Tree-based and ensemble models

Tree-based methods

- Algorithms that stratifying or segmenting the predictor space into a number of simple regions.
- We call these algorithms decision-tree methods because the decisions used to segment the predictor space can be summarized in a tree.
- Decision trees on their own, are very explainable and intuitive, but not very powerful at predicting.
- However, there are extensions of decision trees, such as random forest and boosted trees, which are very powerful at predicting. We will demonstrate two of these in this session.

Decision trees

- Decision Trees by Jared Wilber & Lucía Santamaría

Classification Decision trees

- Use recursive binary splitting to grow a classification tree (splitting of the predictor space into J distinct, non-overlapping regions).
- For every observation that falls into the region R_j , we make the same prediction, which is the majority vote for the training observations in .
- Where to split the predictor space is done in a top-down and greedy manner, and in practice for classification, the best split at any point in the algorithm is one that minimizes the Gini index (a measure of node purity).
- Decision trees are useful because they are very interpretable.
- A limitation of decision trees is that theyn tend to overfit, so in practice we use cross-validation to tune a hyperparameter, , to find the optimal, pruned tree.

Example: the heart data set

- Let's consider a situation where we'd like to be able to predict the presence of heart disease (AHD) in patients, based off 13 measured characteristics.
- The heart data set contains a binary outcome for heart disease for patients who presented with chest pain.

```
1  import pandas as pd
2  heart = pd.read_csv("data/Heart.csv", index_col=0)
3  heart.info()
```

```
<class 'pandas.core.frame.DataFrame'>
Index: 303 entries, 1 to 303
Data columns (total 14 columns):
 #   Column      Non-Null Count  Dtype  
---  ------      --------------  -----  
 0   Age         303 non-null    int64  
 1   Sex         303 non-null    int64  
 2   ChestPain   303 non-null    object 
 3   RestBP      303 non-null    int64  
 4   Chol        303 non-null    int64  
 5   Fbs         303 non-null    int64  
 6   RestECG     303 non-null    int64  
 7   MaxHR       303 non-null    int64  
 8   ExAng       303 non-null    int64  
 9   Oldpeak     303 non-null    float64
 10  Slope       303 non-null    int64  
 11  Ca          299 non-null    float64
 12  Thal        301 non-null    object 
 13  AHD         303 non-null    object 
dtypes: float64(2), int64(9), object(3)
memory usage: 35.5+ KB
```

Example: the heart data set

An angiographic test was performed and a label for AHD of Yes was labelled to indicate the presence of heart disease, otherwise the label was No.

```
1 heart.head()
```

	Age	Sex	ChestPain	RestBP	Chol	Fbs	RestECG	MaxHR	ExAng
1	63	1	typical	145	233	1	2	150	0
2	67	1	asymptomatic	160	286	0	2	108	1
3	67	1	asymptomatic	120	229	0	2	129	1
4	37	1	nonanginal	130	250	0	0	187	0
5	41	0	nontypical	130	204	0	2	172	0

Do we have a class imbalance?

It's always important to check this, as it may impact your splitting and/or modeling decisions.

```
1  heart['AHD'].value_counts(normalize=True)
```

```
AHD
No     0.541254
Yes    0.458746
Name: proportion, dtype: float64
```

This looks pretty good! We can move forward this time without doing much more about this.

Data splitting

Let's split the data into training and test sets:

```
import numpy as np
from sklearn.model_selection import train_test_split

np.random.seed(2024)

heart_train, heart_test = train_test_split(
    heart, train_size=0.8, stratify=heart["AHD"]
)

X_train = heart_train.drop(columns=['AHD'])
y_train = heart_train['AHD']
X_test = heart_test.drop(columns=['AHD'])
y_test = heart_test['AHD']
```

Categorical variables

- This is our first case of seeing categorical predictor variables, can we treat them the same as numerical ones? **No!**
- In `scikit-learn` we must perform **one-hot encoding**

Original Data

Team	Points
A	25
A	12
B	15
B	14
B	19
B	23
C	25
C	29

One-Hot Encoded Data

Team_A	Team_B	Team_C	Points
1	0	0	25
1	0	0	12
0	1	0	15
0	1	0	14
0	1	0	19
0	1	0	23
0	0	1	25
0	0	1	29

Source: https://scales.arabpsychology.com/stats/how-can-i-perform-one-hot-encoding-in-r/

Look at the data again

Which columns do we need to standardize?

