Lab 2 — Global Post-hoc Explainability

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This lab covers three **global post-hoc** explainability techniques applied to black-box classifiers on the Titanic dataset:

Technique	What it explains
Permutation Feature Importance	How much each feature contributes to model performance
Partial Dependence Plot (PDP)	Marginal effect of one (or two) features on the predicted outcome
Global Surrogate Models	A white-box model that approximates a black-box model's predictions

Guide:

- ⚙️ Data preprocessing (Titanic)
- 🔀 Permutation Feature Importance
- 📉 Partial Dependence Plots
- 🪞 Global Surrogate Models

⚙️ Data Preprocessing (~10 min)

We are using the **Titanic** dataset loaded directly from OpenML. This section walks through the full preprocessing pipeline: loading, splitting, imputing, encoding, and scaling.

> 💡 Apply the same good habits from Lab 1: always fit transformations on the **training set only**, then apply them to the test set!

⚙️ Step 1 — Imports & Load

```
# Import the required libraries for this exercise

from sklearn.datasets import fetch_openml
from sklearn.model_selection import train_test_split
from sklearn.impute import SimpleImputer
from sklearn import tree

import pandas as pd
import numpy as np

import seaborn as sns
import matplotlib.pyplot as plt
```

⚙️ Step 2 — Load the Titanic Dataset

```
# Load input features and target variable
df, y = fetch_openml("titanic", version=1, as_frame=True, parser='auto', return_X_y=True)

# The "survived" column contains the target variable
df["survived"] = y
```

⚙️ Step 3 — Stratified Train / Test Split

> 🔑 **Key reminder:** split *before* any transformation. Fitting scalers or imputers on the full dataset causes **data leakage**.

```
# Split the dataset. 80% for training data and 20% for test data. Shuffle the dataset and perform stratification

df_train, df_test = train_test_split(df, test_size=0.2, shuffle=True, random_state=42, stratify=df['survived'])
```

⚙️ Step 4 — Handle Missing Values

> 🔑 **Key reminder:** compute statistics (mean, median...) on the **training set only**, then apply to both sets.

```
print(f'Number of null values in Train before pre-processing: {df_train.age.isnull().sum()}/{len(df_train)}')
print(f'Number of null values in Test before pre-processing: {df_test.age.isnull().sum()}/{len(df_test)}')
```

```
df_train['age'] = df_train['age'].fillna(df_train['age'].mean())
df_test['age'] = df_test['age'].fillna(df_train['age'].mean())

print(f'Number of null values in Train after pre-processing: {df_train.age.isnull().sum()}/{len(df_train)}')
print(f'Number of null values in Test after pre-processing: {df_test.age.isnull().sum()}/{len(df_test)}')
```

```
Number of null values in Train before pre-processing: 209/1047
Number of null values in Test before pre-processing: 54/262
Number of null values in Train after pre-processing: 0/1047
Number of null values in Test after pre-processing: 0/262
```

```
print(f'Number of null values in Train before pre-processing: {df_train.fare.isnull().sum()}/{len(df_train)}')
print(f'Number of null values in Test before pre-processing: {df_test.fare.isnull().sum()}/{len(df_test)}')

df_train['fare'] = df_train['fare'].fillna(df_train['fare'].median())
df_test['fare'] = df_test['fare'].fillna(df_train['fare'].median())

print(f'Number of null values in Train after pre-processing: {df_train.fare.isnull().sum()}/{len(df_train)}')
print(f'Number of null values in Test after pre-processing: {df_test.fare.isnull().sum()}/{len(df_test)}')
```

```
Number of null values in Train before pre-processing: 1/1047
Number of null values in Test before pre-processing: 0/262
Number of null values in Train after pre-processing: 0/1047
Number of null values in Test after pre-processing: 0/262
```

```
print(f'Number of null values in Train before pre-processing: {df_train.embarked.isnull().sum()}/{len(df_train)}
print(f'Number of null values in Test before pre-processing: {df_test.embarked.isnull().sum()}/{len(df_test)}')

imp = SimpleImputer(missing_values=np.nan, strategy='most_frequent')
df_train[['embarked']] = imp.fit_transform(df_train[['embarked']])
df_test[['embarked']] = imp.transform(df_test[['embarked']])

print(f'Number of null values in Train after pre-processing: {df_train.embarked.isnull().sum()}/{len(df_train)}'
print(f'Number of null values in Test after pre-processing: {df_test.embarked.isnull().sum()}/{len(df_test)}')
```

```
Number of null values in Train before pre-processing: 0/1047
Number of null values in Test before pre-processing: 2/262
Number of null values in Train after pre-processing: 0/1047
Number of null values in Test after pre-processing: 0/262
```

⚙️ Step 5 — Drop Uninformative Columns

> 🔑 Remove columns that are not useful for predicting survival, or that leak information about the target variable.

```
df_train = df_train.drop(columns=['name','ticket'])
df_test = df_test.drop(columns=['name','ticket'])

df_train.head()
```

	pclass	sex	age	sibsp	parch	fare	cabin	embarked	boat	body	home.dest	survived
999	3	female	29.604316	0	0	7.7500	NaN	Q	15 16	NaN	NaN	1
392	2	female	24.000000	1	0	27.7208	NaN	C	12	NaN	Lucca, Italy / California	1
628	3	female	11.000000	4	2	31.2750	NaN	S	NaN	NaN	Sweden Winnipeg, MN	0
1165	3	male	25.000000	0	0	7.2250	NaN	C	NaN	NaN	NaN	0
604	3	female	16.000000	0	0	7.6500	NaN	S	16	NaN	Norway Los Angeles, CA	1

