The code for the programming exercises can be found in the `hw_sol_fi_py.ipynb` or `hw_sol_fi_py.pdf` files for Python and in the `hw_sol_fi_R.pdf` file for R.

Solution 1:

a) Permutation Feature Importance compares the performance of the model on the original data with the performance on perturbed data, where the dependence of the variable of interest (let's call it x_j) with the target Y variable is broken.

In order to break the dependence of x_j with y, x_j is replaced with a permuted version $\tilde{x}_j$ which is independent of the target.

However, by permuting the variable we do not only break the dependence with y, but also with all other covariates. As such, we may create unrealistic observations.

For example, time of the year may be dependent with the highest temperature on a day. If we resample the variable time of the year independently of the temperature high, we may create observations where time of the year is winter and temperature high is 40 degrees celsius.

b) If a feature anyway independent of its covarites ($x_j \perp x_{-j}$, then PFI does not extrapolate to unseen regions.

Intuitively, the reason is that no dependence with the covariates is broken, since there were not dependencies between x_j and the remaining variables x_{-j} to begin with..

c) Pseudocode reading in data, estimating a regression model and calculating the MSE

Algorithm 1 getting started

```
df ← read in dataset extrapolation.csv
X, y ← features, target
X_train, X_test ← training data, test data
model ← linear regression model on X_train
return MSE of model predictions
```

d) First, we implement PFI. Here we implement the methods generically, such that the perturbation mechanism can easily be replaced. Therefore, we make use of `f(*args,**kwargs)` and `f(...)` in Python and R, respectively.

Pseudocode of `pfi_fname()`

Algorithm 2 `pfi_fname()`

```
Require: fname: feature of interest name
Require: predict: prediciton function
Require: score: performance metric
Require: X_test: data for the evaluation
Require: y_test: respective labels
Require: ...: further arguments (which are ignored)
X_test_perturbed ← copy X_test and randomly permute column containing feature fname
performance ← score(y_test, predict(X_test_perturbed)) - score(y_test, predict(X_test))
return performance
```

Pseudocode of `fi_naive()`

Algorithm 3 `fi_naive()`

Require: `perf_pert`: function that returns performance for some perturbation.
Require: `predict`: prediciton function
Require: `score`: performance metric
Require: `X_test`: data for the evaluation
Require: `y_test`: respective labels
Require: `...`: further arguments (which are ignored)

```
for fname in columns of X_test do
    imp ← fi_fname(fname, predict, score, X_test, y_test, ...)
    results ← extend by imp
end for
return results
```

Pseudocode of `n_times()`

Algorithm 4 `n_times()`

Require: `n`: number of repetitions
Require: `method`: feature importance method.
Require: `args`: all further arguments that are required for the method
Require: `return_raw`: Whether only the aggregation (mean, stdd) or also the raw results are returned

```
for i in n do
    tmp ← method(args)
    results ← extend by tmp
end for
mean_fi ← mean of results
std_fi ← stdd of results
if return_raw equals True then return mean_fi, std_fi, raw_results
else if return_raw equals False then return mean_fi, std_fi
end if
```

Now we apply the method to our model and dataset.

Algorithm 5 application

```
nr_runs ← 10
fis_mean, fis_std ← n_times(nr_runs, fi_naive, pfi_fname, model prediction function,
    mean_squared_error, X_test, y_test, return_raw=False)
plot bar chart
```

e) X_3 is the most important feature, with X_1 and X_2 sharing the second place. PFI considers X_4 to be irrelevant. According to the PFI interpretation rules, without further assumptions about the data, we know that

- X_1, X_2, X_3 are used by the model for it's prediction
- X_1, X_2, X_3 are dependent with Y and/or dependent with the covariates
- X_4 may be independent of Y and covariates and/or not used by the model. We only know that it is not both dependent and used by the model.

Bonus: If we would additionally analyze the data we find out that X_1, X_2 are dependent but X_3 is independent of all covariates.

As such, we could further conclude that X_3 is dependent with Y (but do not know for X_1, X_2 without looking into the data).

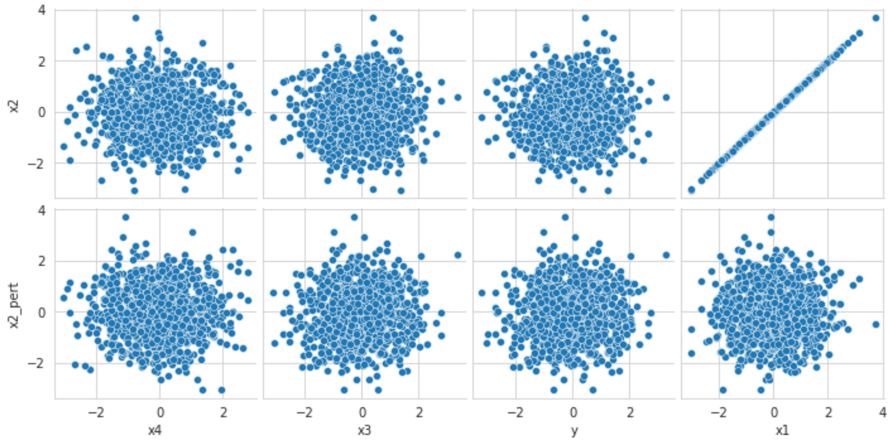
f) Correlation matrix:

	x_1	x_2	x_3	x_4	y
x_1	1.0***	1.0***	0.03	-0.05	0.02
x_2	1.0***	1.0***	0.03	-0.05	0.02
x_3	0.03	0.03	1.0***	-0.0	1.0***
x_4	-0.05	-0.05	-0.0	1.0***	0.0
y	0.02	0.02	1.0***	0.0	1.0***

Our interpretation was correct.

g) If we know the dependence structure of the covariates we can infer whether or not the PFI value is nonzero due to a dependence with the covariates or not. In our example we now know that x_3 is independent of its covariates, so we hypothesize that x_3 is actually dependent with y (and would perform importance tests as a consequence). Since x_1, x_2 are dependent, for those variables we cannot infer anything about the dependence with y with the covariates dependence structure and PFI alone.

h) We use the `extrapolation.csv` dataset. We create a pairplot showing the pairwise scatterplot of the original feature as well as the corresponding perturbed variable with all remaining feature variables (and potentially y).



We can see that the strong correlation of x_2 with x_1 (top row) is broken after permutation (bottom row). All other pairwise (in)dependencies are unchanged. Note: We only assess pairwise, unconditional dependencies. Without assumptions about the data, we cannot know whether further conditional depencies with the remaining covariates were broken.