Which do we need to one-hot encode?

```
1 heart.head()
```

	Age	Sex	ChestPain	RestBP	Chol	Fbs	RestECG	MaxHR	ExAng
1	63	1	typical	145	233	1	2	150	0
2	67	1	asymptomatic	160	286	0	2	108	1
3	67	1	asymptomatic	120	229	0	2	129	1
4	37	1	nonanginal	130	250	0	0	187	0
5	41	0	nontypical	130	204	0	2	172	0

One hot encoding & pre-processing

```
from sklearn.preprocessing import StandardScaler, OneHotEncoder
from sklearn.compose import make_column_transformer, make_column_selector

numeric_feats = ['Age', 'RestBP', 'Chol', 'RestECG', 'MaxHR', 'Oldpeak','Slope', 'Ca']
passthrough_feats = ['Sex', 'Fbs', 'ExAng']
categorical_feats = ['ChestPain', 'Thal']

heart_preprocessor = make_column_transformer(
    (StandardScaler(), numeric_feats),
    ("passthrough", passthrough_feats),
    (OneHotEncoder(handle_unknown = "ignore"), categorical_feats),
)
```

> `handle_unknown = "ignore"` handles the case where categories exist in the test data, which were missing in the training set. Specifically, it sets the value for those to 0 for all cases of the category.

Fitting a dummy classifier

```
from sklearn.dummy import DummyClassifier
from sklearn.pipeline import make_pipeline
from sklearn.model_selection import cross_validate

dummy = DummyClassifier()
dummy_pipeline = make_pipeline(heart_preprocessor, dummy)
cv_10_dummy = pd.DataFrame(
    cross_validate(
        estimator=dummy_pipeline,
        cv=10,
        X=X_train,
        y=y_train
    )
)
cv_10_dummy_metrics = cv_10_dummy.agg(["mean", "sem"])
results = pd.DataFrame({'mean' : [cv_10_dummy_metrics.test_score.iloc[0]],
  'sem' : [cv_10_dummy_metrics.test_score.iloc[1]]},
  index = ['Dummy classifier']
)
results
```

	mean	sem
Dummy classifier	0.541333	0.00299

Fitting a decision tree

```
from sklearn.tree import DecisionTreeClassifier

decision_tree = DecisionTreeClassifier(random_state=2026)

dt_pipeline = make_pipeline(heart_preprocessor, decision_tree)
cv_10_dt = pd.DataFrame(
    cross_validate(
        estimator=dt_pipeline,
        cv=10,
        X=X_train,
        y=y_train
    )
)
cv_10_dt_metrics = cv_10_dt.agg(["mean", "sem"])
results_dt = pd.DataFrame({'mean' : [cv_10_dt_metrics.test_score.iloc[0]],
  'sem' : [cv_10_dt_metrics.test_score.iloc[1]]},
  index = ['Decision tree']
)
results = pd.concat([results, results_dt])
results
```

	mean	sem
Dummy classifier	0.541333	0.00299
Decision tree	0.769167	0.02632

Can we do better?

- We could tune some decision tree parameters (e.g., alpha, maximum tree depth, etc)…
- We could also try a different tree-based method!
- The Random Forest Algorithm by Jenny Yeon & Jared Wilber

The Random Forest Algorithm

1. Build a number of decision trees on bootstrapped training samples.
2. When building the trees from the bootstrapped samples, at each stage of splitting, the best splitting is computed using a randomly selected subset of the features.
3. Take the majority votes across all the trees for the final prediction.

Random forest in `scikit-learn` & missing values

- Does not accept missing values, we need to deal with these somehow…
- We can either drop the observations with missing values, or we can somehow impute them.
- For the purposes of this demo we will drop them, but if you are interested in imputation, see the imputation tutorial in `scikit-learn`

How many rows have missing observations:

```
heart.isna().any(axis=1).sum()
```

```
np.int64(6)
```

Drop rows with missing observations:

```
heart_train_drop_na = heart_train.dropna()

X_train_drop_na = heart_train_drop_na.drop(
    columns=['AHD']
)
y_train_drop_na = heart_train_drop_na['AHD']
```

