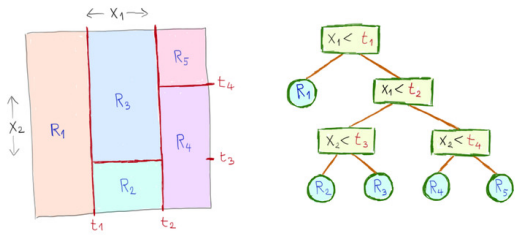
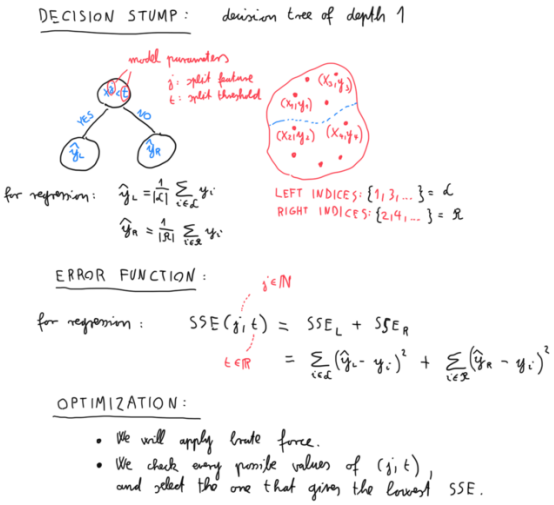
Decision Tree (https://en.wikipedia.org/wiki/Decision_tree_learning)

The decision tree is an old, but still relevant nonlinear learning algorithm. The leaves of the tree represent distinct subsets of the training data. The other nodes compare a given attribute to a threshold value (e.g. is the body temperature > 37 °C). The branches starting from the node are associated with the two possible outcomes of the comparison.



In this notebook, we will prepare the simplest version of the decision tree called decision stump (https://en.wikipedia.org/wiki/Decision_stump), and we will test it on the Boston Housing data set. Moreover, we will explore the capabilities of scikit-learn's decision tree algorithm.



Exercise 2: Implement the training of the decision stump regressor from scratch, and measure the model's root mean squared error (RMSE) on the full Boston Housing data set!

In [1]:

```
# Loading the data.
import pandas as pd
names = ['CRIM', 'ZN', 'INDUS', 'CHAS', 'NOX', 'RM', 'AGE',
         'DIS', 'RAD', 'TAX', 'PTRATIO', 'LSTAT', 'MEDV']
df = pd.read_csv('housing_data.txt', delim_whitespace=True, names=names)
X = df[df.columns[:-1]].values # input matrix
y = df['MEDV'].values          # target vector
```

In [2]:

```
X.shape
```

Out[2]:

```
(506, 12)
```

In [3]:

```
y.shape
```

Out[3]:

```
(506,)
```

In [4]:

```
# Training algorithm.
import numpy as np

n, d = X.shape

sse_min = np.inf

for j in range(d): # iterate over all feature
    x = X[:,j] # select j.th column

    # sort x and y by x
    idxs = x.argsort()
    x_sorted = x[idxs]
    y_sorted = y[idxs]

    # find optimal threshold value
    for i in range(n-1):
        t = (x_sorted[i] + x_sorted[i+1]) /2
        yhat_L = y_sorted[:(i+1)].mean() # preduction for left branch
        yhat_R = y_sorted[(i+1):].mean() # preduction for left branch
        sse_L = ((y_sorted[:(i+1)] - yhat_L)**2).sum()
        sse_R = ((y_sorted[(i+1):] - yhat_R)**2).sum()
        sse = sse_L + sse_R # sum of sequared errors
        # instead of re-computing SSE, updating it would be more efficiant
        if sse < sse_min:
            sse_min = sse
            t_opt = t
            j_opt = j
            print(j, t, sse)
```

```
0 0.007690000000000001 42714.138495049505
0 0.01001 42654.06214285715
0 0.01306 42607.60066733068
0 0.013354999999999999 42487.76150099801
0 0.014065 42237.84195247638
0 0.014355 42153.999678714856
0 0.014700000000000001 42111.73079365079
0 0.015195 41739.21143434343
0 0.016235 41403.70269905533
0 0.017435 41349.519812763305
0 0.01824 41236.26263646922
0 0.01958 41205.95119132654
0 0.020319999999999998 40890.95242258652
0 0.02182 40635.159448559665
0 0.023425 40556.32548257241
0 0.03393 40547.17303427895
0 0.035235 40380.59639339103
0 0.035809999999999995 40254.02162255965
0 0.03637 40253.174434710054
```