Passaggi successivi: New interactive sheet

```
# Remove columns that contain target-leaking info (boat/body) or are mostly missing (cabin, home.dest)
df_train = df_train.drop(columns=['cabin', 'body', 'boat', 'home.dest'])
df_test = df_test.drop(columns=['cabin', 'body', 'boat', 'home.dest'])
```

⚙️ Step 6 — Extract Features & Apply Encoding / Scaling

> 🔑 **Key reminder:** ML models need numbers. We use `OneHotEncoder` for categoricals and `MinMaxScaler` for numerics — both fitted on **train only**.

```
# Extract target variable and input features for the training data
y_train = df_train['survived']              # Target variable training set
X_train = df_train.drop('survived', axis=1)  # Features training set

# Extract target variable and input features for the testing data
```

```
y_test = df_test['survived']                 # Target variable test set
X_test = df_test.drop('survived', axis=1)    # Features test set
```

```
from sklearn.compose import ColumnTransformer
from sklearn.preprocessing import OneHotEncoder, OrdinalEncoder
from sklearn.preprocessing import MinMaxScaler

categorical_columns = ["pclass", "sex", "embarked"]
numerical_columns = ["sibsp", "parch", "fare", "age"]

categorical_encoder = OneHotEncoder(handle_unknown='ignore', drop='if_binary')
minmax_s = MinMaxScaler()

preprocessing = ColumnTransformer(
    [
        ("cat", categorical_encoder, categorical_columns),
        ("num", minmax_s, numerical_columns),
    ],
    verbose_feature_names_out=False,
)
```

> ✅ **Preprocessing complete.** Remember the three rules:
>
> 1. Split *before* fitting any transformer.
> 2. Fit transformers on **train only**, apply to both.
> 3. Use `ColumnTransformer` to cleanly handle mixed-type features in a `Pipeline`.

Exercise 1 — Permutation Feature Importance 🔀

Permutation Feature Importance is a model-agnostic inspection technique that measures how much each feature contributes to model performance.

> A feature is **important** if shuffling its values causes the *model error to increase*. If the model relied on that feature, disrupting it should hurt performance.

Key advantages:

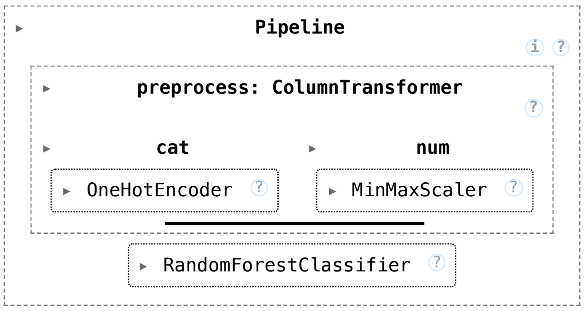
- Direct and intuitive interpretation of the model's behaviour
- Fully **model-agnostic** — works with any fitted estimator
- Does **not require retraining** the model

Main disadvantages:

- Assumes **feature independence** — correlated features can produce biased importance estimates
- Tightly coupled to the chosen **performance metric**

1.1 — Fit the Random Forest Classifier

```
from sklearn.pipeline import Pipeline
from sklearn.ensemble import RandomForestClassifier
from sklearn.inspection import permutation_importance
from sklearn.datasets import make_classification

clf = Pipeline(
    [
        ("preprocess", preprocessing),
        ("classifier", RandomForestClassifier(random_state=42)),
    ]
)
clf.fit(X_train, y_train)
```



1.2 — Model Performance

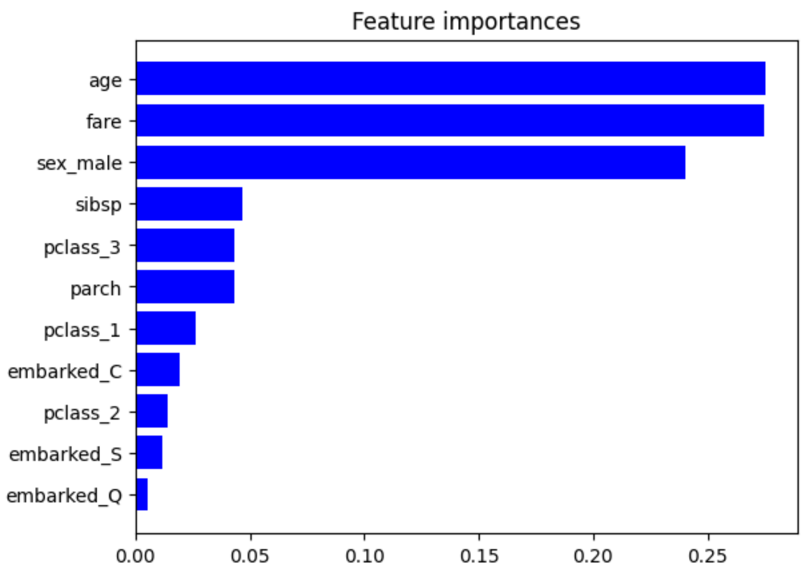
> Before inspecting feature importances, verify the model is predictive enough. A non-predictive model's importances are meaningless.

```
print(f"RF train accuracy: {clf.score(X_train, y_train):.3f}")
print(f"RF test accuracy: {clf.score(X_test, y_test):.3f}")
```

