Overview

This tutorial will focus on Linear Regression

We will include some additional topics, including:

- Basic formulation of supervised learning
- Basic linear regression model
- Train/test set split
- Evaluation of regression models

Overview

The lecture relies on the the following proficiencies and tools:

- Python programming
- Vector computations via the numpy module
- Data handling using the pandas module
- Plotting using matplotlib
- Training and using Machine Learning model via scikit-learn

You will need them only if you plan to handle these tasks yourself

Linear Regression

Loading the Data

Let's start by loading the housing dataset again

In [2]:
```
data = pd.read_csv('data/real_estate.csv', sep=',')
data.head() # Head returns the first 5 elements
```

Out[2]:

	house age	dist to MRT	#stores	latitude	longitude	price per area
0	14.8	393.2606	6	24.96172	121.53812	7.6
1	17.4	6488.0210	1	24.95719	121.47353	11.2
2	16.0	4066.5870	0	24.94297	121.50342	11.6
3	30.9	6396.2830	1	24.94375	121.47883	12.2
4	16.5	4082.0150	0	24.94155	121.50381	12.8

- Our goal is to learn a model that can estimate "price per area"
- But how do we achieve that?

The first step is using Maths to formalize the problem

Input, Output, Examples, Targets

Formally, we say that:

- All columns except the price represent the input x of our model
  - Inputs are often referred to as attributes
- The price represents the output y of our model
- Each row in the table represents one data point, i.e. an example $(\hat{x}_i, \hat{y}_i)$
  - $\hat{x}_i$ is the input value for the i-th example
  - $\hat{y}_i$ is the true output value (or target) for the i-th example

Our goal is to learn a model f such that

- When we feed the input $\hat{x}_i$ of each example to it
- ...The output value $y_i = f(\hat{x}_i)$ is as close as possible to $\hat{y}_i$

This kind of task is known in ML as supervised learning

Supervised Learning and Regression

Supervised Learning is among the most common forms of ML

Our model is a function $f(x, ; w)$ with input x and parameters w

- If the output is numeric, we speak of regression
- ...And we can define the approximation error over the example using, e.g.:

$$MSE(w) = \sum_{i=1}^{m} (f(x_i, ; w) - y_i)^2$$

- "MSE" stands for Mean Squared Error and it's a common error metric

Training in a (MSE) regression problem consists in solving

$$\text{argmin}_w \, MSE(w)$$

- I.e. choosing the parameters w to minimize approximation error

Supervised Learning...And Linear Regression

We speak instead of Linear Regression

...When f is defined as a linear combination of basis functions

$$f(x; w) = \sum_{i=1}^{n} w_j \phi_j(x)$$

In our case each basis function will correspond to a specific input column

$$f(x; w) = w_0\{\text{age}\} + w_1\{\text{MRT dist.}\} + w_2\{\text{\#stores}\} + \\ w_3\{\text{latitude}\} + w_4\{\text{longitude}\}$$

- This is a very common setup when using linear regression

Supervised Learning...And Linear Regression

We speak instead of Linear Regression

...When f is defined as a linear combination of basis functions

$$f(x; w) = \sum_{i=1}^{n} w_j \phi_j(x)$$

Linear regression is one of the simplest supervised learning approaches

...But it is still a very good example!

- Since the model itself is relatively simple
- ...It will allow us to focus on the key challenges when using ML

Separating Input and Output

Our first step will be separating our input and output

In [3]:
```
cols = data.columns
X = data[cols[:-1]] # all columns except the last one
display(X.head())
```

	house age	dist to MRT	#stores	latitude	longitude
0	14.8	393.2606	6	24.96172	121.53812
1	17.4	6488.0210	1	24.95719	121.47353
2	16.0	4066.5870	0	24.94297	121.50342
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We will focus on predicting the logarithm of the price per area

In [4]:
```
y = np.log(data[cols[-1]]) # just the last column
```

- In practice, it's like predicting the order of magnitude

Training and Test Set

The model we learn should work well on all relevant data

Formally, the model should generalize well

- How do we check whether this is the case?
- A typical approach: partitioning our dataset

The basic idea is to split our data in two groups

- The first group will actually be used for training
  - This will be called the training set
- The second group will be used only for model evaluation
  - This will be called the test set (or holdout set)

With this trick, we can assess our model performance on unseen data

Training and Test Set

There are a couple of catches

For this to work:

- The examples in the training set and the test set should be similar
- The test data should be a good match for the data we'll use for real

Ideally, we should have that:

The training data should be representative of the true population

This is the golden rule for building a training set

- Sometimes that's relatively easy to do
- ...But sometimes it may be difficult or impossible

Training and Test Set

In our case, we have a small problem

Our data is sorted by "price per area"

- So if we split our data sequentially in two groups
- ...We will train our model only on low prices
- ...And evaluate its performance only on higher prices

If we do it, the model will generalize poorly

How do we avoid this potential mistake?

Training and Test Set

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How do we avoid this potential mistake?