In [5]:

```
j_opt, t_opt, sse_min
```

Out[5]:

```
(5, 6.941, 23376.74038861689)
```

Exercise 3: Repeat the previous experiment using scikit-learn!

In [6]:

```
from sklearn.tree import DecisionTreeRegressor
```

In [7]:

```
cl = DecisionTreeRegressor(max_depth=1)
cl.fit(X,y)
```

Out[7]:

```
DecisionTreeRegressor
DecisionTreeRegressor(max_depth=1)
```

In [8]:

```
# Internal parameters of the trained model (.tree_.{feature, threshold, value})
print(cl.tree_.feature)
print(cl.tree_.threshold)
print(cl.tree_.value)
```

```
[ 5 -2 -2]
[ 6.94099998 -2.         -2.        ]
[[[22.53280632]]

 [[19.93372093]]

 [[37.23815789]]]
```

Execrice 4: Apply 3-fold cross-validation!

In [9]:

```
from sklearn.model_selection import KFold
from sklearn.metrics import mean_squared_error

re = DecisionTreeRegressor(max_depth=1)
cv = KFold(3, random_state=42, shuffle=True)

scores = []
for tr, te in cv.split(X):
    re.fit(X[tr], y[tr])
    yhat = re.predict(X)
    rmse = (mean_squared_error(y[te], yhat[te]))**0.5
    scores.append(rmse)

np.mean(scores)
```

Out[9]:

```
7.435013307929704
```

In [10]:

```
def evaluate(re, X, y):
    cv = KFold(3, random_state=42, shuffle=True)
    scores = []
    for tr, te in cv.split(X):
        re.fit(X[tr], y[tr])
        yhat = re.predict(X)
        rmse = (mean_squared_error(y[te], yhat[te]))**0.5
        scores.append(rmse)
    return np.mean(scores)
```

In [11]:

```
evaluate(DecisionTreeRegressor(max_depth=1), X, y)
```

Out[11]:

```
7.4350133079297045
```

In [12]:

```
def evaluate(re, X, y):
    cv = KFold(3, random_state=42, shuffle=True)
    scores_te = []
    scores_tr = []
    for tr, te in cv.split(X):
        re.fit(X[tr], y[tr])
        yhat = re.predict(X)
        scores_tr.append((mean_squared_error(y[tr], yhat[tr]))**0.5)
        scores_te.append((mean_squared_error(y[te], yhat[te]))**0.5)
    return np.mean(scores_tr), np.mean(scores_te)
```