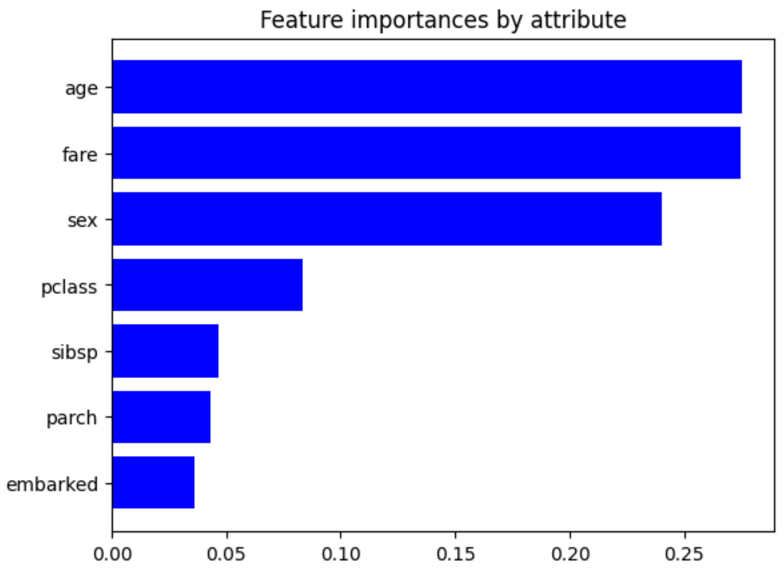
```
RF train accuracy: 0.969
RF test accuracy: 0.779
```

1.3 — Built-in Feature Importances

```
# Plot the feature importance (raw, per one-hot column)

importance = clf[-1].feature_importances_
feature_names = clf[:-1].get_feature_names_out()

sorted_idx = importance.argsort()

plt.barh(feature_names[sorted_idx], importance[sorted_idx], color='blue')
plt.title("Feature importances")
plt.show()
```



```
# Plot the feature importance aggregated by original attribute

importance = clf[-1].feature_importances_
feature_names = clf[:-1].get_feature_names_out()

feature_importances = {}
for feature_name, imp in zip(feature_names, importance):
    key = feature_name.split("_")[0] if "_" in feature_name else feature_name
    feature_importances[key] = feature_importances.get(key, 0) + imp

feature_importances = dict(sorted(feature_importances.items(), key=lambda x: x[1], reverse=False))

plt.barh(list(feature_importances.keys()), list(feature_importances.values()), color='blue')
plt.title("Feature importances by attribute")
plt.show()
```



The impurity-based feature importance ranks the **numerical features** to be the **most important** features.

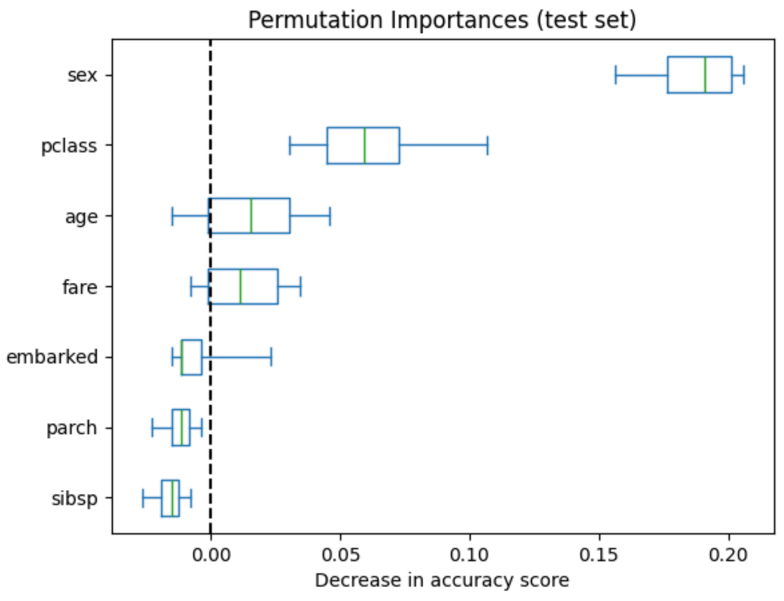
This stems from two known **limitations** of impurity-based importances:

- Importances are biased towards *high-cardinality features* (e.g. `fare`, `age`).
- Importances are computed on **training set statistics** and may not reflect generalisation ability.

1.4 — Permutation Importance on the Test Set

```
from sklearn.inspection import permutation_importance

# Calculate the permutation importance of each feature — test set
result = permutation_importance(clf, X_test, y_test, n_repeats=10, random_state=42)

sorted_importances_idx = result.importances_mean.argsort()
importances = pd.DataFrame(
    result.importances[sorted_importances_idx].T,
    columns=X_test.columns[sorted_importances_idx],
)
ax = importances.plot.box(vert=False, whis=5)
ax.set_title("Permutation Importances (test set)")
ax.axvline(x=0, color="k", linestyle="--")
ax.set_xlabel("Decrease in accuracy score")
```

```
Text(0.5, 0, 'Decrease in accuracy score')
```