Random forest in `scikit-learn`

```
from sklearn.ensemble import RandomForestClassifier

random_forest = RandomForestClassifier(random_state=2026)
rf_pipeline = make_pipeline(heart_preprocessor, random_forest)
cv_10_rf = pd.DataFrame(
    cross_validate(
        estimator=rf_pipeline,
        cv=10,
        X=X_train_drop_na,
        y=y_train_drop_na
    )
)

cv_10_rf_metrics = cv_10_rf.agg(["mean", "sem"])
results_rf = pd.DataFrame({'mean' : [cv_10_rf_metrics.test_score.iloc[0]],
  'sem' : [cv_10_rf_metrics.test_score.iloc[1]]},
  index = ['Random forest']
)
results = pd.concat([results, results_rf])
results
```

	mean	sem
Dummy classifier	0.541333	0.002990
Decision tree	0.769167	0.026320
Random forest	0.818297	0.017362

Can we do better?

- Random forest can be tuned a several important parameters, including:
  - `n_estimators`: number of decision trees (higher = more complexity)
  - `max_depth`: max depth of each decision tree (higher = more complexity)
  - `max_features`: the number of features you get to look at each split (higher = more complexity)
- We can use `GridSearchCV` to search for the optimal parameters for these, as we did for in -nearest neighbors.

Tuning random forest in `scikit-learn`

```
from sklearn.model_selection import GridSearchCV

rf_param_grid = {'randomforestclassifier__n_estimators': [200],
                 'randomforestclassifier__max_depth': [1, 3, 5, 7, 9],
                 'randomforestclassifier__max_features': [1, 2, 3, 4, 5, 6, 7]}

rf_tune_grid = GridSearchCV(
    estimator=rf_pipeline,
    param_grid=rf_param_grid,
    cv=10,
    n_jobs=-1 # tells computer to use all available CPUs
)
rf_tune_grid.fit(
    X_train_drop_na,
    y_train_drop_na
)

cv_10_rf_tuned_metrics = pd.DataFrame(rf_tune_grid.cv_results_)
results_rf_tuned = pd.DataFrame({'mean' : rf_tune_grid.best_score_,
  'sem' : pd.DataFrame(rf_tune_grid.cv_results_)['std_test_score'][6] / 10**(1/2)},
  index = ['Random forest tuned']
)
results = pd.concat([results, results_rf_tuned])
```

Random Forest results

How did the Random Forest compare against the other models we tried?

```
1 results
```

	mean	sem
Dummy classifier	0.541333	0.002990
Decision tree	0.769167	0.026320
Random forest	0.818297	0.017362
Random forest tuned	0.860688	0.022223

Boosting

- No randomization.
- The key idea is combining many simple models called weak learners, to create a strong learner.
- They combine multiple shallow (depth 1 to 5) decision trees.
- They build trees in a serial manner, where each tree tries to correct the mistakes of the previous one.

Tuning `GradientBoostingClassifier` with `scikit-learn`

- `GradientBoostingClassifier` can be tuned a several important parameters, including:
  - `n_estimators`: number of decision trees (higher = more complexity)
  - `max_depth`: max depth of each decision tree (higher = more complexity)
  - `learning_rate`: the shrinkage parameter which controls the rate at which boosting learns. Values between 0.01 or 0.001 are typical.
- We can use `GridSearchCV` to search for the optimal parameters for these, as we did for the parameters in Random Forest.

Tuning `GradientBoostingClassifier` with `scikit-learn`

```
from sklearn.ensemble import GradientBoostingClassifier

gradient_boosted_classifier = GradientBoostingClassifier(random_state=2026)
gb_pipeline = make_pipeline(heart_preprocessor, gradient_boosted_classifier)
gb_param_grid = {'gradientboostingclassifier__n_estimators': [200],
              'gradientboostingclassifier__max_depth': [1, 3, 5, 7, 9],
              'gradientboostingclassifier__learning_rate': [0.001, 0.005, 0.01]}
gb_tune_grid = GridSearchCV(
    estimator=gb_pipeline,
    param_grid=gb_param_grid,
    cv=10,
    n_jobs=-1 # tells computer to use all available CPUs
)
gb_tune_grid.fit(
    X_train_drop_na,
    y_train_drop_na
)

cv_10_gb_tuned_metrics = pd.DataFrame(gb_tune_grid.cv_results_)
results_gb_tuned = pd.DataFrame({'mean' : gb_tune_grid.best_score_,
  'sem' : pd.DataFrame(gb_tune_grid.cv_results_)['std_test_score'][6] / 10**(1/2)},
  index = ['Gradient boosted classifier tuned']
)
results = pd.concat([results, results_gb_tuned])
```

