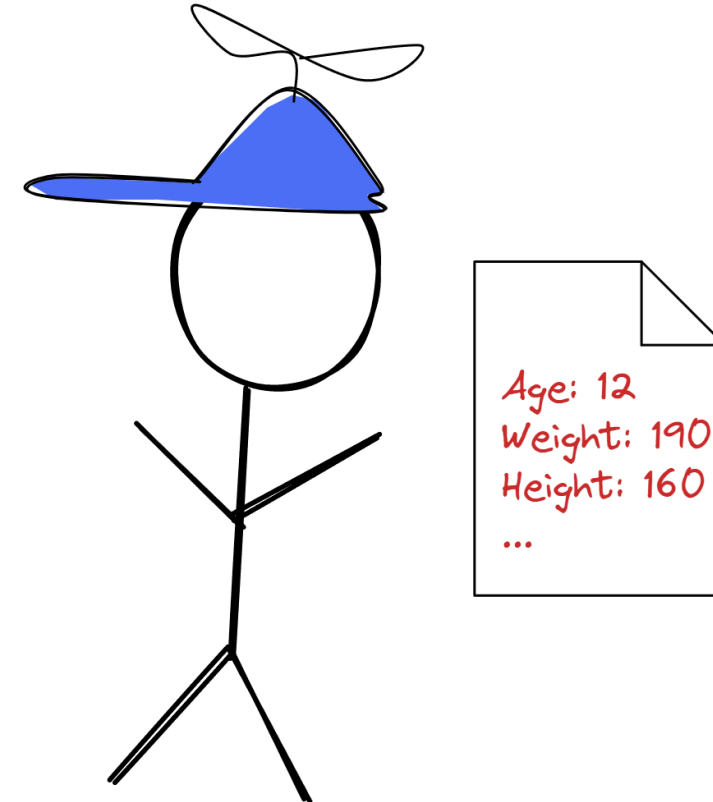
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Survey data