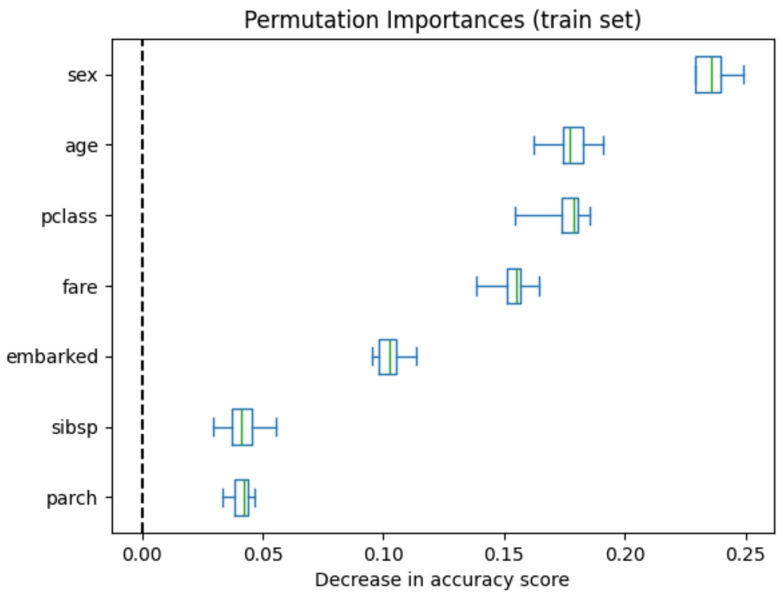


The low-cardinality categorical features `sex` and `pclass` are now ranked as the **most important** features. Permuting their values causes the **largest drop in accuracy** on the test set — confirming they drive the model's generalisation.

1.5 — Permutation Importance on the Training Set

```
# Calculate the permutation importance of each feature — train set
result = permutation_importance(clf, X_train, y_train, n_repeats=10, random_state=42)

sorted_importances_idx = result.importances_mean.argsort()
importances = pd.DataFrame(
    result.importances[sorted_importances_idx].T,
    columns=X_train.columns[sorted_importances_idx],
)
ax = importances.plot.box(vert=False, whis=5)
ax.set_title("Permutation Importances (train set)")
ax.axvline(x=0, color="k", linestyle="--")
ax.set_xlabel("Decrease in accuracy score")
```

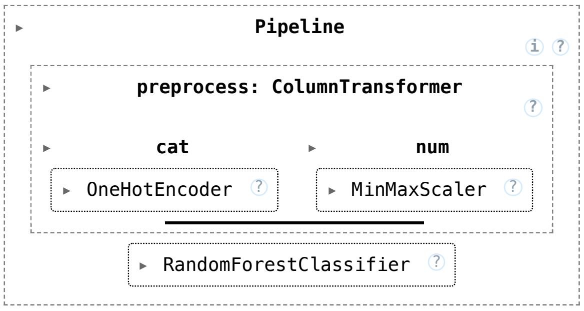
```
Text(0.5, 0, 'Decrease in accuracy score')
```



> `fare` gets a **significantly higher** importance ranking on the training set than on the test set. This discrepancy is a clear sign of **overfitting**: the Random Forest has enough capacity to use `fare` to memorise training examples, but this does not generalise.

1.6 — Regularised Random Forest (`min_samples_leaf=20`)

```
# Limit tree capacity to prevent overfitting
clf = Pipeline(
    [
        ("preprocess", preprocessing),
        ("classifier", RandomForestClassifier(random_state=42, min_samples_leaf=20)),
    ]
)
clf.fit(X_train, y_train)
clf.fit(X_train, y_train)
```



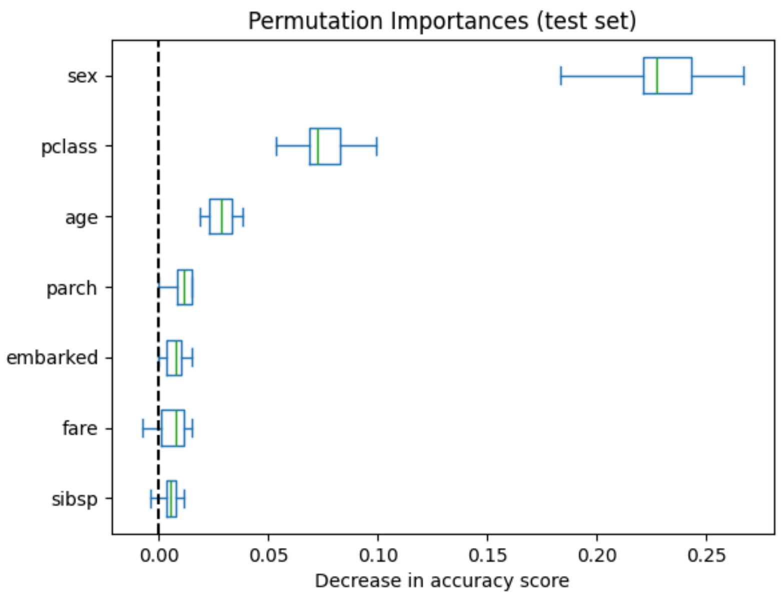
```
print(f"RF train accuracy: {clf.score(X_train, y_train):.3f}")
print(f"RF test accuracy: {clf.score(X_test, y_test):.3f}")
```

```
RF train accuracy: 0.808
RF test accuracy: 0.847
```

Train and test accuracy are now very close — the model is **no longer overfitting**. We can now trust the permutation importance results.