`GradientBoostingClassifier` results

How did the `GradientBoostingClassifier` compare against the other models we tried?

```
1 results
```

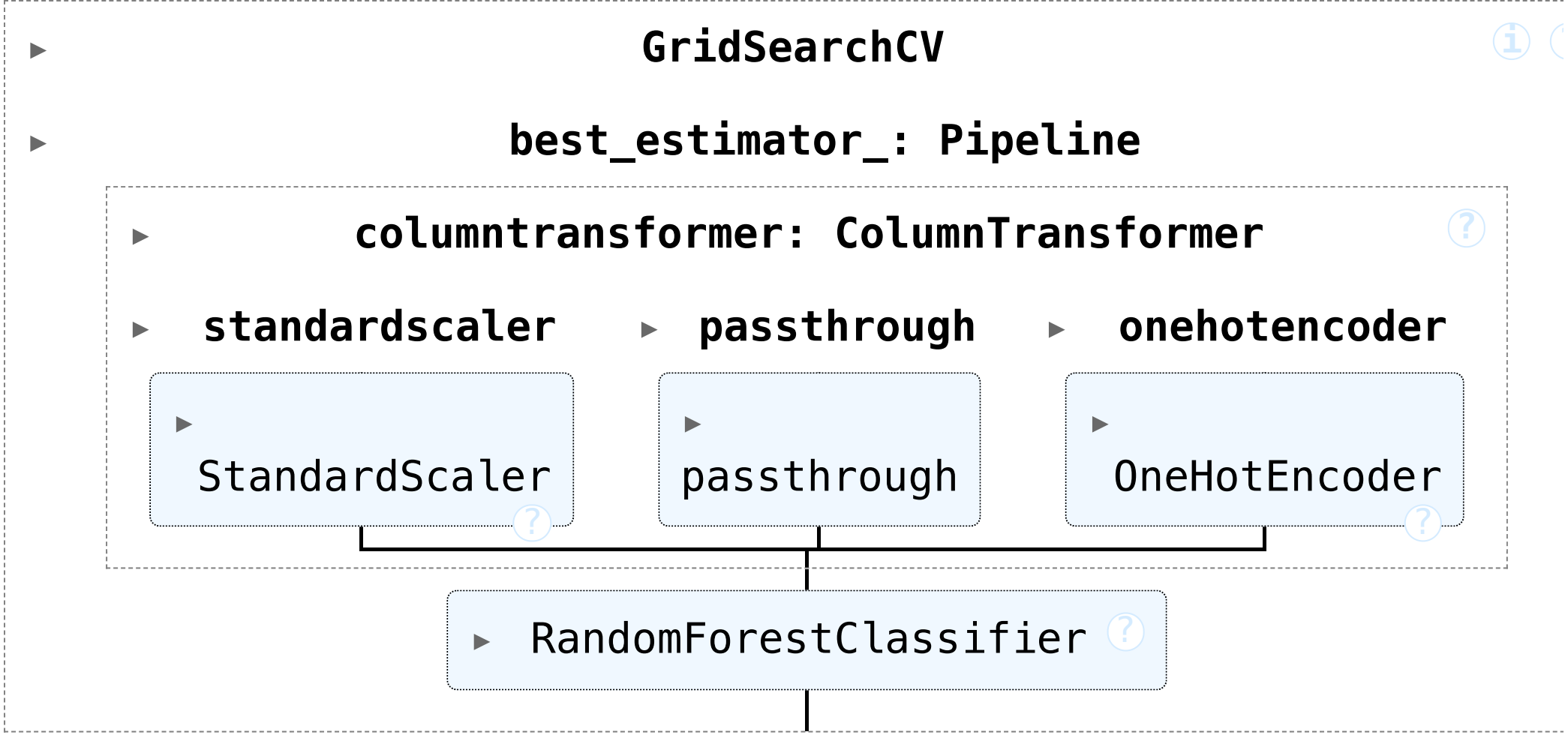
	mean	sem
Dummy classifier	0.541333	0.002990
Decision tree	0.769167	0.026320
Random forest	0.818297	0.017362
Random forest tuned	0.860688	0.022223
Gradient boosted classifier tuned	0.851993	0.025671

How do we choose the final model?