In [ ]:

```

```

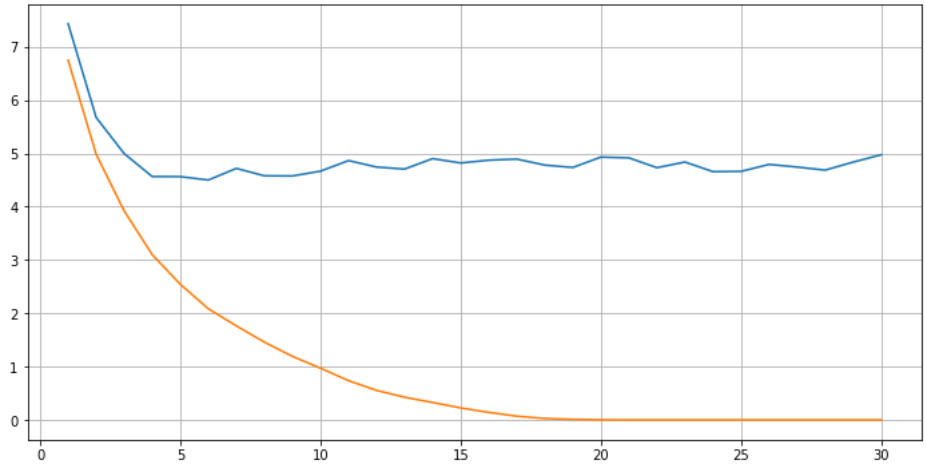
Exercise 5: Determine what maximal depth gives the lowest RMSE!

In [13]:

```
# loop over different max_depth values...
n = 30
rmse_te = dict()
rmse_tr = dict()

for i in range(n):
    a,b = evaluate(DecisionTreeRegressor(max_depth=i+1), X, y)
    rmse_tr[i+1] = a
    rmse_te[i+1] = b
```

In [14]:

```
# plot training and test RMSE as a function of max_depth
# select the max_depth that gives the lowest test RMSE

import matplotlib.pyplot as plt

plt.figure(figsize=(12, 6))
plt.plot(list(rmse_te.keys()), list(rmse_te.values()))
plt.plot(list(rmse_tr.keys()), list(rmse_tr.values()))
plt.grid(True)
```

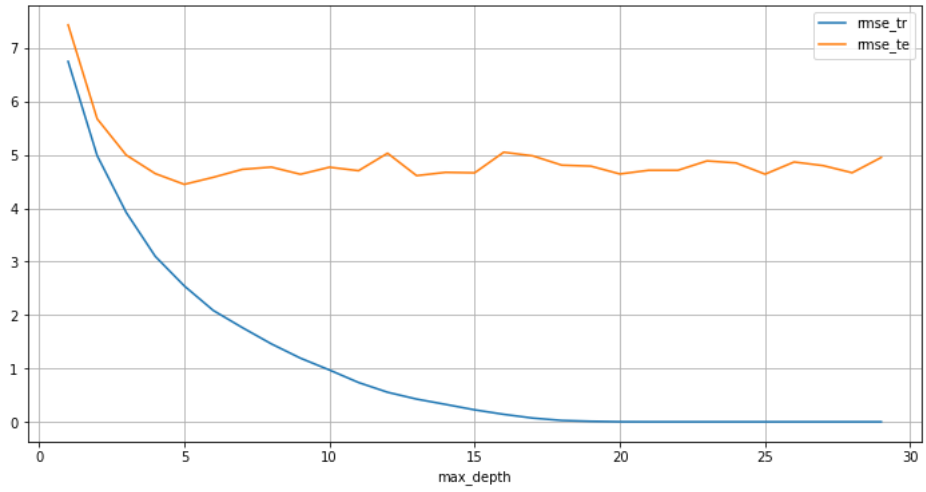


In [15]:

```
# Professor solution
res = []
for max_depth in range(1, 30):
    rmse_tr, rmse_te = evaluate(DecisionTreeRegressor(max_depth=max_depth), X, y)
    res.append({
        'max_depth': max_depth,
        'rmse_tr': rmse_tr,
        'rmse_te': rmse_te
    })

df_res = pd.DataFrame(res).set_index('max_depth')
df_res.plot(figsize=(12, 6), grid=True)
```

Out[15]:

```
<AxesSubplot: xlabel='max_depth'>
```



In [16]:

```
# Optimal max_depth.
df_res['rmse_te'].idxmin()
```

Out[16]:

```
5
```

In [ ]:

```

```

Exercise 6: Train a decision tree of depth 3 and visualize the trained model!