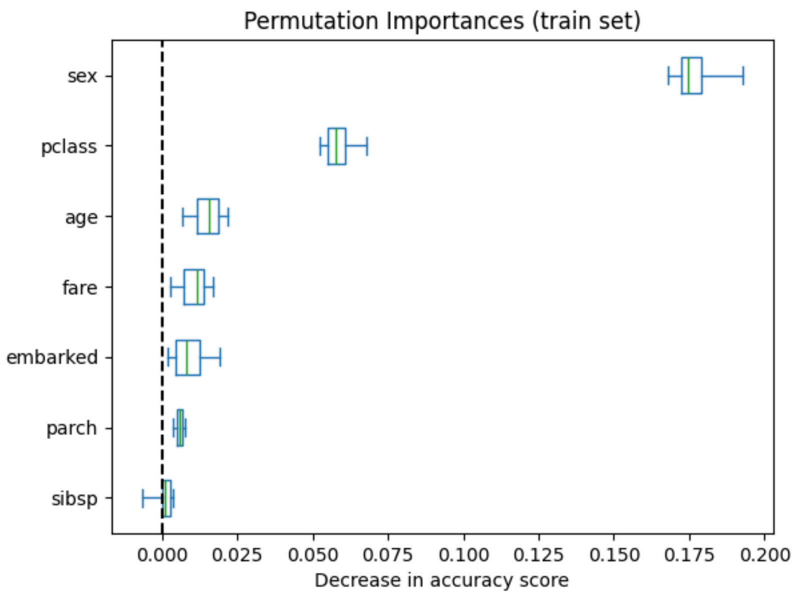
```
# Permutation importance (test set) — regularised model
result = permutation_importance(clf, X_test, y_test, n_repeats=10, random_state=42)

sorted_importances_idx = result.importances_mean.argsort()
importances = pd.DataFrame(
    result.importances[sorted_importances_idx].T,
    columns=X_test.columns[sorted_importances_idx],
)
ax = importances.plot.box(vert=False, whis=5)
ax.set_title("Permutation Importances (test set)")
ax.axvline(x=0, color="k", linestyle="--")
ax.set_xlabel("Decrease in accuracy score")
```

```
Text(0.5, 0, 'Decrease in accuracy score')
```



```
# Permutation importance (train set) — regularised model
result = permutation_importance(clf, X_train, y_train, n_repeats=10, random_state=42)

sorted_importances_idx = result.importances_mean.argsort()
importances = pd.DataFrame(
    result.importances[sorted_importances_idx].T,
    columns=X_train.columns[sorted_importances_idx],
)
ax = importances.plot.box(vert=False, whis=5)
ax.set_title("Permutation Importances (train set)")
ax.axvline(x=0, color="k", linestyle="--")
ax.set_xlabel("Decrease in accuracy score")
```

```
Text(0.5, 0, 'Decrease in accuracy score')
```



Exercise 2 — Partial Dependence Plots 📉

A **Partial Dependence Plot** (PDP) shows the **marginal effect** of one (or two) features on the predicted outcome of a machine learning model.

- It is a **global method**: it considers *all instances* and describes the global relationship between a feature and the prediction.
- PDPs are easy to visualise and intuitively interpretable.

Key advantages:

- Computation is intuitive and the visualisation is easy to read.
- Provides a global view of how a feature influences the prediction.

Main disadvantages:

- Assumes **feature independence** — correlated features distort the marginal estimates.
- Only practical for **at most two features** at a time.

2.1 — Imports

```
from sklearn.inspection import permutation_importance, partial_dependence, PartialDependenceDisplay
from sklearn.ensemble import RandomForestClassifier
from sklearn.tree import DecisionTreeClassifier
from sklearn.datasets import make_classification
```

2.2 — Fit RF & DT Classifiers

```
# Random Forest classifier
rf = Pipeline(
    [
        ("preprocess", preprocessing),
        ("classifier", RandomForestClassifier(random_state=42)),
    ]
)
rf.fit(X_train, y_train)

print(f"RF train accuracy: {rf.score(X_train, y_train):.3f}")
print(f"RF test accuracy:  {rf.score(X_test, y_test):.3f}")
```

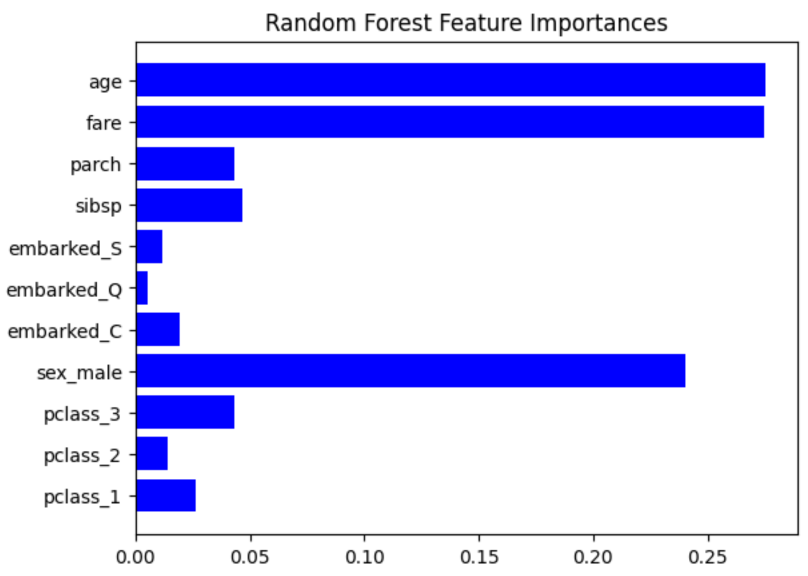
```
RF train accuracy: 0.969
RF test accuracy:  0.779
```

```
# Decision Tree classifier
dt = Pipeline(
    [
        ("preprocess", preprocessing),
        ("classifier", DecisionTreeClassifier(random_state=42)),
    ]
)
dt.fit(X_train, y_train)

print(f"DT train accuracy: {dt.score(X_train, y_train):.3f}")
print(f"DT test accuracy:  {dt.score(X_test, y_test):.3f}")
```