- A sample respondent:
 - 12 years old
 - 160 cm tall
 - weighs 190 pounds

A respondent

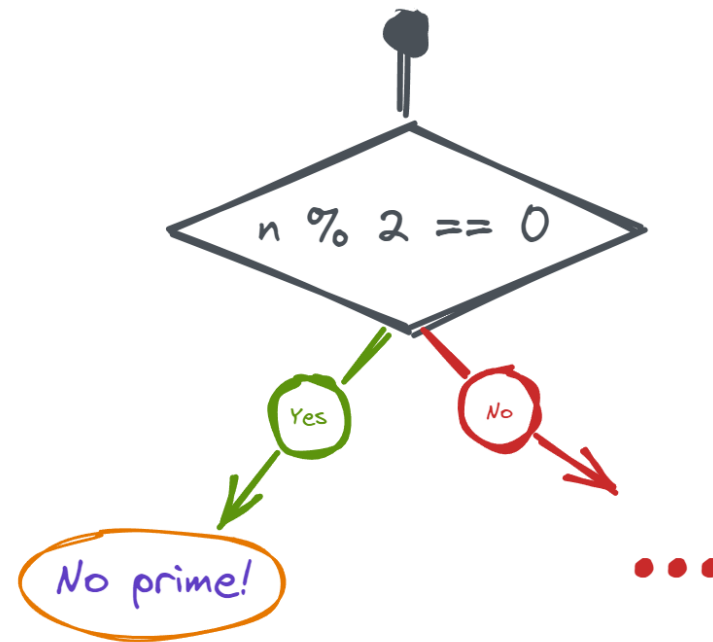


Multivariate anomalies

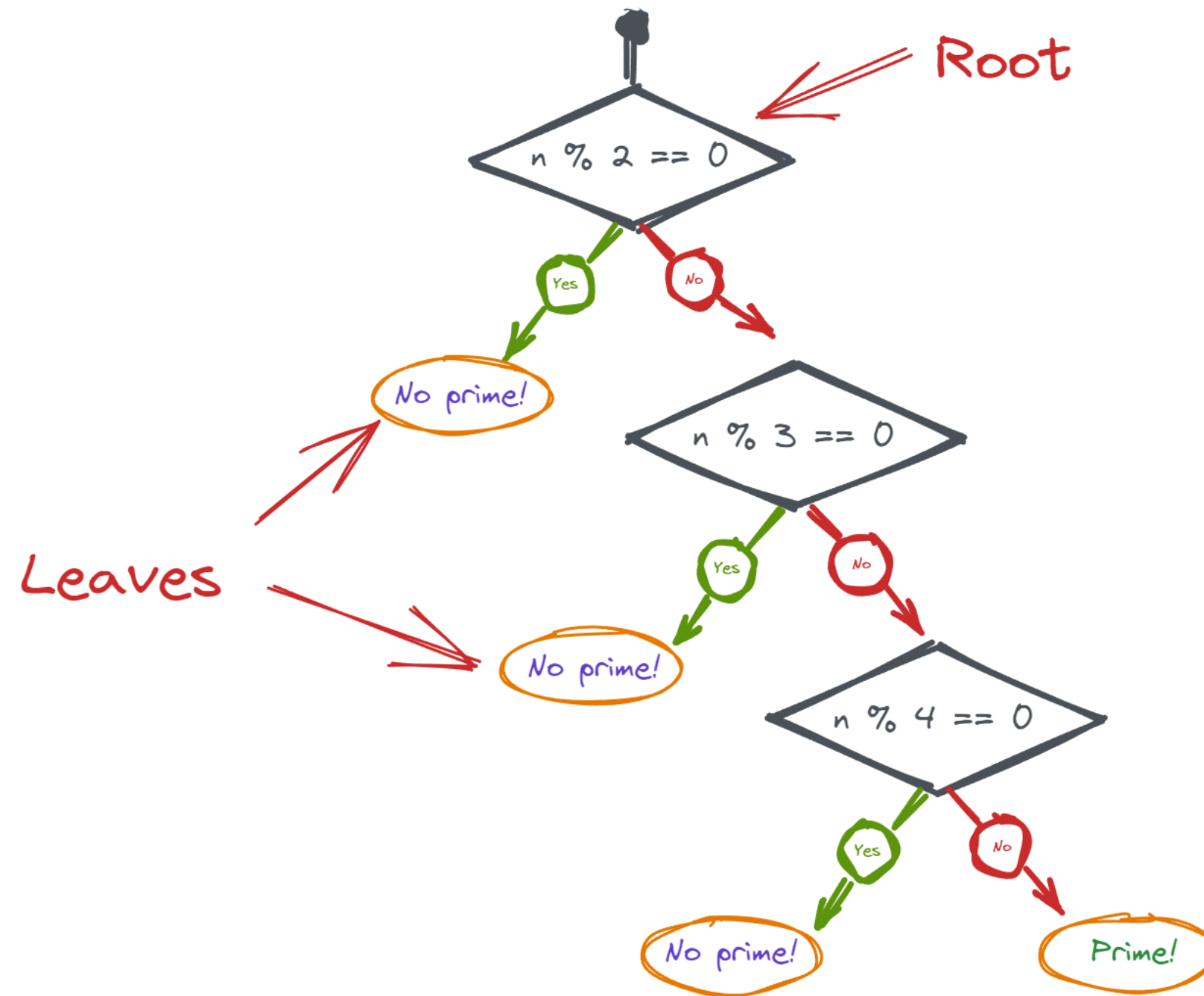
Multivariate anomalies:

- have two or more attributes
- attributes are not necessarily anomalous
- only anomalous when all attributes are considered

