Modeling tasks and first approaches

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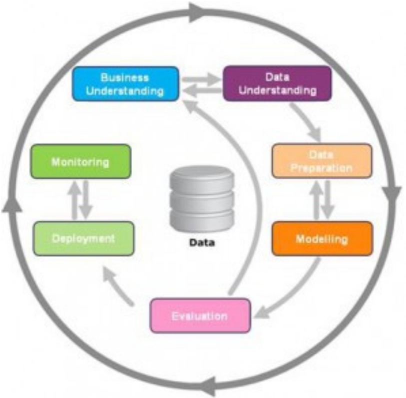
Back to CRISP-DM

- The first phases of CRISP-DM
  - Business Understanding
  - Data Understanding
  - Data Preparation
  - Modelling (or Modeling)



What is modeling?

- Reality
  - You **obtain** the selling price of a house or apartment
  - You also **know and can observe the house** by
    - inspection,
    - asking questions to neighbours,
    - looking at the floor plan,
    - seeing photos,
    - seeing its location, etc.

What is modeling?

- **Model** (in this case)
  - a **function** that given an objective description of a house or apartment gives you a specific value as an **estimation** of the value of the apartment.

What is modeling?

- **Model**
  - a useful **representation** of real entities or phenomena
  - often: a **mathematical object**
    - e.g., a function, an equation, logical formulae

What is modeling?

- **Model** in Machine Learning / Data Mining
  - Is obtained from **data**
    - often: **learned**
  - Using an **algorithm**
  - It can be used to solve specific **tasks**
    - prediction, classification, segmentation, association, recommendation
  - It **approximates** an observed phenomenon
  - It can be **evaluated**

Machine Learning tasks

- **Classification**
  - Given a sample of pairs $< Obj, Class >$, where
    - $Obj \in Objects$
    - $Class \in Classes$
  - obtain a function $f : Objects \rightarrow Classes$
- **Regression**
  - Given a sample of pairs $< Obj, Val >$, where
    - $Obj \in Objects$
    - $Val \in Values \subseteq \mathbb{R}$
  - obtain a function $f : Objects \rightarrow Values$

Machine Learning tasks

- **Supervised machine learning**
    - Classification and regression are supervised
    - Each object is **labeled** by a “teacher”
    - also called **directed machine learning**
- Other supervised ML **tasks**
    - Recommendation
    - Outlier detection (if examples are labeled)
    - (open)

Machine Learning tasks

- **Unsupervised machine learning**
  - Will be studied later
  - Examples have no labels
    - Most of the data
  - also called **undirected machine learning**
- Unsupervised ML **tasks**
  - Clustering
  - Dimensionality reduction
  - Discovering relevant patterns
  - Outlier detection (if examples are not labeled)
  - (open)

Learning tasks: an example

In a bank, the credit office needs routinely to decide if a loan can be given to the buyers of a house or apartment. The bank can never lend above the value of the house, so they have to decide what is its value. The office has access to thousands of records of houses and apartments that were sold in the market in the past. To alleviate the effort of the bank evaluation experts and reduce operational costs in 10%, management decided to obtain a model that can automatically evaluate a given house with enough precision.

- What is the **business problem**?
- What is the **machine learning problem**?
- What are the **business success criteria**?
- What are the **machine learning success criteria**?

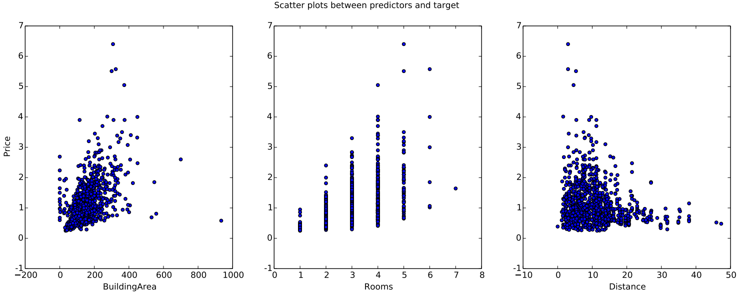
A regression example: data understanding

- Let's look at the data (using part of **Melbourne Housing** data set)
  - Predictors: **BuildingArea**, **Rooms** and **Distance**
  - Target: **Price** (Median value of homes)

	BuildingArea	Rooms	Distance
11039	144.0	3	4.5
9984	131.0	3	13.5
8259	67.0	1	8.8
9156	150.0	2	2.1
6567	87.0	2	8.7

A regression example: data understanding

- Can we predict *Price* from the predictors?
  - What do plots tell us?



