Ensemble Models

Ensemble Models

We finished the earlier notebook with the following considerations

- DTs are non-linear models and quite prone to overfitting
- This can be mitigated (e.g. by reducing depth), but often with a loss of accuracy
- There is no easy fix by using a single DT

What about using multiple DTs?

For example, we could think of training several, different, DTs

- Each disting DT would risk overfitting, but in a different way
- Intuitively, overfitting would then appear as random noise
- ...Which could be canceled out via aggregation (averaging, voting)

This is the key idea behind ensemble DT models

We will (briefly) discuss a few of the main approach in this class

Random Forests

Random Forests work exactly as we have described

We assume we built m be different trees (estimators):

- Let $f_i(x)$ be the output of the i-th tree
- Let $\mathbb{I}(f_i(x) = k)$ is the indicator function for $f_i(x) = k$
- ...which is equal to 1 if $f_i(x) = k$ and 0 otherwise

Then the output of a RF for classification is given by:

$$f(x) = \mathrm{argmax}_{k \in K} \sum_{i=1}^{m} \mathbb{I}(f_i(x) = k)$$

- Intuitively: every tree "votes" for a class
- ...And we pick the class with the largest number of votes

Random Forests

We can use Random Forests for regression, too

In this case the model output is just an average:

$$f(x) = \frac{1}{m} \sum_{i=1}^{m} f_i(x)$$

We obtain different trees

...By using slighly different daset to train them. In particular we use:

- Bootstrapping: we select random subsets of the examples
- Bagging: we select random subsets of the attributes

They are called Random Forests due to:

- The use of multiple trees
- The introduction of random elements

Random Forests

We can learn a Random Forest model as usual

First we build a model object

```
In [5]: from sklearn.ensemble import RandomForestRegressor
        rfm = RandomForestRegressor(n_estimators=150, max_depth=20)
```

- We can specify the number of estimators (along the usual parameters)

Then we train the model:

```
In [6]: rfm.fit(X_tr, y_tr);
```

...And finally we obtain the predictions:

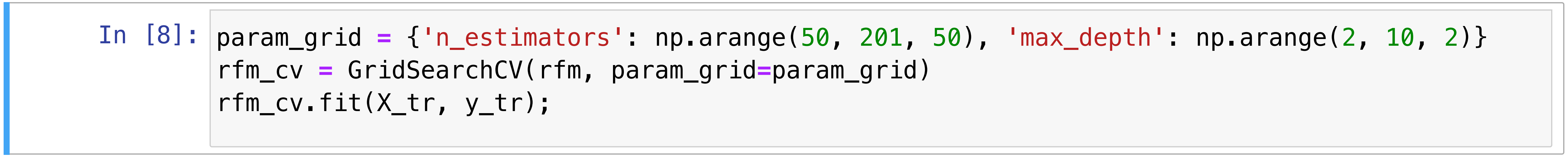
```
In [7]: rfm_pred_tr, rfm_pred_ts = rfm.predict(X_tr), rfm.predict(X_ts)
        print(f'R2: {r2_score(y_tr, rfm_pred_tr):.3} (training), {r2_score(y_ts, rfm_pred_ts):.3} (
```

```
R2: 0.967 (training), 0.743 (test)
```

Random Forests

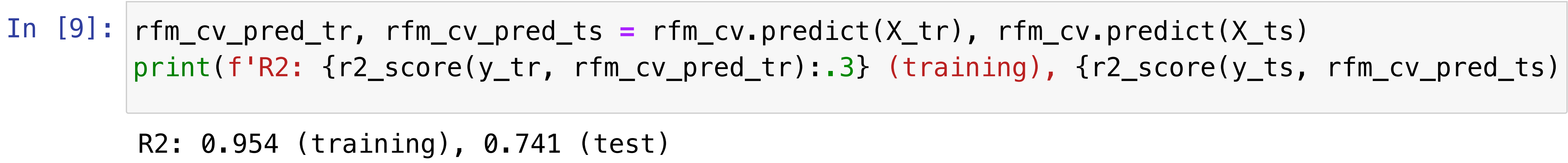
We can optimize the parameters using grid search and cross validation

This is interesting to check how RF differ from simple DTs



```
In [8]: param_grid = {'n_estimators': np.arange(50, 201, 50), 'max_depth': np.arange(2, 10, 2)}
        rfm_cv = GridSearchCV(rfm, param_grid=param_grid)
        rfm_cv.fit(X_tr, y_tr);
```