Decision trees



Decision trees

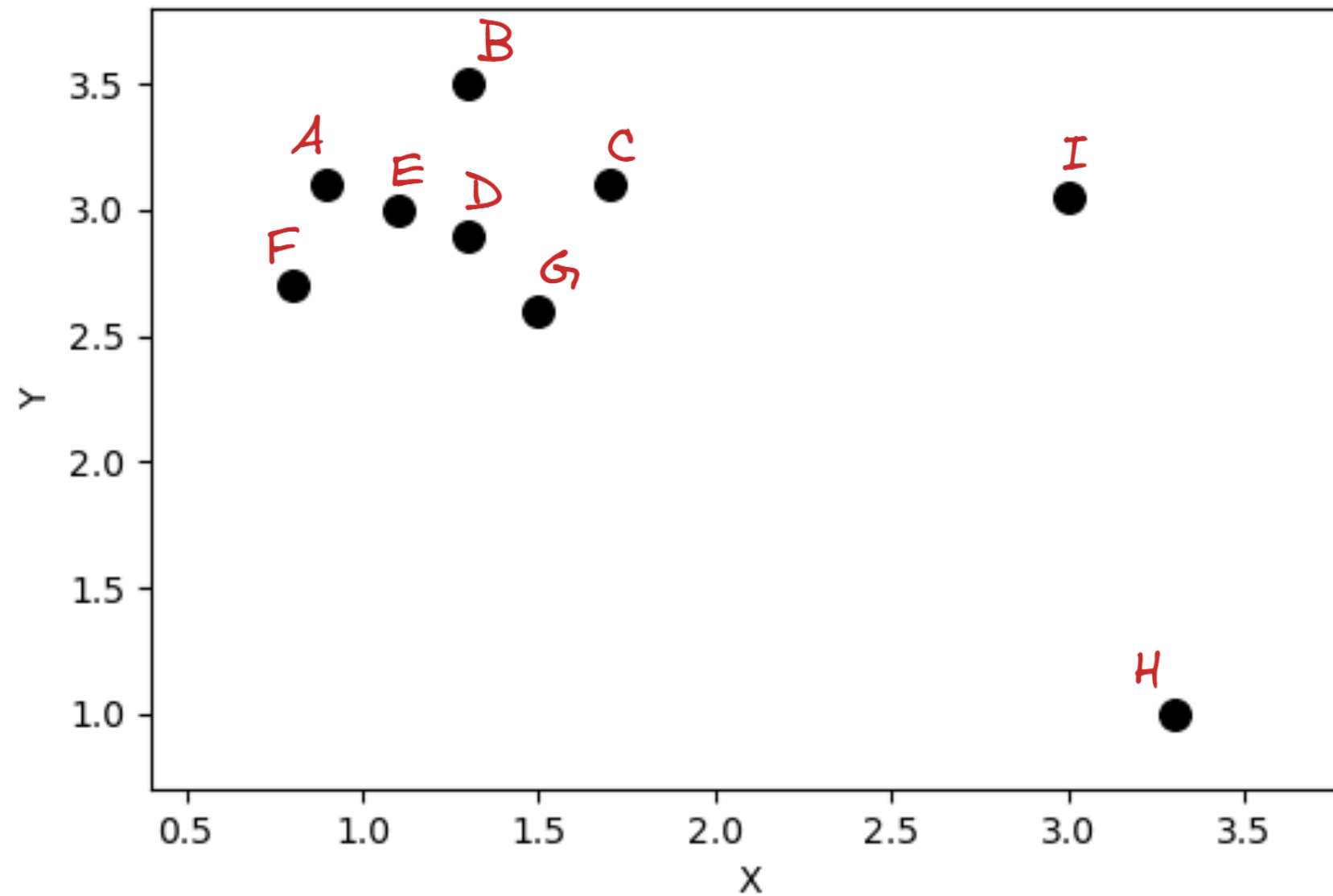


Isolation Trees

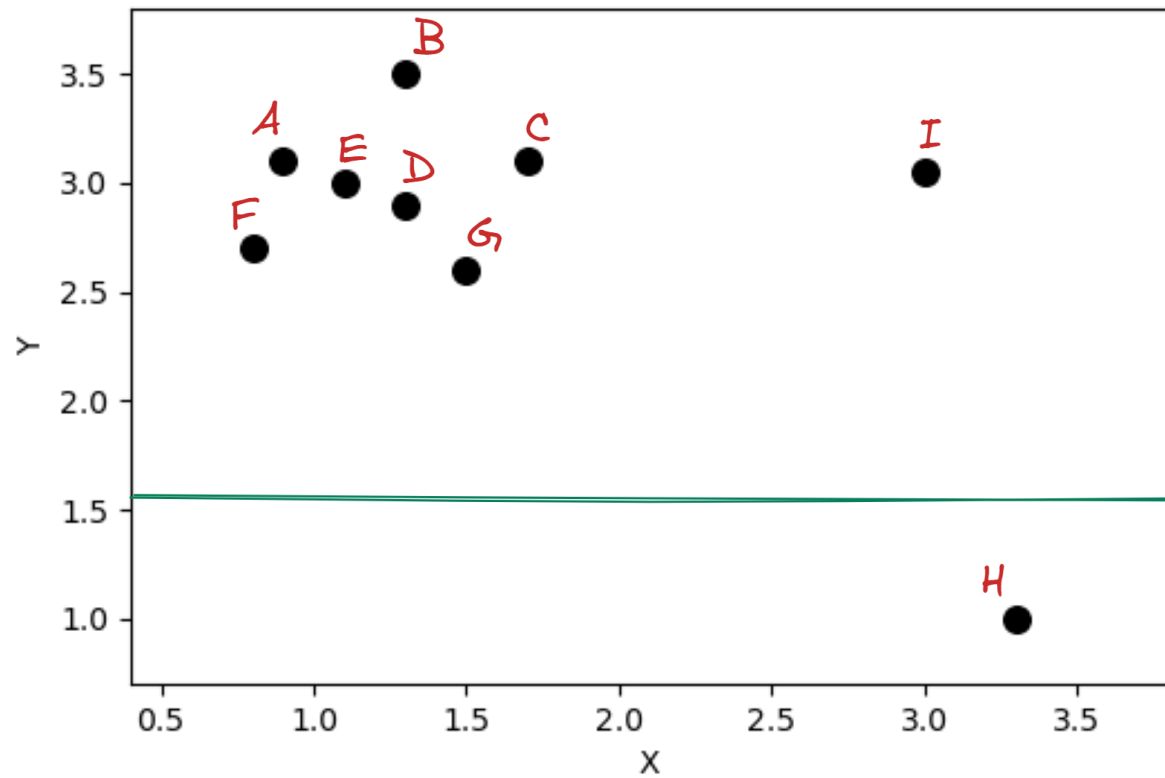
iTrees:

- short for isolation trees
- randomized versions of decision trees
- splitting (branching) occurs randomly
- random split is more likely to occur in inlier/outlier gap