A regression example: modeling: Linear Regression

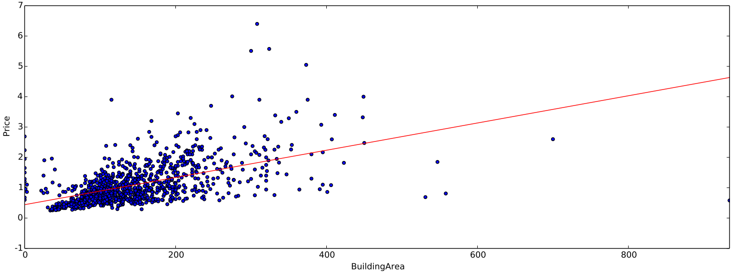
- We can obtain a **linear function** f from the data such that
  - $\widehat{Price} = f(BuildingArea, Rooms, Distance)$
  - that can be done using **Linear Regression**
- If we have m attributes

$$\hat{y} = f(x_1, x_2, \ldots, x_m) = \beta_0 + \sum_{i=1}^{m} \beta_i . x_i$$

- There is an **algorithm** that, given the data, finds the **parameters** β_i - it is based on a centuries old mathematical procedure

A regression example: modeling: Linear Regression

- Linear Regression
  - Let's visualize the effect of LR with one predictor: *BuildingArea*
  - This is called **simple regression**
  - The red line was **algorithmically** obtained from the data



A regression example: modeling: Linear Regression

- Linear Regression
    - Let's see the function obtained

```
Model slope:      4487.65167729

Model intercept: 441450.158562
```

$$\widehat{Price} = 44150.16 + 4487.65 \times BuildingArea$$

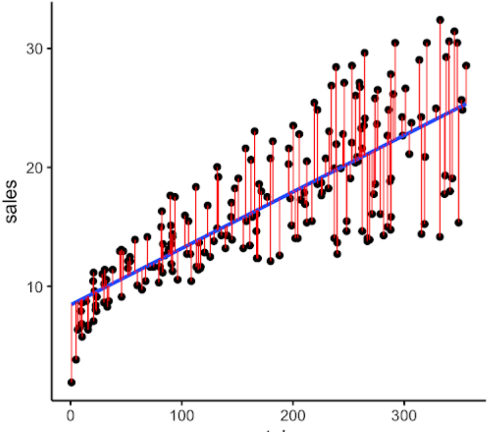
A regression example: modeling: Linear Regression

- Linear Regression
  - **how good** is the model?
  - we can measure R^2 (r-squared), a measure of **fit**
    - 0 is the worst fit (predicting average)
    - 1 is the best fit (got them all)
    - a low value indicates **underfit**
  - a fit well above 0 may be useful
    - depending on the problem
    - in this case it is above zero but not high

```
Model R2:      0.29210253038
```

A regression example: modeling: R squared

- What is R^2 measuring?
  - How much the predicted $\hat{y}$ are close to the actual y
  - The difference $e_i = \hat{y}_i - y_i$ is a **residual** or error
    - Best fit has $e_i = 0$ for all i