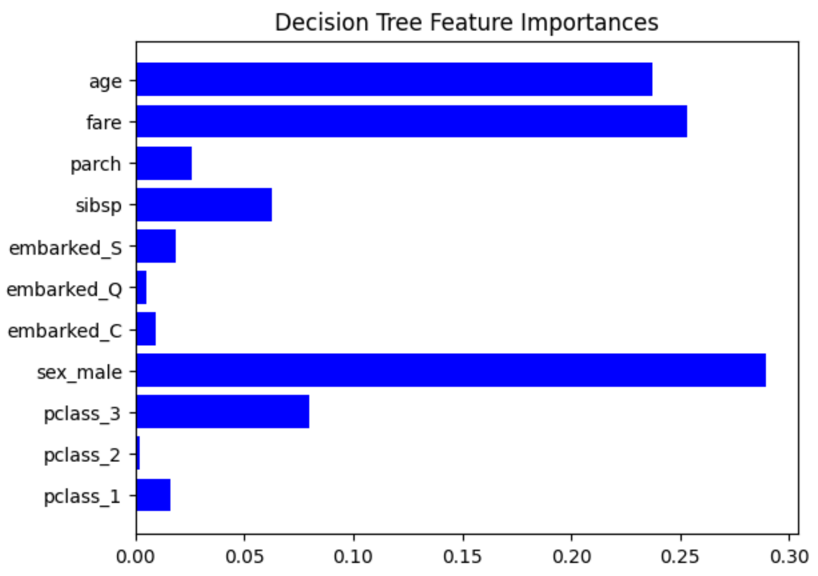
```
DT train accuracy: 0.969
DT test accuracy:  0.771
```

2.3 — Feature Importances

```
# Feature importance — Random Forest
importance = rf[-1].feature_importances_
feature_names = rf[:-1].get_feature_names_out()

plt.barh(feature_names, importance, color='blue')
plt.title("Random Forest Feature Importances")
plt.show()
```



```
# Feature importance — Decision Tree
importance = dt[-1].feature_importances_
feature_names = dt[:-1].get_feature_names_out()

plt.barh(feature_names, importance, color='blue')
plt.title("Decision Tree Feature Importances")
plt.show()
```



2.4 — Partial Dependence Plots

```
X_train.columns.tolist()
```

```
['pclass', 'sex', 'age', 'sibsp', 'parch', 'fare', 'embarked']
```

```
categorical_columns
```

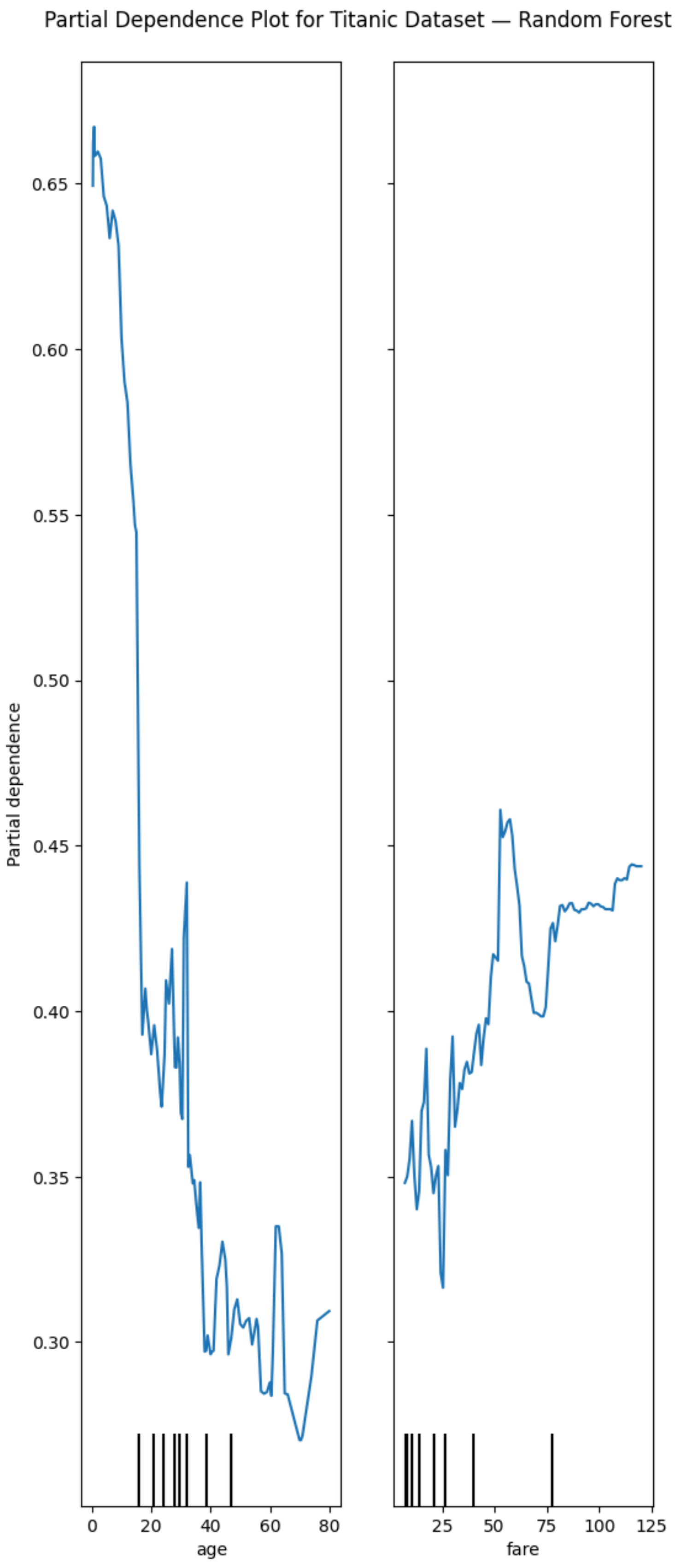
```
['pclass', 'sex', 'embarked']
```

```
feature_names
```