Example 2D data

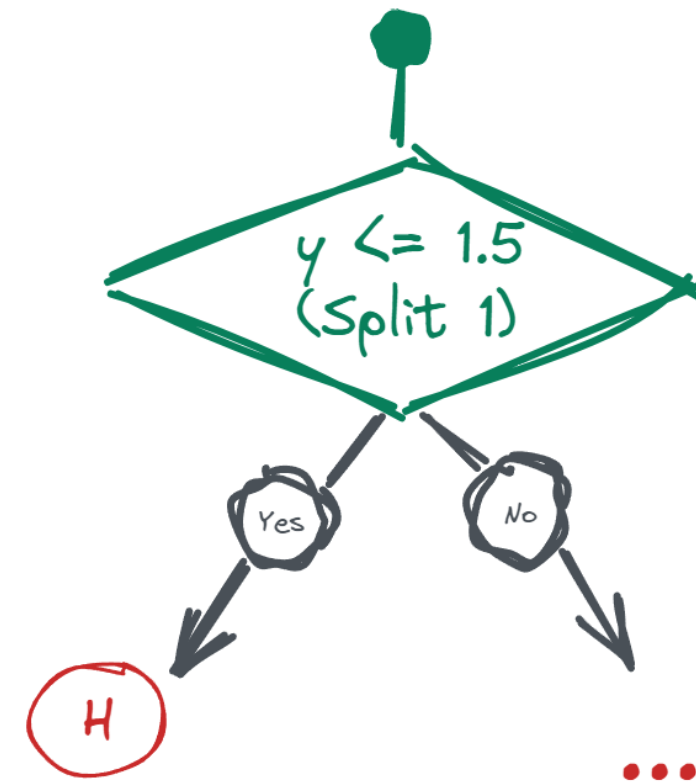


Fitting an iTree

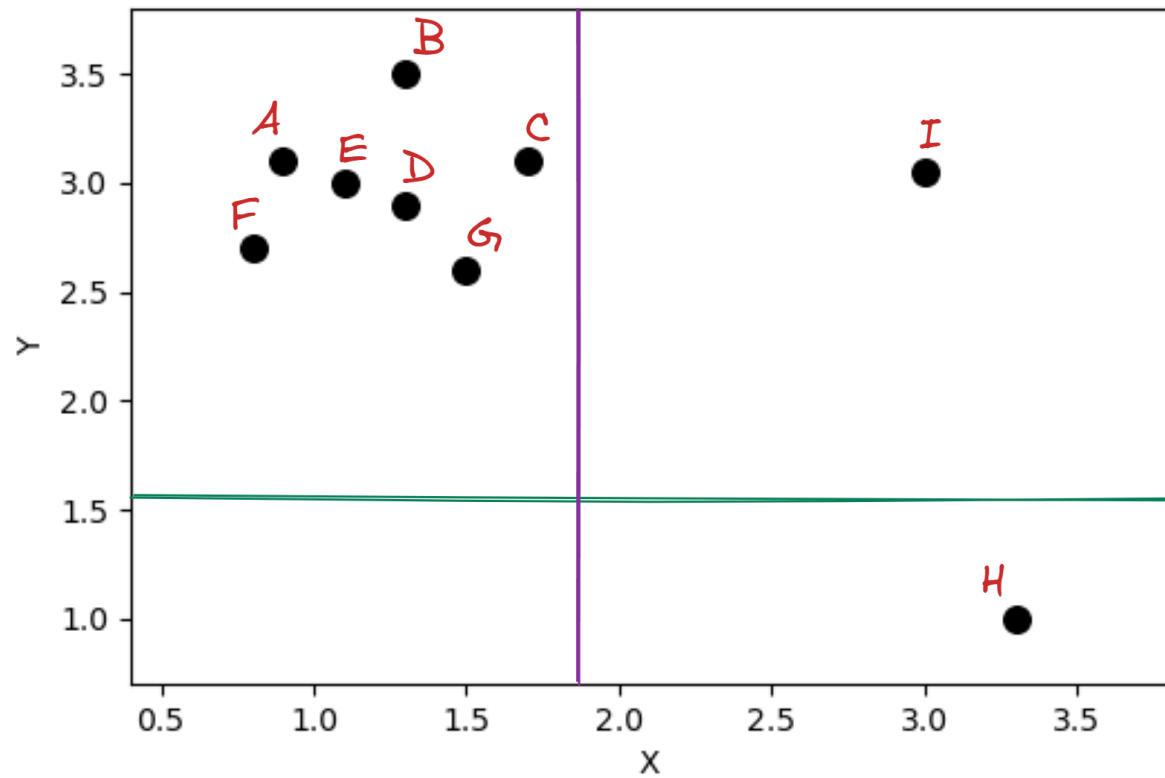


Splits

Split 1