A regression example: modeling: R squared

- The **sum of the squares** of the residuals is a measure of total **error**

$$SS_{res} = \sum_{i=1}^{n} e_i^2$$

- We **normalize** this error with the error predicting the mean $SS_{tot} = \sum_{i=1}^{n}(y_i - \overline{y})^2$
- And subtract to 1

$$R^2 = 1 - \frac{SS_{res}}{SS_{tot}}$$

A regression example: modeling: multivariate regression

- Use more predictors
  - the prediction is now **hyperplane** on a 3 dimensional space
  - the value of R^2 increases considerably

```
LinearRegression(copy_X=True, fit_intercept=True, normalize=Fa
Predictors: ['BuildingArea', 'Rooms', 'Distance']
Coefficients (alphas):     [   2727.02768147  303464.96545695
Model intercept: 211030.895258
Model R2:     0.488415717231
```

Regression: finding the model

- The regression model is found **analytically**
  - $\overrightarrow{\beta} = [\ \beta_0, \beta_1, \ldots, \beta_m\ ]$
  - the i^{th} case is $x_i = [1, x_1^i, \ldots, x_m^i]$
  - then, we can use the dot product for estimating y_i

$$\hat{y}_i = \overrightarrow{\beta}.x_i$$

  - X is the $n \times (m+1)$ matrix of independent variables with a left column of 1s
  - Y is the $n \times 1$ matrix of target/dependent values

$$\overrightarrow{\beta} = (X^T X)^{-1} X^T Y$$

Regression: finding the model

- Where does this equation **come from**?
- Aim is to find β_i that **minimize** the squares of the residuals
  - **least squares** approach

$$\min_{\overrightarrow{\beta}} \sum_{i=1}^{n} (\overrightarrow{\beta}.x_i - y_i)^2$$

- by deriving and equaling to zero we get to the $\overrightarrow{\beta}$ equation

Regression: finding the model : complexity

- **Computational complexity** analysis
- How **hard** is it to compute the β_i ?
  - matrix multiplications can be $O(n.m^2)$
  - matrix **inversion** can be $O(m^3)$
- **not so bad**
  - linear with the number of cases (great)
  - problematic with many predictors (**usually** not a problem)

More on regression

- Lasso regression
- Ridge regression
- Polynomial regression
- Logistic regression

The nearest neighbor approach

- The aim of modeling is to **discover the hidden function** f
  - f is able to **estimate** the target y for new cases x
- Linear regression approach
  - f is **assumed** to have a linear form
  - all we have to find are the **parameters** β_i
  - they are found **analytically** from the data

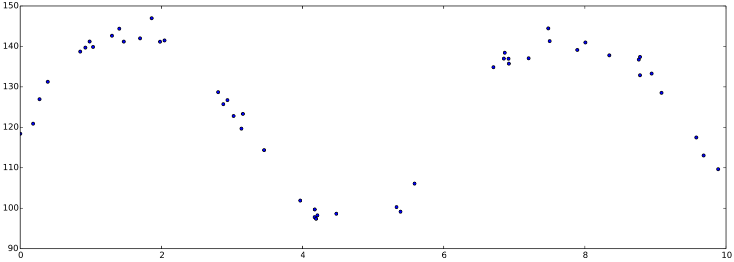
The nearest neighbor approach

- **Nearest neighbor** approach
  - f is assumed to be **locally smooth**
  - *nearby* cases tend have **similar values** for f
    - if $sim(x_1, x_2)$ is small then $f(x_1) \approx f(x_2)$
  - we can estimate $f(x)$ from the neighbors of x

The nearest neighbor approach

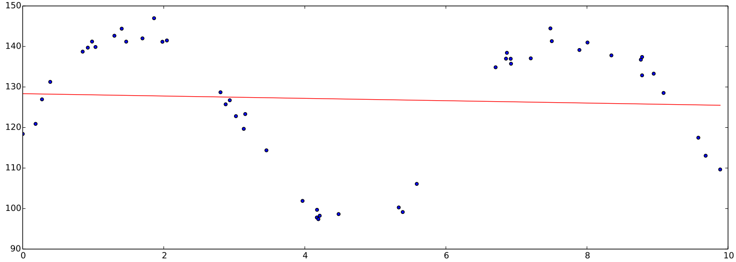
- Suppose we want to model the number of customers in a shop given the time of the day
  - These are the observations (the data)

```
(0, 10)
```