The solution is to shuffle the data before partitioning

- With this simple trick, the training and test distribution
- ...Are statistically guaranteed to be similar

Training and Test Set

As tool for learning our model, we will use scikit-learn

...Which provides a function to handle shuffling and training/test splitting:

```
In [5]: from sklearn.model_selection import train_test_split

        X_tr, X_ts, y_tr, y_ts = train_test_split(X, y, test_size=0.34, random_state=42)

        print(f'Size of the training set: {len(X_tr)}')
        print(f'Size of the test set: {len(X_ts)}')

        Size of the training set: 273
        Size of the test set: 141
```

The function `train_test_split`

- Randomly shuffles the data (optionally with a fixed seed `random_state`)
- Puts a fraction `test_size` of the data in the test set
- ...And the remaining data in the training set
- Both the input and the output data is processed in this fashion

Training and Test Set

Using separate test set is extremely important

...Because we want our model to work on new data

- We have no use for a model that learns the input data perfectly
- ...But that behaves poorly on unseen data
- In these cases, we say that the model does not generalize

By keeping a separate test set we can simulate this evaluation

However, beware of exception!

Sometimes, you it impossible to guarantee train/test similarity

- E.g. when making forecasts over time, the historical system behavior
- ...Can be different from the future system behavior
- In that case, the train/test split should simulate the expected difference

The trick is to think of what the train and test data will be at deployment time

Fitting the Model

We can now train a linear model

In [6]:
```
from sklearn.linear_model import LinearRegression

m = LinearRegression()
m.fit(X_tr, y_tr)
```

Out[6]:
```
LinearRegression()
```

We obtain the estimated output via the `predict` method:

In [7]:
```
y_pred_tr = m.predict(X_tr)
y_pred_ts = m.predict(X_ts)
```

- The predictions (unlike the targets) are not guaranteed to be integers
- ...But that is still fine, since it's easy to interpret them

Evaluation

Finally, we need to evaluate the prediction quality

A common approach is using metrics. Here are a few examples:

- The Mean Absolute Error is given by:

$$MAE = \frac{1}{m} \sum_{i=1}^{m} |f(x_i) - y_i|$$

- The Root Mean Squared Error is given by:

$$RMSE = \sqrt{\frac{1}{m} \sum_{i=1}^{m} (f(x_i) - y_i)^2}$$

Both the RMSE and MAE a simple error measures

Evaluation

- The coefficient of determination (R^2 coefficient) is given by:

$$R^2 = 1 - \frac{\sum_{i=1}^{m}(f(x_i) - y_i)^2}{\sum_{i=1}^{m}(y_i - \tilde{y})^2}$$

where $\tilde{y}$ is the average of the y values

The coefficient of determination is a useful, but more complex metric:

- Its maximum is 1: an $R^2 = 1$ implies perfect predictions
- Having a known maximum make the metric very readable
- It can be arbitrarily low (including negative)
- It can be subject to a lot of noise if the targets y have low variance

Using the MSE directly for evaluation is usually a bad idea

...Since it is a square, and therefore not easy to parse for a human

Evaluation

Let's see the values for our example

In [8]:
```python
from sklearn.metrics import r2_score, mean_absolute_error, mean_squared_error

print(f'MAE on the training data: {mean_absolute_error(y_tr, y_pred_tr):.3}')
print(f'MAE on the test data: {mean_absolute_error(y_ts, y_pred_ts):.3}')
print(f'RMSE on the training data: {np.sqrt(mean_squared_error(y_tr, y_pred_tr)):.3}')
print(f'RMSE on the test data: {np.sqrt(mean_squared_error(y_ts, y_pred_ts)):.3}')
print(f'R2 on the training data: {r2_score(y_tr, y_pred_tr):.3}')
print(f'R2 on the test data: {r2_score(y_ts, y_pred_ts):.3}')
```

```
MAE on the training data: 0.143
MAE on the test data: 0.177
RMSE on the training data: 0.207
RMSE on the test data: 0.253
R2 on the training data: 0.691
R2 on the test data: 0.645
```

- In general, we have better predictions on the training set than on the test set
- This is symptomatic of some overfitting
- I.e. we are learning patterns that don't translate to unseen data

Later on, we will see some techniques to deal with this situation

Evaluation

As an (important!) alternative to metrics, we can use scatter plots

We can show the true vales on the x-axis, the predictions on the y-axis

In [9]:
```
plt.figure(figsize=figsize)
plt.scatter(y_ts, y_pred_ts, alpha=0.2)
plt.plot(plt.xlim(), plt.ylim(), linestyle=':', color='tab:orange')
plt.tight_layout(); plt.grid(':')
```

A Jupyter widget could not be displayed because the widget state could not be found. This could happen if the kernel storing the widget is no longer available, or if the widget state was not saved in the notebook. You may be able to create the widget by running the appropriate cells.

This gives us a better idea of which kind of mistakes the model is making

Conclusions and Take-Home Messages

- Basic formulation of supervised learning
  - I.e. learning a model from available examples
  - ...When the examples contain values for both the input and the output
- Basic linear regression model
  - One the simplest approaches for supervised learning
  - I.e. the output is a linear combination of the input values
  - Regression = we estimate a numeric quantity
- Train/test set split
  - Needed to evaluate our model on unseen data (generalization)
- Evaluation of regression models
  - Make sure to compare the performance on both training and test data
  - Metrics (e.g. RMSE, MAE) provide a compact evaluation
  - Scatter plot for a more fine-grained evaluation