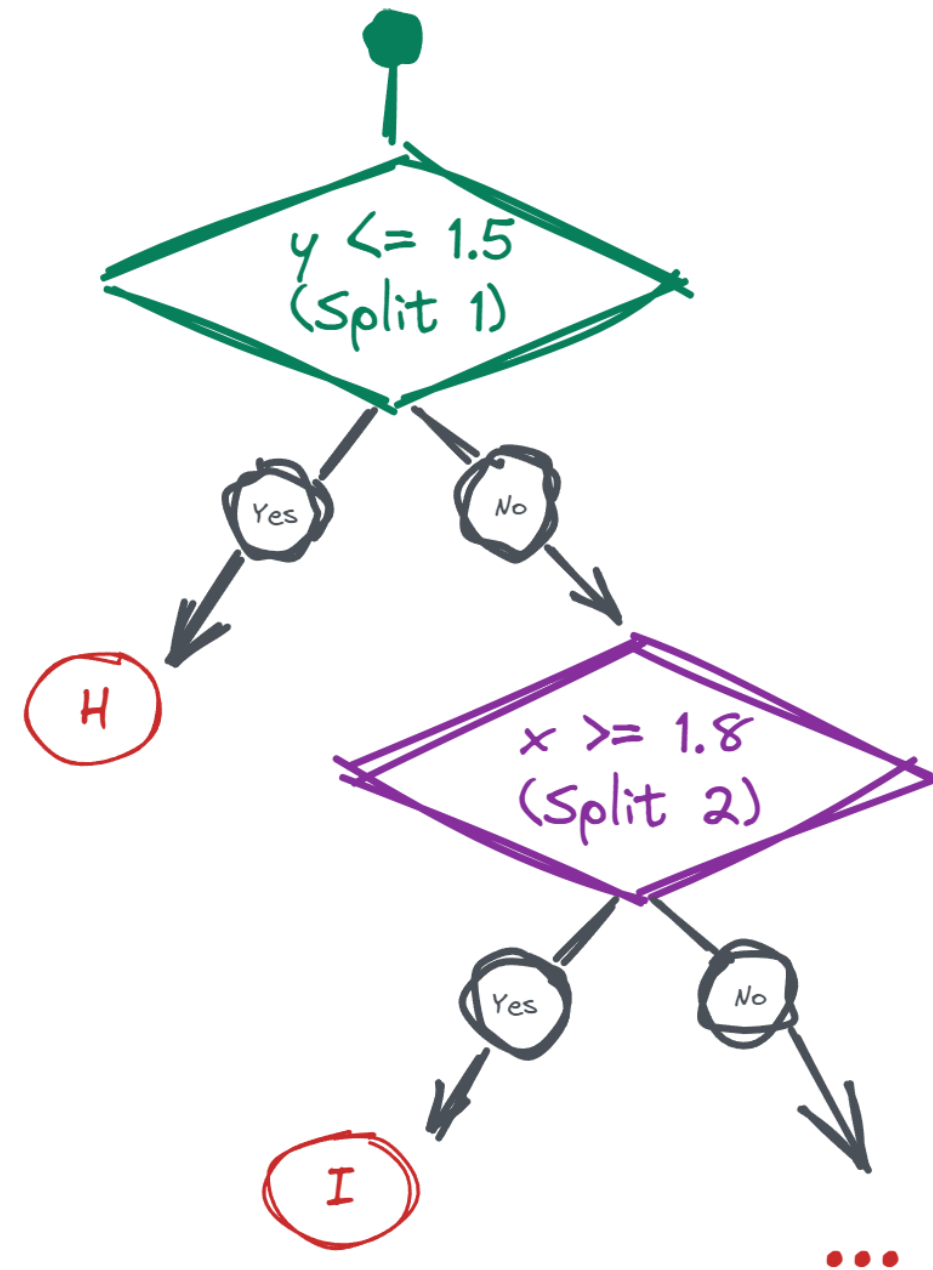


Fitting an iTree

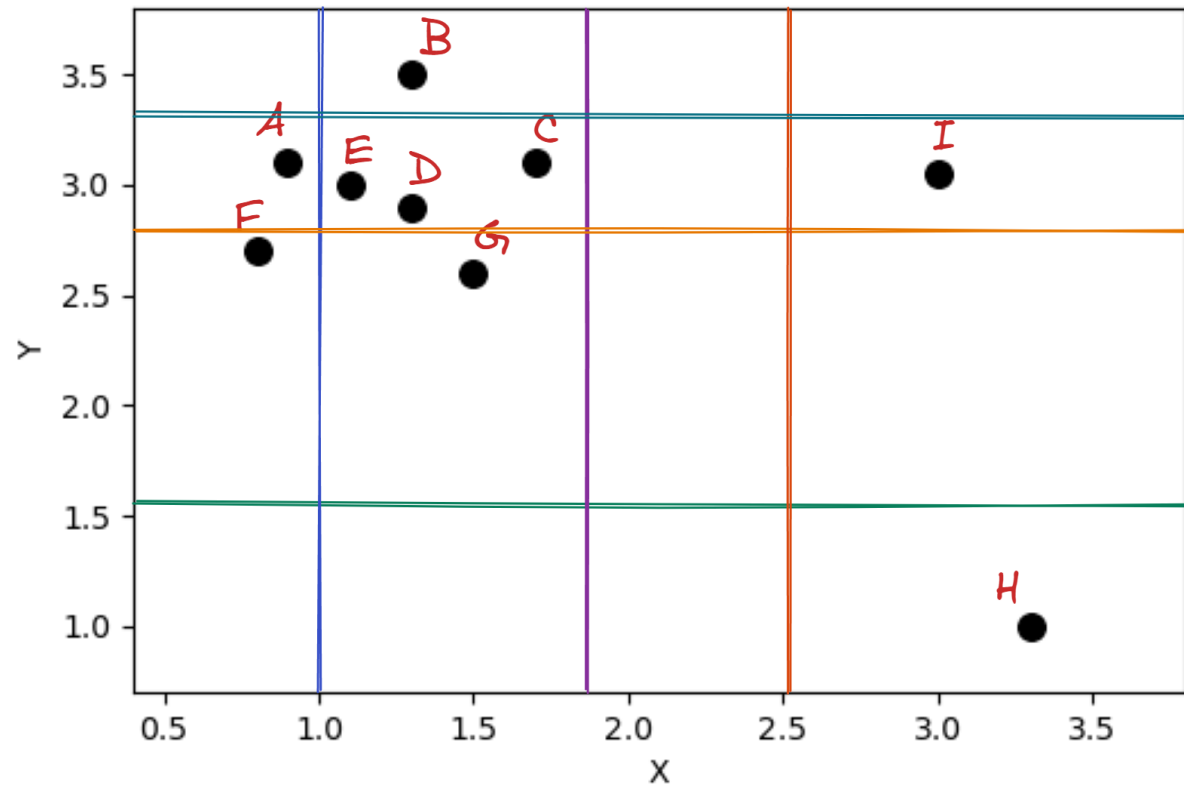


Splits

Split 1
Split 2

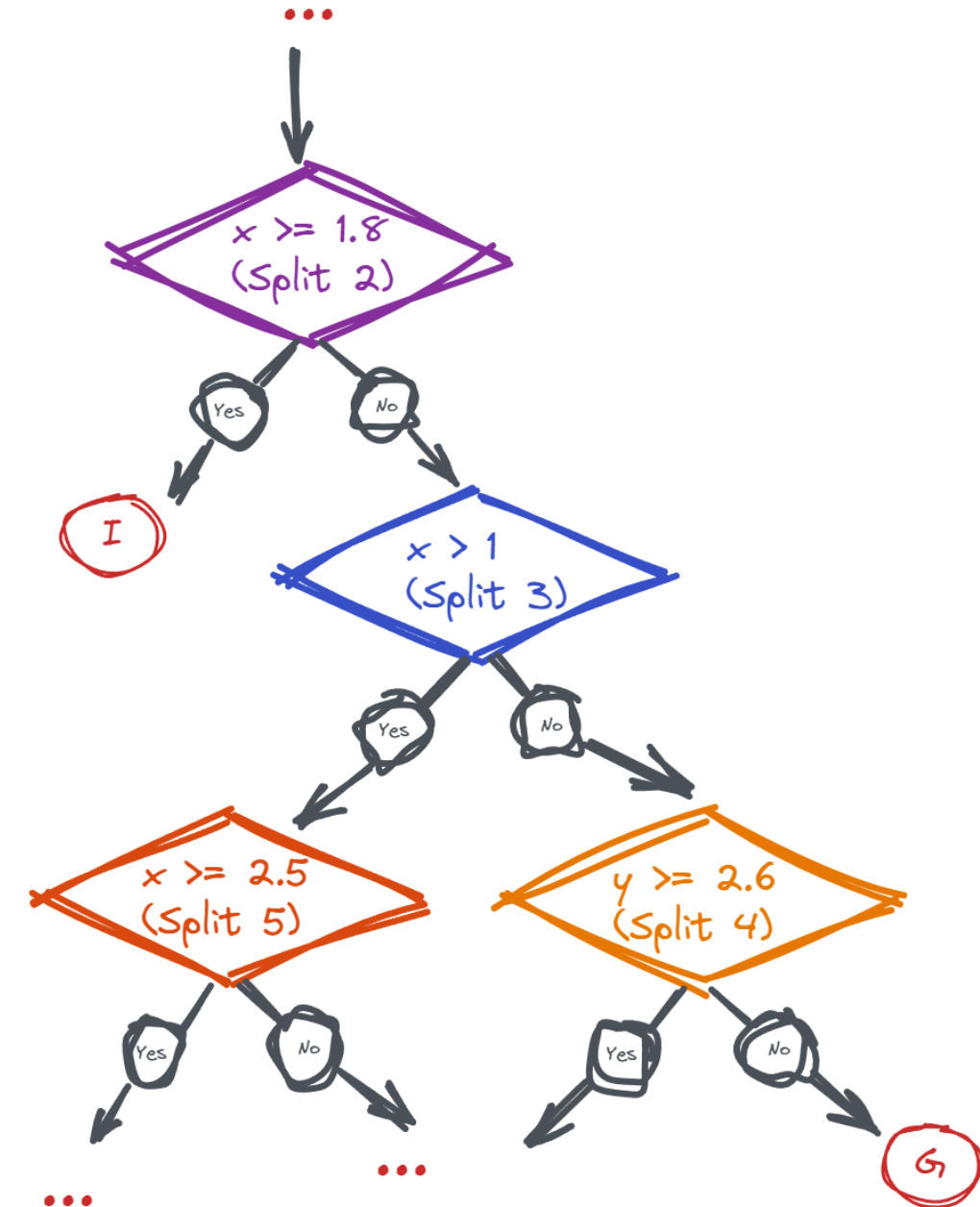