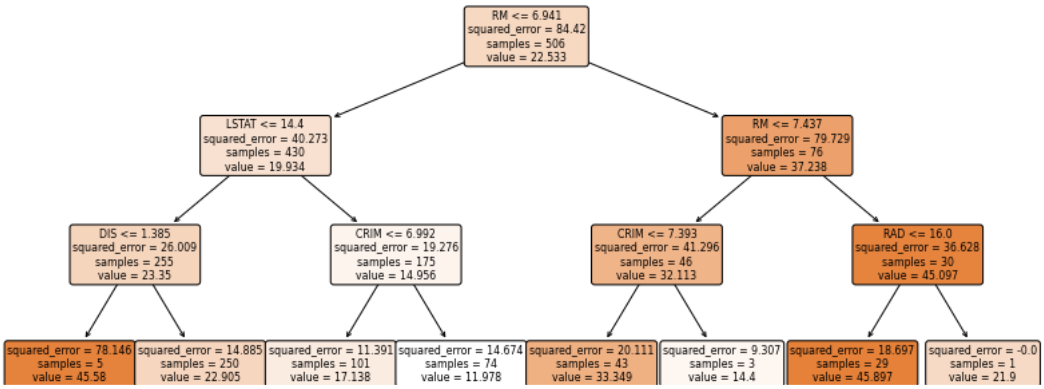
In [17]:

```
from sklearn.tree import plot_tree
import matplotlib.pyplot as plt
```

In [18]:

```
re = DecisionTreeRegressor(max_depth=3)
re.fit(X ,y)
plt.figure(figsize=(14, 6))
plot_tree(re, rounded=True, filled=True, feature_names=names)
```

```
 Text(0.9375, 0.125, 'squared_error = -0.0\nsamples = 1\nvalue = 21.9')]
```



In [19]:

```
# Number of parameters in the tree.
(re.tree_.feature >= 0).sum() * 2
```

Out[19]:

```
14
```

In [20]:

```
# Total size of the set
X.shape[0] * (X.shape[1]+1)
```

Out[20]:

```
6578
```

In [21]:

```
re.tree_.threshold
```

Out[21]:

```
array([ 6.94099998, 14.4000001 ,  1.38484997, -2.        , -2.        ,
        6.99237013, -2.        , -2.        ,  7.43700004,  7.39342499,
       -2.        , -2.        , 16.        , -2.        , -2.        ])
```

In [22]:

```
re.tree_.feature
```

Out[22]:

```
array([ 5, 11,  7, -2, -2,  0, -2, -2,  5,  0, -2, -2,  8, -2, -2],
      dtype=int64)
```

Decision Trees for Classification

- Decision trees can also be applied to classification problems.
- The necessary modification is that instead of sum of squared error, a different split criterion should be applied (e.g. misclassification count, Gini impurity (https://en.wikipedia.org/wiki/Decision_tree_learning#Gini_impurity), information gain (https://en.wikipedia.org/wiki/Decision_tree_learning#Information_gain)), and the leaf predictions should be changed to class probabilities.
- Decision trees can handle multiclass problems too.

Exercise 7: Apply a decision tree classifier for the Wisconsin Breast Cancer data set! Use 5-fold cross-validation! The evaluation metric should be the ratio of correct classifications. Determine the maximal depth that gives the highest accuracy! Compare the best decision tree against logistic regression!

In [23]:

```
# Load the data to DataFrame.
import pandas as pd
names = [
    'Sample_code_number', 'Clump_Thickness', 'Uniformity_of_Cell_Size',
    'Uniformity_of_Cell_Shape', 'Marginal_Adhesion', 'Single_Epithelial_Cell_Size',
    'Bare_Nuclei', 'Bland_Chromatin', 'Normal_Nucleoli', 'Mitoses', 'Class'
]
df = pd.read_csv('wisconsin_data.txt', sep=',', names=names, na_values='?')
df['Bare_Nuclei'].fillna(0, inplace=True)
df.head()
```

Out[23]:

	Sample_code_number	Clump_Thickness	Uniformity_of_Cell_Size	Uniformity_of_Cell_Shape	Marginal_Adhesion	Single_Epithelial_Cell_Size	Bare_Nuclei
0	1000025	5	1	1	1	2	1.0
1	1002945	5	4	4	5	7	10.0
2	1015425	3	1	1	1	2	2.0
3	1016277	6	8	8	1	3	4.0
4	1017023	4	1	1	3	2	1.0

In [24]:

```
# Input matrix.
X = df[names[1:-1]].values
X.shape
```

Out[24]:

```
(699, 9)
```

In [25]:

```
# Target vector.
y = df['Class'].values // 2 -1
```

In [26]:

```
from sklearn.tree import DecisionTreeClassifier
from sklearn.metrics import accuracy_score
from sklearn.model_selection import KFold
```

In [27]:

```
# Model evaluation function.
def evaluate(cl, X, y):
    cv = KFold(5, random_state=42, shuffle=True)

    scores_tr = []
    scores_te = []
    for tr, te in cv.split(X):
        cl.fit(X[tr], y[tr])
        yhat = cl.predict(X)
        scores_tr.append(accuracy_score(y[tr], yhat[tr]))
        scores_te.append(accuracy_score(y[te], yhat[te]))

    return np.mean(scores_tr), np.mean(scores_te)
```

In [28]:

```
evaluate(DecisionTreeClassifier(max_depth=1), X, y)
```

Out[28]:

```
(0.9288250702785585, 0.8941212744090441)
```

In [ ]:

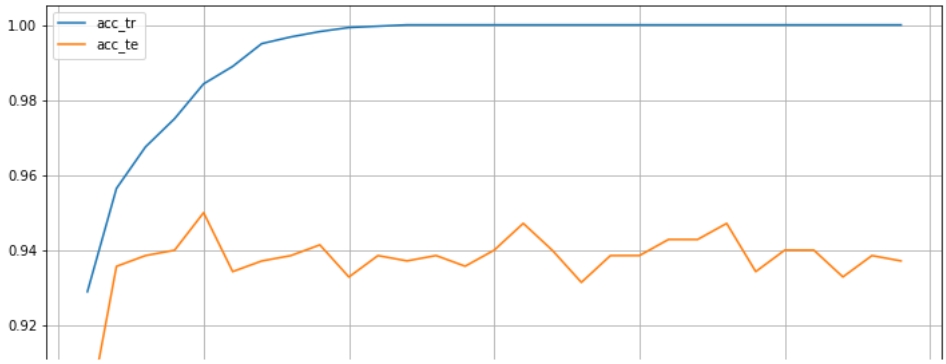
```
```

In [29]:

```
# Trying different max_depth values.
res = []
for max_depth in range(1, 30):
    acc_tr, acc_te = evaluate(DecisionTreeClassifier(max_depth=max_depth), X, y)
    res.append({
        'max_depth': max_depth,
        'acc_tr': acc_tr,
        'acc_te': acc_te
    })

df_res = pd.DataFrame(res).set_index('max_depth')
df_res.plot(figsize=(12, 6), grid=True)
```

Out[29]:

```
<AxesSubplot: xlabel='max_depth'>
```



In [30]:

```
# Optimal max_depth.
df_res['acc_te'].idxmax()
```

Out[30]:

```
5
```

In [31]:

```
df_res.loc[8]
```

Out[31]:

```
acc_tr    0.996783
acc_te    0.938448
Name: 8, dtype: float64
```

In [32]:

```
# Comparison to logistic regression.

from sklearn.linear_model import LogisticRegression
evaluate(LogisticRegression(), X, y)
```