- Remember, what is your question or application?
- A good rule when models are not very different, what is the simplest model that does well?
- Look at other metrics that are important to you (not just the metric you used for tuning your model), remember precision & recall, for example.
- Remember - no peaking at the test set until you choose! And then, you should only look at the test set for one model!

Precision and recall on the tuned random forest model

```
from sklearn.metrics import make_scorer, precision_score, recall_score

scoring = {
    'accuracy': 'accuracy',
    'precision': make_scorer(precision_score, pos_label='Yes'),
    'recall': make_scorer(recall_score, pos_label='Yes')
}

rf_tune_grid = GridSearchCV(
    estimator=rf_pipeline,
    param_grid=rf_param_grid,
    cv=10,
    n_jobs=-1,
    scoring=scoring,
    refit='accuracy'
)

rf_tune_grid.fit(X_train_drop_na, y_train_drop_na)
```


GridSearchCV
best_estimator_: Pipeline
columntransformer: ColumnTransformer
standardscaler
passthrough
onehotencoder
StandardScaler
passthrough
OneHotEncoder
RandomForestClassifier

Precision and recall cont'd

- What do we think? Is this model ready for production in a diagnostic setting?
- How could we improve it further?

```
cv_results = pd.DataFrame(rf_tune_grid.cv_results_)

mean_precision = cv_results['mean_test_precision'].iloc[rf_tune_grid.best_index_]
sem_precision = cv_results['std_test_precision'].iloc[rf_tune_grid.best_index_] / np.sqrt(10)
mean_recall = cv_results['mean_test_recall'].iloc[rf_tune_grid.best_index_]
sem_recall = cv_results['std_test_recall'].iloc[rf_tune_grid.best_index_] / np.sqrt(10)

results_rf_tuned = pd.DataFrame({
    'mean': [rf_tune_grid.best_score_, mean_precision, mean_recall],
    'sem': [cv_results['std_test_accuracy'].iloc[rf_tune_grid.best_index_] / np.sqrt(10), sem_precision, sem_
}, index=['accuracy', 'precision', 'recall'])

results_rf_tuned
```

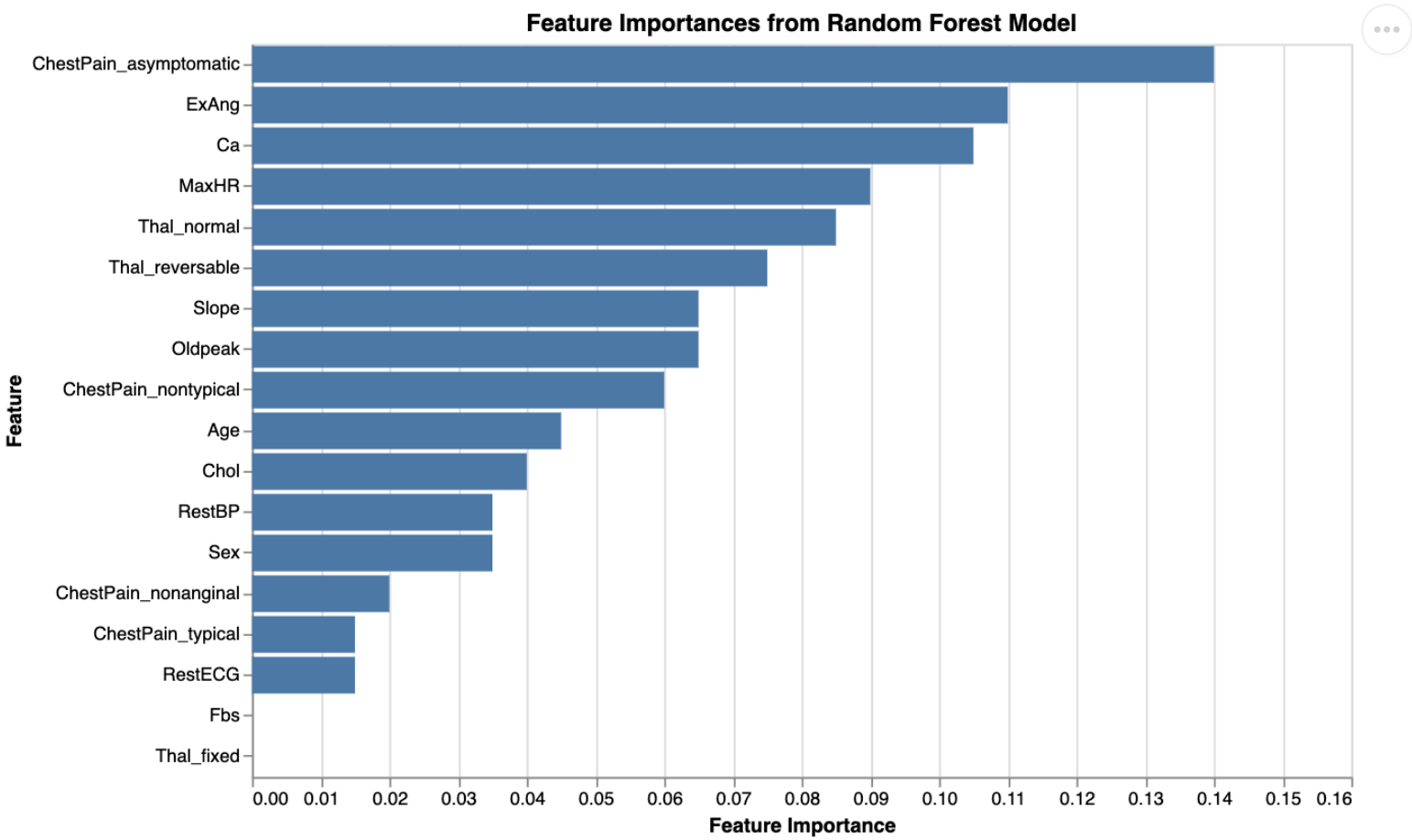
	mean	sem
accuracy	0.860688	0.018576
precision	0.920505	0.022982
recall	0.770909	0.038928