Fitting an iTree



Splits

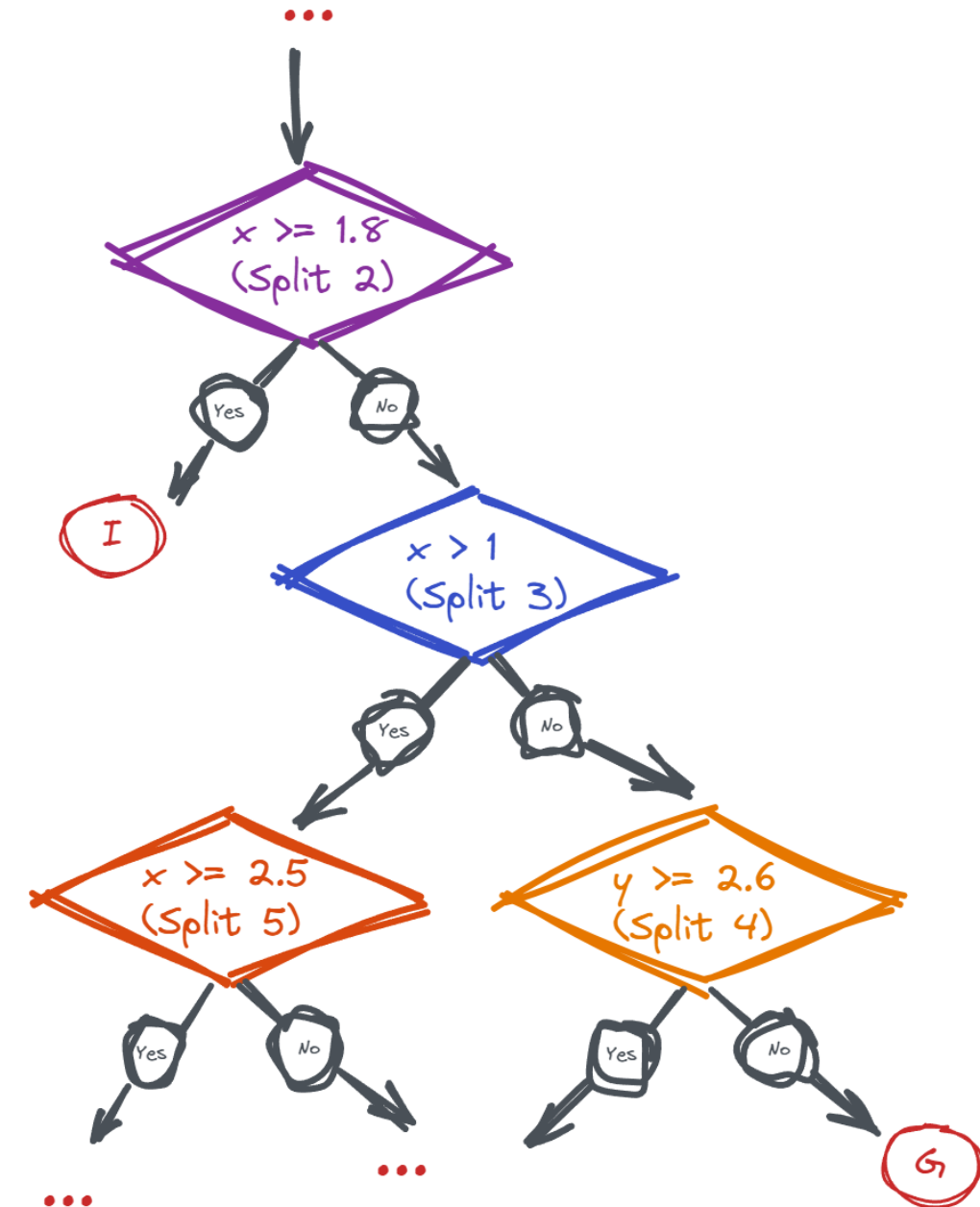
- Split 1
- Split 2
- Split 3
- Split 4
- Split 5
- Split 6