Out[32]:

```
(0.9703136979299771, 0.9627954779033916)
```

In [33]:

```
# Another compartion with Linear regression

# Loading the data.
import pandas as pd
names = ['CRIM', 'ZN', 'INDUS', 'CHAS', 'NOX', 'RM', 'AGE',
         'DIS', 'RAD', 'TAX', 'PTRATIO', 'LSTAT', 'MEDV']
df = pd.read_csv('../_data/housing_data.txt', delim_whitespace=True, names=names)
X = df[df.columns[:-1]].values # input matrix
y = df['MEDV'].values          # target vector
```

In [34]:

```
from sklearn.model_selection import KFold
from sklearn.metrics import mean_squared_error

def evaluate(re, X, y):
    cv = KFold(3, random_state=42, shuffle=True)

    scores_tr = []
    scores_te = []
    for tr, te in cv.split(X):
        re.fit(X[tr], y[tr])
        yhat = re.predict(X)
        scores_tr.append(mean_squared_error(y[tr], yhat[tr])**0.5)
        scores_te.append(mean_squared_error(y[te], yhat[te])**0.5)

    return np.mean(scores_tr), np.mean(scores_te)

evaluate(DecisionTreeRegressor(max_depth=1), X, y)
```

Out[34]:

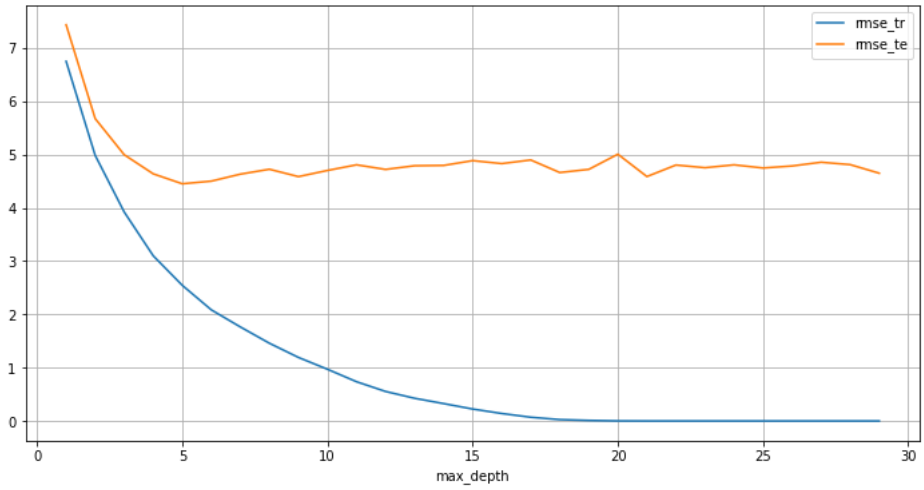
```
(6.748971341330223, 7.4350133079297045)
```

In [35]:

```
res = []
for max_depth in range(1, 30):
    rmse_tr, rmse_te = evaluate(DecisionTreeRegressor(max_depth=max_depth), X, y)
    res.append({
        'max_depth': max_depth,
        'rmse_tr': rmse_tr,
        'rmse_te': rmse_te
    })

df_res = pd.DataFrame(res).set_index('max_depth')
df_res.plot(figsize=(12, 6), grid=True)
```

Out[35]:

```
<AxesSubplot: xlabel='max_depth'>
```



In [36]:

```
# Optimal max_depth.
df_res['rmse_te'].idxmin()
```

Out[36]:

```
5
```

In [37]:

```
df_res.loc[df_res['rmse_te'].idxmin()]
```

Out[37]:

```
rmse_tr    2.545337
rmse_te    4.451221
Name: 5, dtype: float64
```

In [38]:

```
# Comparison against ridge regression.
from sklearn.linear_model import Ridge
evaluate(Ridge(), X, y)
```

Out[38]:

```
(4.736093991350386, 4.8792312907094795)
```

Decision Trees vs. Linear Models

Decision trees

- ...are insensitive to the scale of the input features 😀
- ...are easier to explain 😀
- ...can learn complex patterns 😀
- ...do not handle sparse data efficiently ☹
- ...tend to overfit more ☹

In [ ]:

```

```