Feature importances

Feature importances in `scikit-learn`

```
# Access the best pipeline
best_pipeline = rf_tune_grid.best_estimator_

# Extract the trained RandomForestClassifier from the pipeline
best_rf = best_pipeline.named_steps['randomforestclassifier']

# Extract feature names after preprocessing
# Get the names of features from each transformer in the pipeline
numeric_features = numeric_feats
categorical_feature_names = best_pipeline.named_steps['columntransformer'].transformers_[2][1].get_feature_na
passthrough_features = passthrough_feats

# Combine all feature names into a single list
feature_names = np.concatenate([numeric_features, passthrough_features, categorical_feature_names])

# Calculate feature importances
feature_importances = best_rf.feature_importances_

# Create a DataFrame to display feature importances
importances_df = pd.DataFrame({
    'Feature': feature_names,
    'Importance': feature_importances
})

```

Visualizing the results



Evaluating on the test set

Predict on the test set:

```
heart_test_drop_na = heart_test.dropna()
X_test_drop_na = heart_test_drop_na.drop(columns=['AHD'])
y_test_drop_na = heart_test_drop_na['AHD']

heart_test_drop_na["predicted"] = rf_tune_grid.predict(
    X_test_drop_na
)
```

Evaluating on the test set

Examine accuracy, precision and recall:

```
rf_tune_grid.score(
    X_test_drop_na,
    y_test_drop_na
)
```

```
0.7868852459016393
```

```
precision_score(
    y_true=heart_test_drop_na["AHD"],
    y_pred=heart_test_drop_na["predicted"],
    pos_label='Yes'
)
```

```
np.float64(0.8)
```

```
recall_score(
    y_true=heart_test_drop_na["AHD"],
    y_pred=heart_test_drop_na["predicted"],
    pos_label='Yes'
)
```