How points are classified

Points are outliers:

- if close to the root node
- or require fewer splits



US Airbnb data

```
import pandas as pd

airbnb_df = pd.read_csv("airbnb.csv")
```

US Airbnb data

```
airbnb_df.info()
```

```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 10000 entries, 0 to 9999
Data columns (total 6 columns):
#   Column                                Non-Null Count  Dtype  
---  -
0   minimum_nights                        10000 non-null  int64   
1   number_of_reviews                     10000 non-null  int64   
2   reviews_per_month                     10000 non-null  float64  
3   calculated_host_listings_count        10000 non-null  int64   
4   availability_365                      10000 non-null  int64   
5   price                                10000 non-null  int64   
dtypes: float64(1), int64(5)
```

fit_predict

```
from pyod.models.iforest import IForest

iforest = IForest()
labels = iforest.fit_predict(airbnb_df)

print(labels)
```

```
array([0, 0, 0, ..., 1, 0, 0])
```

Filter outliers

```
outliers = airbnb_df[labels == 1]  
  
print(outliers.shape)
```

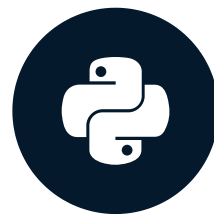
```
(1000, 6)
```

Let's practice!

ANOMALY DETECTION IN PYTHON

Overview of Isolation Forest hyperparameters

ANOMALY DETECTION IN PYTHON



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Most important hyperparameters

Hyperparameters which influence `IForest` the most:

- `contamination`
- `n_estimators`
- `max_samples`
- `max_features`

What is contamination?

How `IForest` classifies data points:

1. Raw anomaly scores are generated
2. Set a threshold called `contamination`
3. The highest percentage of anomaly scores denoted with `contamination` are chosen as outlying datapoints

Setting contamination

```
from pyod.models.iforest import IForest  
  
# Accepts a value between 0 and 0.5  
iforest = IForest(contamination=0.05)
```

What is n_estimators?

```
# More trees for larger datasets  
iforest = IForest(n_estimators=1000)  
  
iforest.fit(airbnb_df)
```

max_samples and max_features

```
iforest = IForest(n_estimators=200, max_samples=0.6, max_features=0.9)  
  
iforest.fit(airbnb_df)
```

Tree growth

- iTrees:
 - grow in a randomized fashion
 - split is chosen randomly between feature min and max
 - grow until:
 - all points are isolated
 - maximum depth is reached

Max tree depth

- Equals the logarithm of the sample size

IForest advantages

- Very efficient on large datasets
- Doesn't need all normal instances like other algorithms
- No statistical assumptions
- Performs well out-of-the-box

Challenges of outlier detection

- Supervised-learning models rely on metrics like RMSE or log loss
- Outlier detection is an unsupervised-learning problem
- Outlier classifiers should be combined with supervised-learning models

Let's practice!

ANOMALY DETECTION IN PYTHON

Hyperparameter tuning of Isolation Forest

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Tuning contamination

- No determined way of tuning it
- Have to rely on:
 - intuition
 - EDA insights
 - domain knowledge
 - business expectations

Survey example

- Research similar surveys
- Learn the proportion of the poorest and the wealthiest
- Research is better than blindly choosing a value

Big Mart sales data

```
import pandas as pd
```

```
big_mart = pd.read_csv("big_mart_sales.csv")  
big_mart.info()
```

```
<class 'pandas.core.frame.DataFrame'>  
RangeIndex: 7060 entries, 0 to 7059  
Data columns (total 5 columns):  
#   Column                Non-Null Count  Dtype  
0   weight                7060 non-null  float64  
1   fat_content           7060 non-null  object  
2   type                  7060 non-null  object  
3   max_retail_price      7060 non-null  float64  
4   sales                 7060 non-null  float64  
dtypes: float64(3), object(2)
```

