Regression Trees

Decision Trees for Regression

Decision Trees can be used for Regression, in which case:

- Leaves are labeled with the mean of the associated examples:

$$\text{mean}(y) = \frac{1}{n}\sum_{j=1}^{n} y_j$$

- We split so as to reduce the weighed variance:

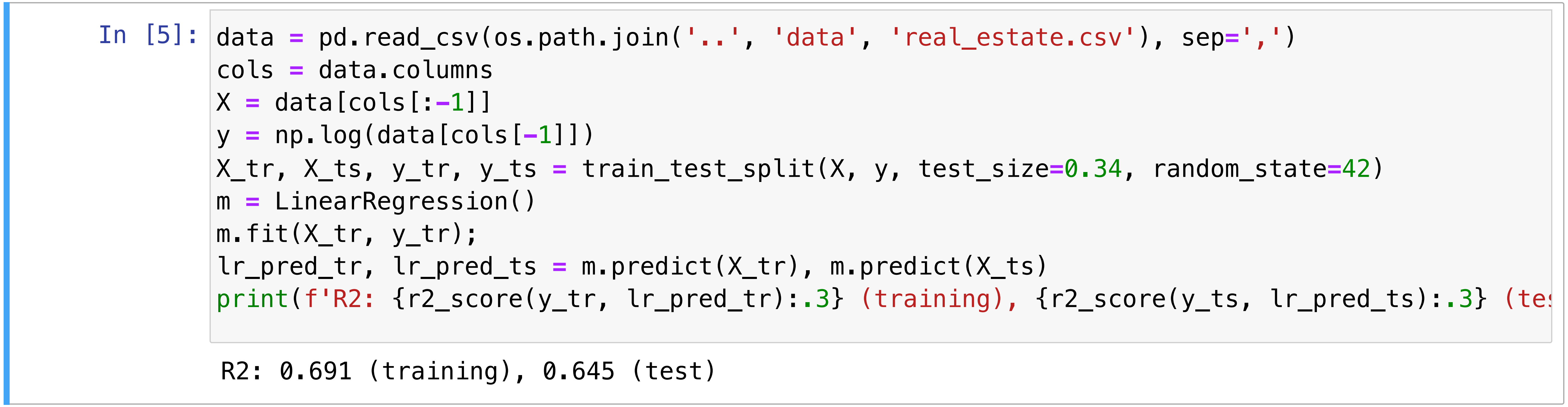
$$\frac{|y_{x_j \le \theta}|}{|y|}\text{Var}(y_{x_j \le \theta}) + \frac{|y_{x_j > \theta}|}{|y|}\text{Var}(y_{x_j > \theta})$$

$$\text{with: } \text{Var}(y) = \frac{1}{n}\sum_{j=1}^{n}(y_j - \text{mean}(y))^2$$

A Practical Example

We will apply DT regression to the housing price dataset

...But first, let's repeat our Linear Regression approach as a baseline:



In [5]:

```
data = pd.read_csv(os.path.join('..', 'data', 'real_estate.csv'), sep=',')
cols = data.columns
X = data[cols[:-1]]
y = np.log(data[cols[-1]])
X_tr, X_ts, y_tr, y_ts = train_test_split(X, y, test_size=0.34, random_state=42)
m = LinearRegression()
m.fit(X_tr, y_tr);
lr_pred_tr, lr_pred_ts = m.predict(X_tr), m.predict(X_ts)
print(f'R2: {r2_score(y_tr, lr_pred_tr):.3} (training), {r2_score(y_ts, lr_pred_ts):.3} (tes
```

```
R2: 0.691 (training), 0.645 (test)
```

We will attempt to improve over these results

A Practical Example

We proceed as usual for scikit learn

First we build a model object:

```
In [6]: from sklearn.tree import DecisionTreeRegressor
        rtm = DecisionTreeRegressor()
```

Then we call the `fit` method:

```
In [7]: rtm.fit(X_tr, y_tr);
```

...And finally we evaluate the performance:

```
In [8]: rtm_pred_tr, rtm_pred_ts = rtm.predict(X_tr), rtm.predict(X_ts)
        print(f'R2: {r2_score(y_tr, rtm_pred_tr):.3} (training), {r2_score(y_ts, rtm_pred_ts):.3} (
```

```
R2: 0.994 (training), 0.655 (test)
```

Non-Linear Estimators

The performance gap is very significant

...At least on the training set

- This happens even if DTs are training using a greedy heuristic
- ...While Linear Regression is trained to optimality