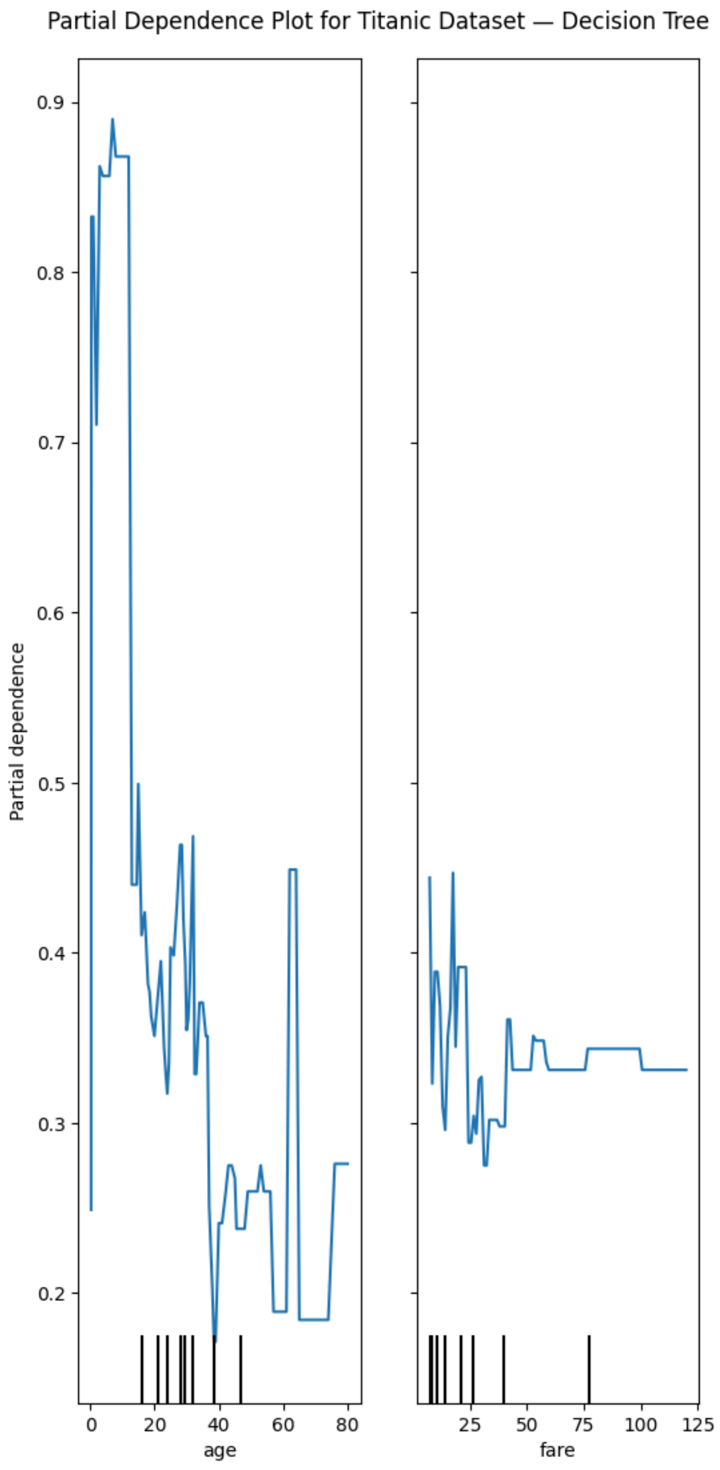
```
array(['pclass_1', 'pclass_2', 'pclass_3', 'sex_male', 'embarked_C',
       'embarked_Q', 'embarked_S', 'sibsp', 'parch', 'fare', 'age'],
      dtype=object)
```

```
# Select a subset of features to display in the PDP
selected_features = ['age', 'fare']

# PDP — Random Forest
fig, ax = plt.subplots(figsize=(6, 14))
```

```
display = PartialDependenceDisplay.from_estimator(
    rf,
    X_train,
    features=selected_features,
    n_cols=4,
    categorical_features=categorical_columns,
    ax=ax
)

display.figure_.suptitle('Partial Dependence Plot for Titanic Dataset — Random Forest')
display.figure_.subplots_adjust(hspace=0.4, top=0.95)
plt.show()
```



```
feature_names = X_train.columns

# PDP — Decision Tree
fig, ax = plt.subplots(figsize=(6, 12))

display = PartialDependenceDisplay.from_estimator(
    dt,
    X_train,
    features=selected_features,
    n_cols=2,
    categorical_features=categorical_columns,
    ax=ax
)

display.figure_.suptitle('Partial Dependence Plot for Titanic Dataset — Decision Tree')
display.figure_.subplots_adjust(hspace=0.4, top=0.95)
plt.show()
```



Exercise 3 — Global Surrogate Models

A **global surrogate model** is an *interpretable* model trained to **approximate** the predictions of a black-box model as accurately as possible.