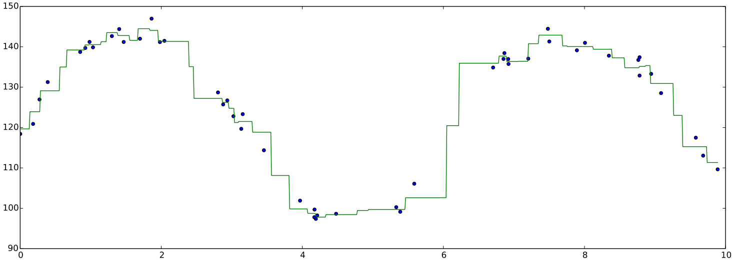
The nearest neighbor approach

- Linear regression **does not find** a good solution
  - the linear assumption is **too strong**



The nearest neighbor approach

- A nearest neighbour approach finds a **better** solution
  - using 2 nearest neighbors
  - the corresponding f adapts to the data
  - **be careful!** - it may **overfit**
    - in a future lecture we will see how to measure **overfitting**



The k nearest neighbor approach: kNN

- **Input**:
  - data X, y
  - parameter k, number of neighbors
  - distance measure d
  - new case x_{new}
- **Output**:
  - estimated value $\hat{y}(x_{new})$
- **Algorithm**:
  - calculate $d(x_i, x_{new})$ for each $x_i \in X$
  - obtain the k $x_{(1)}, \ldots, x_{(k)}$ points that minimize d
  - output $\hat{y}(x_{new}) = avg_i \;\; x_{(i)}$

The nearest neighbor approach

- no model is produced
  - **lazy** learning
    - only use the data when you have to predict
  - opposed to **eager** learning
    - build the model as soon as you have the data

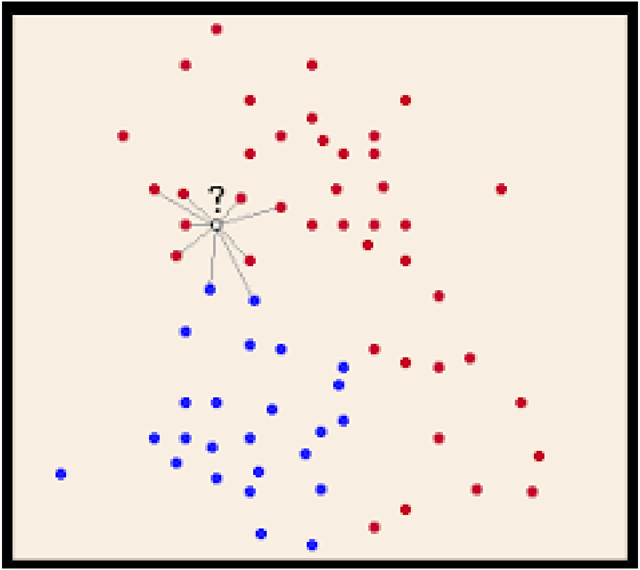
A classification example

- The kNN approach can also be used for **classification**
  - *The credit office of the bank also has records of previous loan applications and the outcome of the credit (payed with no difficulty, not an easy payment process). The aim is to find a model that automatically supports the decision of the bank credit office for loans*
- This is a **two class** problem
  - class1='easy', class2='difficult'

A classification example: kNN

- The kNN approach for **classification**
  - given a new application x_{new}
  - find the k applications closer to x_{new}
  - output the **majority** class in those cases

A classification example: kNN



Look ahead

- We will see other
  - ML methods for learning **classifiers**
  - ML methods for learning **regression models**
- Linear regression
  - *learns* by finding the values **analytically**
- kNN
  - *learns* by **memorizing** all the past data
- other methods
  - may use other strategies
    - mostly search and optimization

Relevant issues

- **Non-numerical** variables in regression
  - categorical can be binarized (dummy variables)
- The importance of **distance functions** in kNN
  - hybrid distances
- The importance of **normalization** in kNN
  - the $<$age,salary$>$ example
- How do these methods cope with **missing data**?
  - matrix operations
  - distance functions

References

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