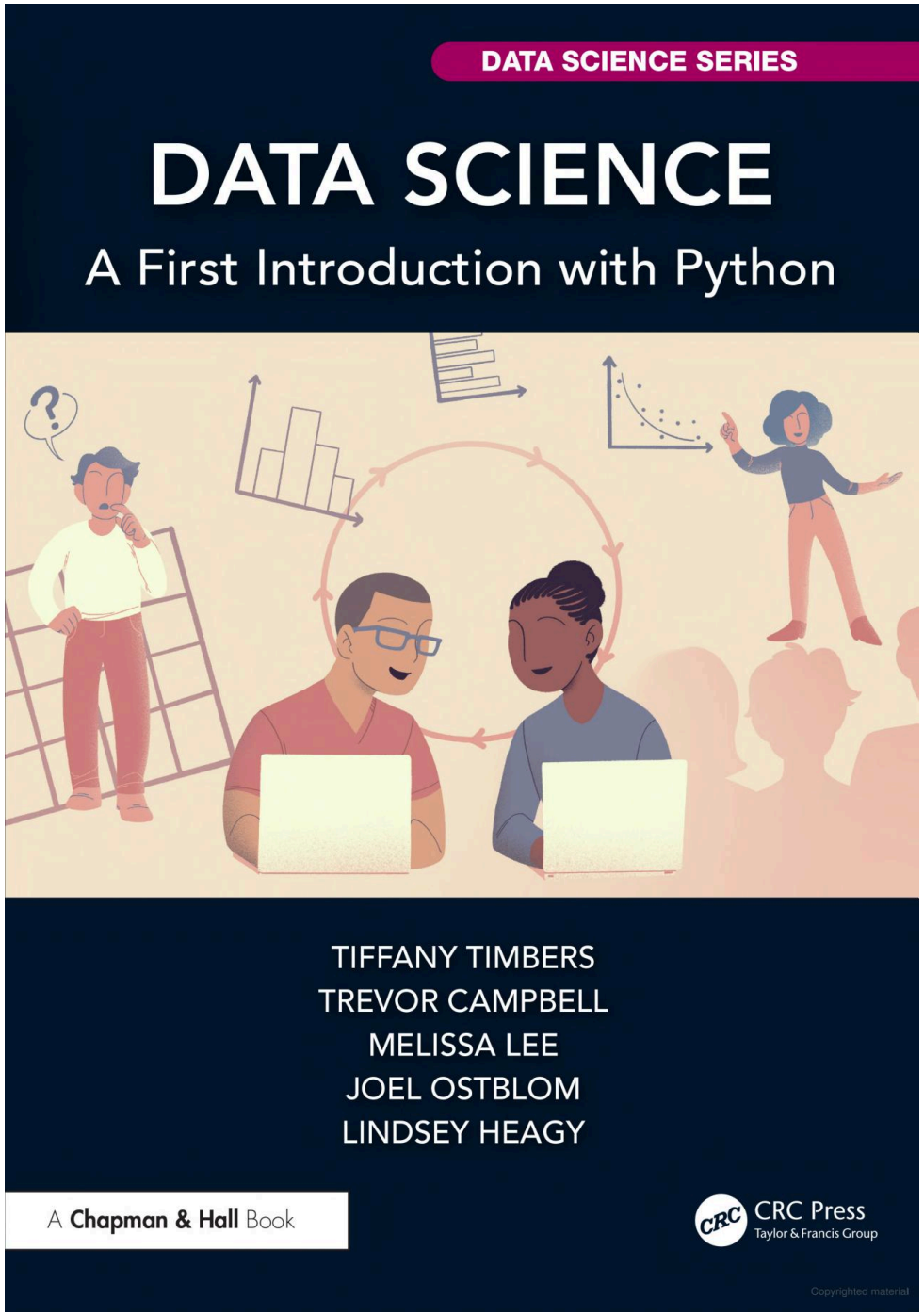
```
np.float64(0.7142857142857143)
```

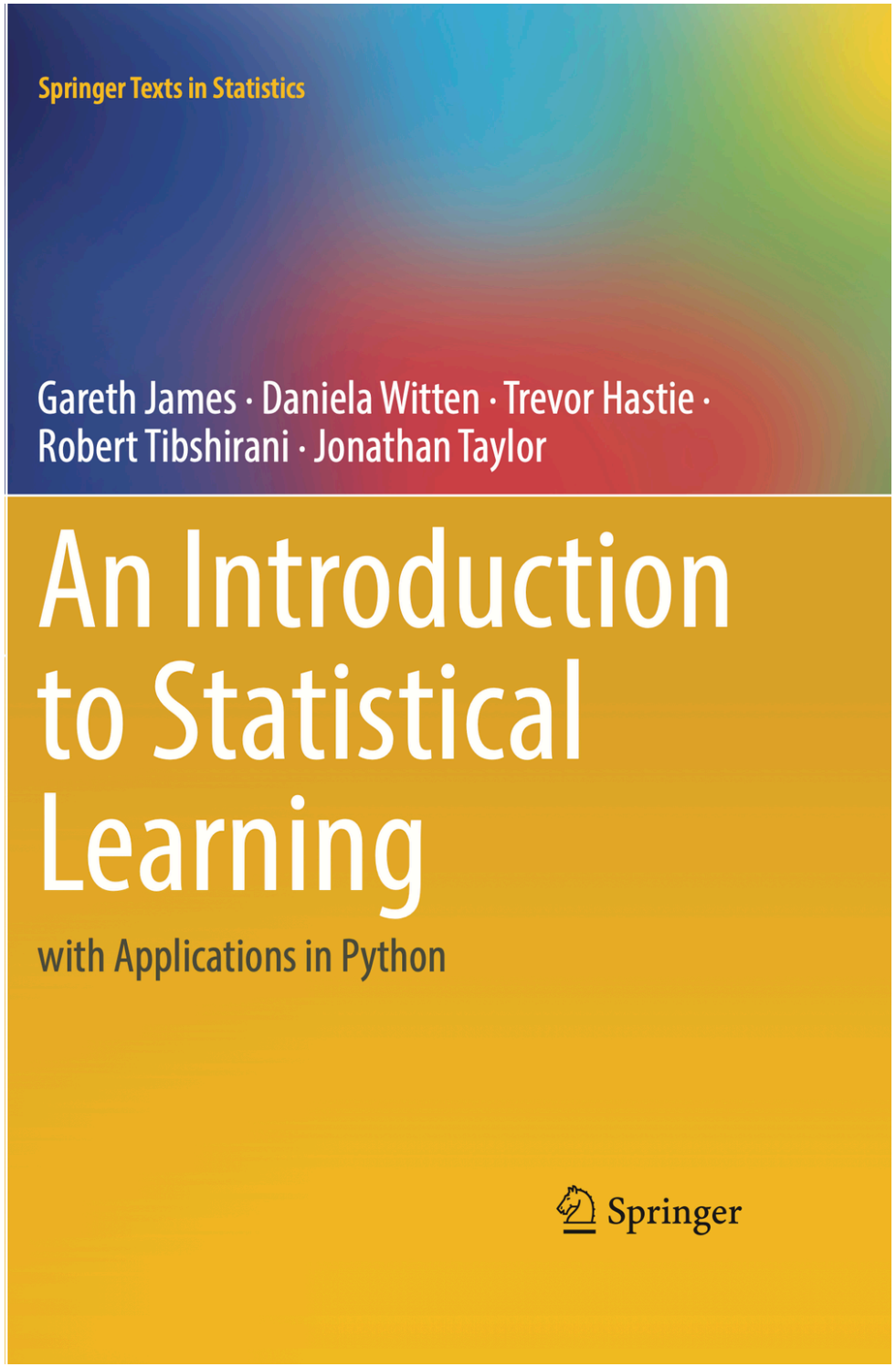
```
conf_matrix = pd.crosstab(
    heart_test_drop_na["AHD"],
    heart_test_drop_na["predicted"]
)
print(conf_matrix)
```

```
predicted  No  Yes
AHD
No         28    5
Yes         8   20
```

Other boosting models:

Keep learning!





https://python.datasciencebook.ca/

Local installation

1. Using Docker: Data Science: A First Introduction (Python Edition) Installation Instructions
2. Using conda: UBC MDS Installation Instructions

Additional resources

- The UBC DSCI 573 (Feature and Model Selection notes) chapter of Data Science: A First Introduction (Python Edition) by Varada Kolhatkar and Joel Ostblom. These notes cover classification and regression metrics, advanced variable selection and more on ensembles.
- The `scikit-learn` website is an excellent reference for more details on, and advanced usage of, the functions and packages in the past two chapters. Aside from that, it also offers many useful tutorials to get you started.
- *An Introduction to Statistical Learning* {cite:p}`james2013introduction` provides a great next stop in the process of learning about classification. Chapter 4 discusses additional basic techniques for classification that we do not cover, such as logistic regression, linear discriminant analysis, and naive Bayes.

References

Gareth James, Daniela Witten, Trevor Hastie, Robert Tibshirani and Jonathan Taylor. An Introduction to Statistical Learning with Applications in Python. Springer, 1st edition, 2023. URL: https://www.statlearning.com/.

Kolhatkar, V., and Ostblom, J. (2024). UBC DSCI 573: Feature and Model Selection course notes. URL: https://ubc-mds.github.io/DSCI_573_feat-model-select

Pedregosa, F. et al., 2011. Scikit-learn: Machine learning in Python. Journal of machine learning research, 12(Oct), pp.2825–2830.