> The key idea: you don't need to peek inside the black box — only its **prediction function** and a dataset are required.

How to build a surrogate:

1. Select a dataset X.
2. Get the **black-box predictions** for X.
3. Choose an **interpretable model type** (linear model, decision tree, ...).
4. Train the interpretable model on X using the black-box predictions as labels.
5. Measure how well the surrogate **replicates** the black-box predictions (reconstruction error).

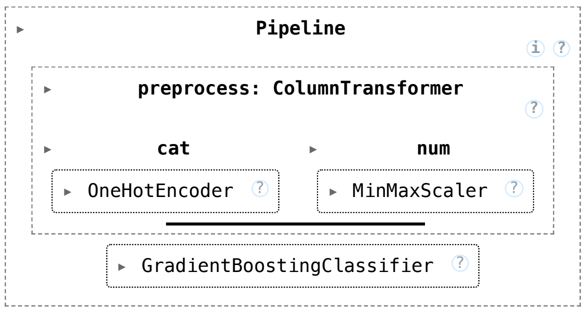
The surrogate is **model-agnostic** — it makes no assumptions about the inner workings of the black-box model.

3.1 — Imports

```
from sklearn.ensemble import GradientBoostingClassifier
import numpy as np
from sklearn.datasets import load_digits
from sklearn.model_selection import train_test_split
from sklearn.linear_model import LogisticRegression
from sklearn.metrics import accuracy_score
```

3.2 — Train the Black-Box Model

```
# Train the black-box model (GradientBoostingClassifier)
black_box_model = Pipeline(
    [
        ("preprocess", preprocessing),
        ("classifier", GradientBoostingClassifier(n_estimators=100, random_state=42)),
    ]
)
black_box_model.fit(X_train, y_train)
```



3.3 — Train the White-Box Surrogate

```
# Train the white-box surrogate (Logistic Regression) on the black-box predictions
white_box_model = Pipeline(
    [
        ("preprocess", preprocessing),
        ("classifier", LogisticRegression(max_iter=1000, random_state=42)),
    ]
)

black_box_train_predictions = black_box_model.predict(X_train)

# The surrogate is trained to replicate the black-box output, not the true labels
white_box_model.fit(X_train, black_box_train_predictions)
```

▸ **Pipeline**

▸ **preprocess: ColumnTransformer**

3.4 — Inspect Surrogate Coefficients

```
# Extract coefficients and compute odds ratios
coefficients = white_box_model[1].coef_[0]
feature_names = white_box_model[:-1].get_feature_names_out()

odds_ratios = np.exp(coefficients)

results_df = pd.DataFrame({
    'Feature': feature_names,
    'Weight': coefficients,
    'Odds Ratio': odds_ratios
})

print(results_df)
```

```
       Feature    Weight  Odds Ratio
0     pclass_1  1.405170    4.076221
1     pclass_2  0.530692    1.700108
2     pclass_3 -1.925615    0.145786
3     sex_male -4.247295    0.014303
4   embarked_C  0.518761    1.679945
5   embarked_Q  0.258913    1.295521
6   embarked_S -0.767426    0.464206
7        sibsp -1.025828    0.358499
8        parch  0.271571    1.312025
9         fare  0.208645    1.232008
10         age -3.382159    0.033974
```

3.5 — Evaluate Both Models

```
# Accuracy of the black-box and white-box models on true labels
black_box_train_accuracy = accuracy_score(y_train, black_box_train_predictions)
black_box_test_accuracy  = accuracy_score(y_test, black_box_model.predict(X_test))
white_box_train_accuracy = accuracy_score(y_train, white_box_model.predict(X_train))
white_box_test_accuracy  = accuracy_score(y_test, white_box_model.predict(X_test))

print(f"Black-box train accuracy: {black_box_train_accuracy:.3f}")
print(f"Black-box test  accuracy: {black_box_test_accuracy:.3f}")
print(f"White-box train accuracy: {white_box_train_accuracy:.3f}")
print(f"White-box test  accuracy: {white_box_test_accuracy:.3f}")
```

```
Black-box train accuracy: 0.861
Black-box test  accuracy: 0.813
White-box train accuracy: 0.790
White-box test  accuracy: 0.832
```

3.6 — Reconstruction Error

```
# Reconstruction error: how well does the white-box replicate the black-box predictions?
white_box_reconstruction_error_train = 1 - accuracy_score(
    black_box_train_predictions, white_box_model.predict(X_train)
)
white_box_reconstruction_error_test = 1 - accuracy_score(
    black_box_model.predict(X_test), white_box_model.predict(X_test)
)

print("White-Box Surrogate - Reconstruction Error:")
print(f"  Train: {white_box_reconstruction_error_train:.3f}")
print(f"  Test:  {white_box_reconstruction_error_test:.3f}")
```

```
White-Box Surrogate - Reconstruction Error:
  Train: 0.107
  Test:  0.103
```

🔍 Reflection Questions

1. **Permutation Feature Importance:** Why does permutation importance on the *training set* give a different result than on the *test set* for the unconstrained Random Forest? What does `min_samples_leaf=20` change, and why?
2. **PDP:** The PDP shows the *average* marginal effect. If `fare` and `pclass` are correlated, what risk do you run when interpreting each PDP independently? How could you detect this problem?
3. **Surrogate Model:** A high reconstruction error means the white-box model cannot replicate the black-box well. In that case, is the