The difference is due to non-linearity

Linear Regression can capture only linear input-output correlations

- We need careful feature engineering to handle non-linearity
- ...And still we cannot easily capture non-linar over multiple attributes

Decisition Trees have no such restriction

- By partitioning the training data
- ...They can learn an any piecewise constant input-output relation

Overfitting Issues

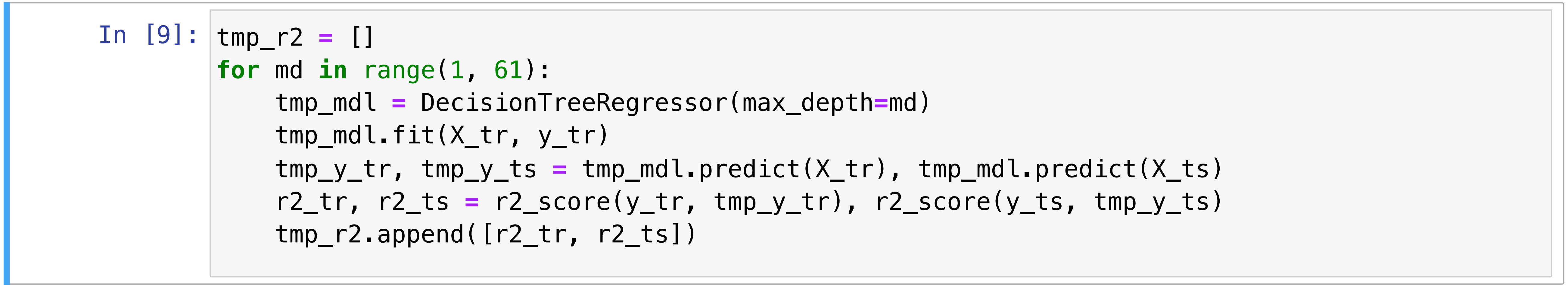
That said, our test-set result are not so go: we have a lot of overfitting

This is typical with all simple Decision Tree models

- DTs are very expressive models (often too much!)
- So, we could mitigate the issue by reducing how expressive they are

Typically, we play with the termination condition

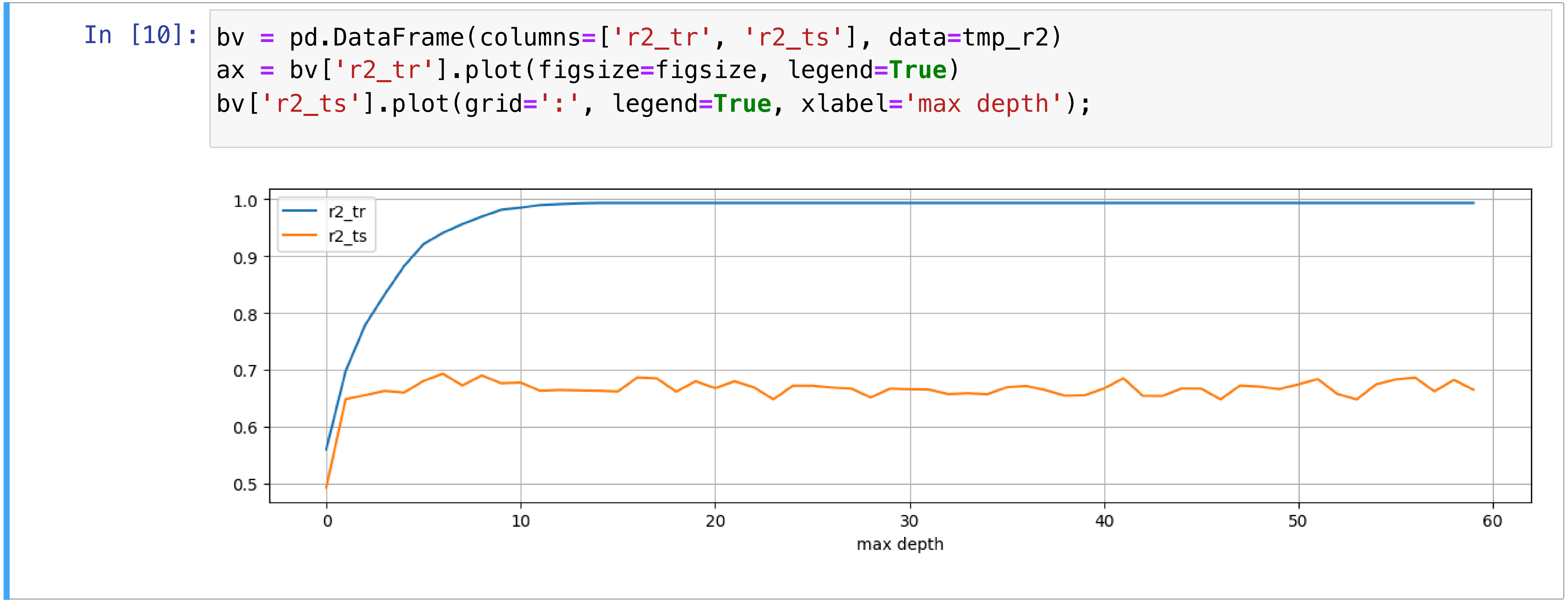
- Let's try controlling the maximum tree depth
- ...And see what kind of results we get on the training and test set



```
In [9]: tmp_r2 = []
        for md in range(1, 61):
            tmp_mdl = DecisionTreeRegressor(max_depth=md)
            tmp_mdl.fit(X_tr, y_tr)
            tmp_y_tr, tmp_y_ts = tmp_mdl.predict(X_tr), tmp_mdl.predict(X_ts)
            r2_tr, r2_ts = r2_score(y_tr, tmp_y_tr), r2_score(y_ts, tmp_y_ts)
            tmp_r2.append([r2_tr, r2_ts])
```