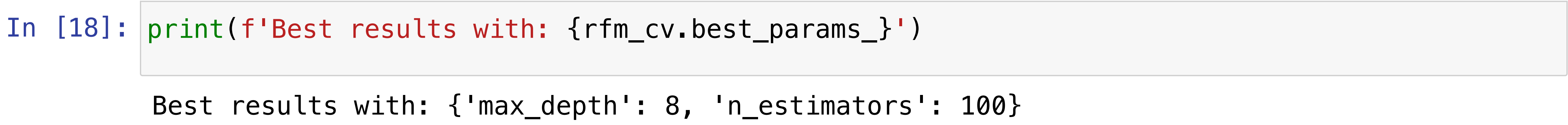
The results are not necessarily better



```
In [9]: rfm_cv_pred_tr, rfm_cv_pred_ts = rfm_cv.predict(X_tr), rfm_cv.predict(X_ts)
        print(f'R2: {r2_score(y_tr, rfm_cv_pred_tr):.3} (training), {r2_score(y_ts, rfm_cv_pred_ts)

        R2: 0.954 (training), 0.741 (test)
```

...But the optimal parameters tend to be more reliable



```
In [18]: print(f'Best results with: {rfm_cv.best_params_}')

         Best results with: {'max_depth': 8, 'n_estimators': 100}
```

Random Forests

RF and DTs operate in a very different way

The basic ingredient is still a DT

- DTs need to be deep in order to be expressive
- ...But deeper DTs are also very prone to overfitting

RFs have an innate mechanism to counter overfitting

- ...And therefore they can afford being much deeper
- This makes them much more reliable at learning complex relations

They are a bit slower to train

- ...But still fast compared to other complex ML models

Gradient Boosted Trees

Gradient Boosted Trees also employ multiple DTs, but in a different fashion

Technically, the output of a GBT model is just the sum of the individual ouputs

$$f(x) = \sum_{i=1}^{m} f_i(x)$$

- Where the notation is the same we used for random forests

However, the trees are trained sequentially:

- The first tree (i.e. $f_1(x)$) is trained as usual
- The second tree is trained to apply a correction over $f_1(x)$
- The third to apply a correction over $f_1(x) + f_2(x)$, etc.

Gradient Boosted Trees

The corrections are incremental:

- Each new tree does not try to completely fix the previous predictions
- ...But rather to make a step in the right direction
- ...As given by an exact or approximate gradient

There is no need for randomization, in principle:

- The incremental training process already yields different trees
- However, the scikit-learn implementation has some random elements

The idea of using a "chain" of corrective models is general

- It is called gradient boosting and can be applied with other model types
- ...But GBTs are the probably the best known example

Gradient Boosted Trees

We can learn Gradient Boosted Trees model as usual

First we build a model object

```
In [19]: from sklearn.ensemble import GradientBoostingRegressor
         gbm = GradientBoostingRegressor(n_estimators=100, max_depth=3)
```

- We can specify the number of estimators (along the usual parameters)

Then we train the model:

```
In [20]: gbm.fit(X_tr, y_tr);
```

...And finally we obtain the predictions:

```
In [21]: gbm_pred_tr, gbm_pred_ts = gbm.predict(X_tr), gbm.predict(X_ts)
         print(f'R2: {r2_score(y_tr, gbm_pred_tr):.3} (training), {r2_score(y_ts, gbm_pred_ts):.3} (

         R2: 0.944 (training), 0.724 (test)
```

Gradient Boosted Trees

We can optimize the parameters using grid search and cross validation

This is interesting to check how GBTs differ from RFs

```
In [22]: param_grid = {'n_estimators': np.arange(50, 200, 50), 'max_depth': np.arange(2, 10, 2)}
         gbm_cv = GridSearchCV(gbm, param_grid=param_grid)
         gbm_cv.fit(X_tr, y_tr);
```

The results should be more or less comparable with RFs

```
In [23]: gbm_cv_pred_tr, gbm_cv_pred_ts = gbm_cv.predict(X_tr), gbm_cv.predict(X_ts)
         print(f'R2: {r2_score(y_tr, gbm_cv_pred_tr):.3} (training), {r2_score(y_ts, gbm_cv_pred_ts)
```

```
R2: 0.95 (training), 0.748 (test)
```

...But the optimal are very different!

```
In [24]: print(f'Best results with: {gbm_cv.best_params_}')
```

```
Best results with: {'max_depth': 4, 'n_estimators': 50}
```

Gradient Boosted Trees

GBTs use multiple trees, like RFs, but operate very differently

Random Forests need to be deep in order to be expressive

- Since all trees trying to learn the same input-output relation
- Depth is needed to capture complexity

Gradient Boosted Trees have an innate mechanism (summation) to:

- Counter overfitting
- and improve expressivity

As a result, individual trees in GBT can be much shallower

- Typically shallow trees tend to work better

What works best between RFs and GBTs is application-dependent

...But both are among the best ML models for tabular datasets!