Encode categoricals

```
big_mart = pd.get_dummies(big_mart)
```

	weight	max_retail_price	sales	fat_content_low_fat	fat_content_regular
0	9.30	249.8092	3735.1380	1	0
1	5.92	48.2692	443.4228	0	1
2	17.50	141.6180	2097.2700	1	0
3	19.20	182.0950	732.3800	0	1
4	8.93	53.8614	994.7052	1	0

evaluate_outlier_classifier

```
def evaluate_outlier_classifier(model, data):  
    # Get labels  
    labels = model.fit_predict(data)  
  
    # Return inliers  
    return data[labels == 0]
```

evaluate_regressor

```
from sklearn.linear_model import LinearRegression
from sklearn.model_selection import train_test_split
from sklearn.metrics import mean_squared_error
```

evaluate_regressor

```
def evaluate_regressor(inliers):  
    X = inliers.drop("sales", axis=1)  
    y = inliers[['sales']]  
  
    X_train, X_test, y_train, y_test = train_test_split(X, y, random_state=10)  
  
    lr = LinearRegression()  
    lr.fit(X_train, y_train)  
  
    preds = lr.predict(X_test)  
    rmse = mean_squared_error(y_test, preds, squared=False)  
  
    return round(rmse, 3)
```

Tuning contamination

```
contaminations = [0.05, 0.1, 0.2, 0.3]
scores = dict()

for c in contaminations:
    # Instantiate IForest with the current c
    iforest = IForest(contamination=c, random_state=10)

    # Get inliers with the current IForest
    inliers = evaluate_outlier_classifier(iforest, big_mart)

    # Calculate and store RMSE into scores
    scores[c] = evaluate_regressor(inliers)
```

Look at the output

```
print(scores)
```

```
{0.05: 1148.555, 0.1: 1147.48, 0.2: 1082.307, 0.3: 1029.33}
```

Tuning multiple hyperparameters

```
estimators = [100, 200, 300,]  
max_samples = [0.6, 0.8, 1]  
scores = dict()
```

Cartesian product

```
from itertools import product
```

```
list(product(estimators, max_samples))
```

```
[(100, 0.6),  
 (100, 0.8),  
 (100, 1),  
 (200, 0.6),  
 (200, 0.8),  
 (200, 1),  
 (300, 0.6),  
 (300, 0.8),  
 (300, 1)]
```

Inside the loop

```
estimators = [100, 200, 300,]
max_samples = [0.6, 0.8, 1]
scores = dict()

for e, m in product(estimators, max_samples):
    # Instantiate an IForest
    iforest = IForest(n_estimators=e, max_samples=m, contamination=.3)

    # Get the inliers with the current IForest
    inliers = evaluate_outlier_classifier(iforest, big_mart)

    # Calculate and store RMSE into scores
    scores[(e, m)] = evaluate_regressor(inliers)
```


Looking at the output

```
print(scores)
```

```
{(100, 0.6): 959.398,  
 (100, 0.8): 986.056,  
 (100, 1): 1195.875,  
 (200, 0.6): 947.628,  
 (200, 0.8): 933.115,  
 (200, 1): 1195.875,  
 (300, 0.6): 949.412,  
 (300, 0.8): 935.962,  
 (300, 1): 1195.875}
```

Parallel execution

```
# Faster computation with n_jobs=-1
iforest = IForest(n_estimators=1000, n_jobs=-1)

iforest.fit(big_mart)
```

Let's practice!

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Interpreting the output of IForest

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An alternative

```
from pyod.models.iforest import IForest

iforest = IForest(contamination=0.2, max_features=0.5, random_state=1)

iforest = iforest.fit(airbnb_df)

labels = iforest.labels_
print(labels)
```

```
array([0, 0, 0, ..., 1, 0, 0])
```

Predictions on new data

```
import numpy as np

new_data = [[34, 40, 0.44, 3, 2, 90]]

iforest.predict(new_data)
```

```
array([0])
```

Probability scores

```
all_probs = iforest.predict_proba(airbnb_df)
print(all_probs)
```

```
array([[0.71401381, 0.28598619],
       [0.75553703, 0.24446297],
       [0.6844169 , 0.3155831 ],
       ...,
       ])
```

```
print(all_probs.shape)
```

```
(10000, 2)
```

Outlier probability scores

```
outliers = airbnb_df[iforest.labels_ == 1]
outlier_probs = iforest.predict_proba(outliers)

print(outlier_probs[:10])
```

```
array([[0.51999538, 0.48000462],
       [0.61789522, 0.38210478],
       [0.61802032, 0.38197968],
       [0.35184434, 0.64815566],
       [0.57533286, 0.42466714],
       [0.59038933, 0.40961067],
       [0.57677613, 0.42322387],
       [0.54158826, 0.45841174],
       [0.49118093, 0.50881907],
       [0.21387357, 0.78612643]])
```


Abandoning contamination

```
# Fit to Airbnb
iforest = IForest(max_features=0.5, random_state=1)
iforest.fit(airbnb_df)

# Calculate probabilities
probs = iforest.predict_proba(airbnb_df)

# Probs for outliers
outlier_probs = probs[:, 1]
```

Abandoning contamination

```
# Filter only when probability is higher than 65%  
outliers = airbnb_df[outlier_probs >= 0.65]  
  
print(len(outliers))
```

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