Bias vs Variance

Let's plot the R2 values over maximum depth



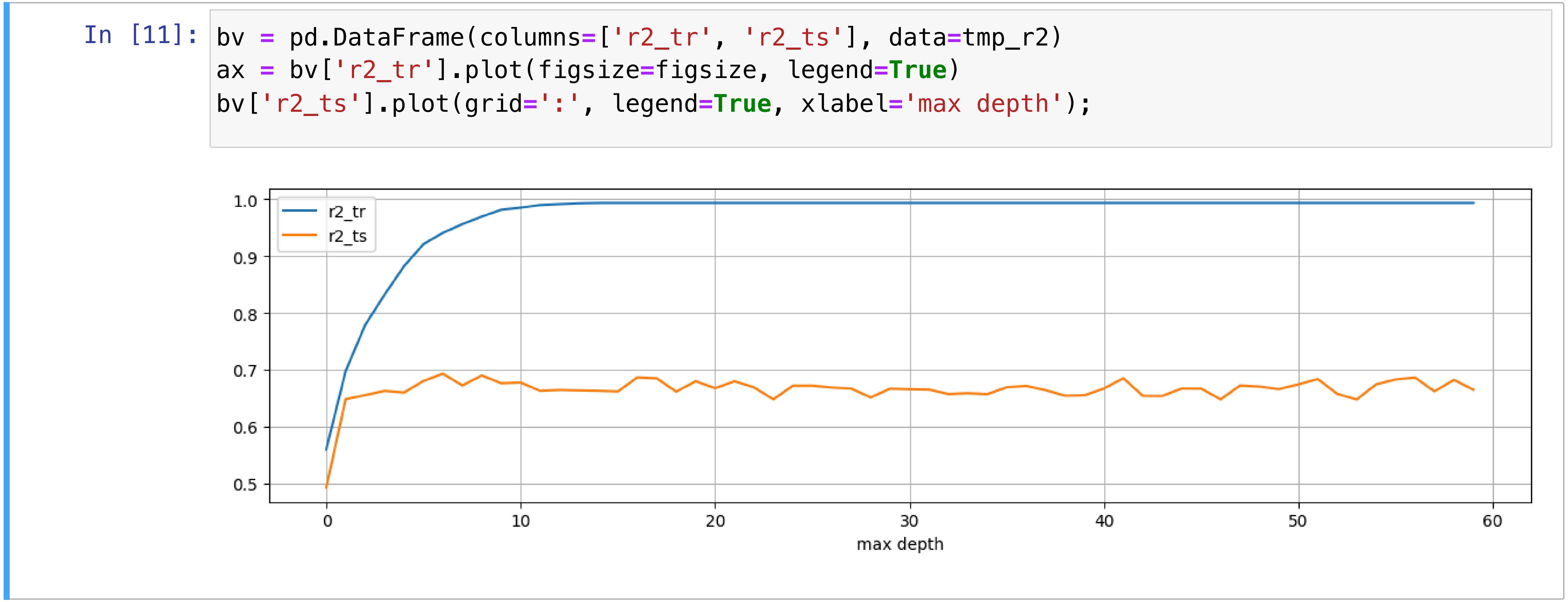
In [10]:

```
bv = pd.DataFrame(columns=['r2_tr', 'r2_ts'], data=tmp_r2)
ax = bv['r2_tr'].plot(figsize=figsize, legend=True)
bv['r2_ts'].plot(grid=':', legend=True, xlabel='max depth');
```

- Low-depth trees are less capable of learning the I/O map from the training data
- ...But they have more consistent results on unseen examples

Bias vs Variance

Let's plot the R2 values over maximum depth



In [11]:

```
bv = pd.DataFrame(columns=['r2_tr', 'r2_ts'], data=tmp_r2)
ax = bv['r2_tr'].plot(figsize=figsize, legend=True)
bv['r2_ts'].plot(grid=':', legend=True, xlabel='max depth');
```

- High-depth trees can learn the I/O map from the training data
- ...But they become noisy (or even perform worse!) on unseen examples

Bias vs Variance

We call:

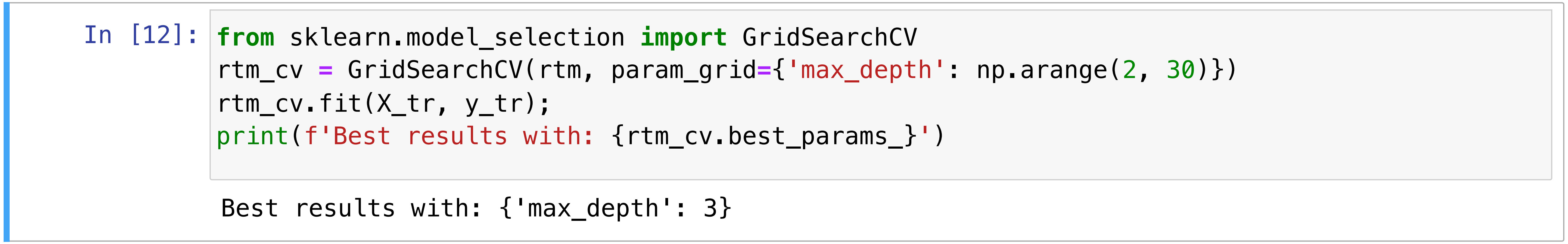
- Bias the tendency of an ML model to behave in a certain, stable way
- Variance the ability to change the output rapidly with input changes

Low-depth leads to higher bias and lower variance (and vice-versa)

Depth optimization with DTs is usually a good idea

...Just don't use the test set for that

- Use cross-validation instead!
- For the optimization part, we will use a simple grid search



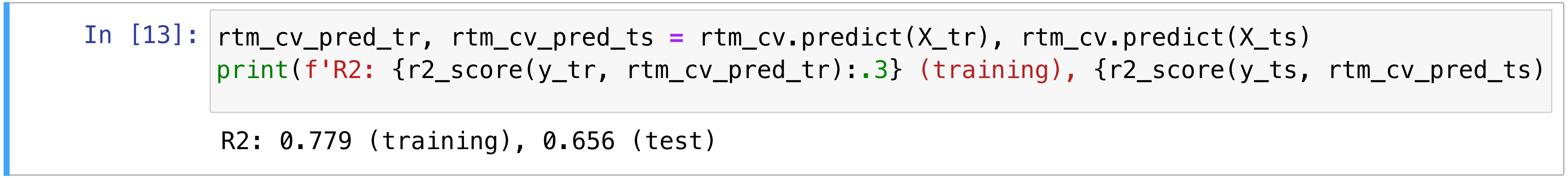
```
In [12]: from sklearn.model_selection import GridSearchCV
         rtm_cv = GridSearchCV(rtm, param_grid={'max_depth': np.arange(2, 30)})
         rtm_cv.fit(X_tr, y_tr);
         print(f'Best results with: {rtm_cv.best_params_}')
```

```
Best results with: {'max_depth': 3}
```

Results for the Calibrated DT

Let's check the results for our calibrated DT

We can obtain them directly from the `GridSearchCV` object



```
In [13]: rtm_cv_pred_tr, rtm_cv_pred_ts = rtm_cv.predict(X_tr), rtm_cv.predict(X_ts)
         print(f'R2: {r2_score(y_tr, rtm_cv_pred_tr):.3} (training), {r2_score(y_ts, rtm_cv_pred_ts)

         R2: 0.779 (training), 0.656 (test)
```

We have less overfitting, but the results are also slighly worse

The reason is in the bias/variance link

- DTs are very prone to overfitting
- We can increase their bias to reduce that risk
- ...But typically that has also a big impact on variance

In summary, using simple DTs there is no easy fix for this issue