Introduction to Machine Learning

Lecture 3: Regression

Alexis Zubiolo
alexis.zubiolo@gmail.com

Data Science Team Lead @ Adcash

November 3, 2016

Before we start

Would you be interested in a more advanced course? I can propose

- Machine learning from scratch (how to implement an ML algorithm with no library)
- A more advanced version of this course (with more theoretical technical details)
- Large-scale machine learning

Regression in Machine Learning

This lecture is about regression in Machine learning.

Reminder: In regression, the output y is **continous**.

Example:

- **Price estimation**: $y =$ price (*e.g.* 50000 BGN for a house)
- **Predicting the future** (*e.g.* weather forecast): $y =$ temperature or amount of rain

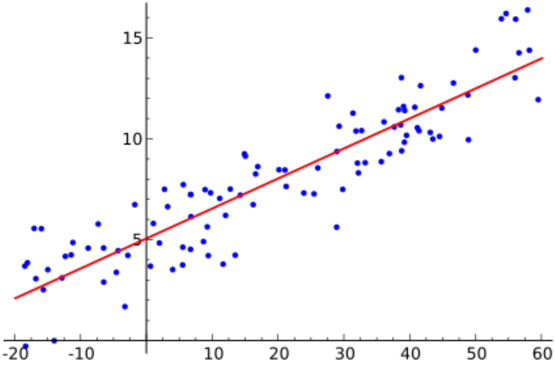
Regression in Machine Learning: Applications

Domains of application:

- Price estimation/prediction
- Weather forecast
- Production quantity estimation
- Stock option price prediction
- Fit statistical model to data
- Physics & chemistry
- . . . and others

Linear and polynomial regression

Purpose of regression: **approximate solutions** of **overdetermined systems**.



In this course, we will see

- Linear regression
- Polynomial regression

Linear regression

Linear regression

Principal components:

- Old problem (least-squares method usually credited to Carl Friedrich Gauss in 1795)
- Several ways to approximate the data
  - Linear model
  - Polynomial model (remember kernels from SVMs)
  - Fit a distribution
  - ...
- Several ways to formulate the problem
  - Least Squares
  - Support Vector regression
  - ...
- Several ways to solve the problem

Linear regression with ordinary least-squares

Linear regression: Estimate y as a **linear** function of x:

$$\hat{y} = w^T x$$

Least squares: Penalty (loss) is a **quadratic** function

$$\ell(\hat{y}, y) = (\hat{y} - y)^2$$

living area (m^2)	**# bedrooms**	price (1000's euros)
50	**1**	30
76	**2**	48
26	**1**	12
102	**3**	90

living area (m^2)	**# bedrooms**	price (1000's euros)
50	**1**	30
76	**2**	48
26	**1**	12
102	**3**	90
61	**2**	?

Variable standardization

Variables have various magnitudes. Example:

- Living area: Up to a few hundreds m^2
- Price: Up to a few 100 000s BGN (and even more)

This can be an issue when training a regression model.

Variable standardization

Variables have various magnitudes. Example:

- Living area: Up to a few hundreds m^2
- Price: Up to a few 100 000s BGN (and even more)

This can be an issue when training a regression model.

It is possible to calculate the **standard score** z of a variable x

$$z = \frac{x - \mu}{\sigma}$$

where

- μ is the mean of the variable
- σ is its standard deviation

Variable standardization

Variables have various magnitudes. Example:

- Living area: Up to a few hundreds m^2
- Price: Up to a few 100 000s BGN (and even more)

This can be an issue when training a regression model.

It is possible to calculate the **standard score** z of a variable x

$$z = \frac{x - \mu}{\sigma}$$

where

- μ is the mean of the variable
- σ is its standard deviation

Another option: Scale between 0 and 1

$$z = \frac{x - \mathrm{min}}{\mathrm{max} - \mathrm{min}}$$

Overfitting and underfitting

Illustration on a generated example: Try to fit the function

$$y = f(x) = \cos\left(\frac{3\pi}{2}x\right) + \text{noise}$$

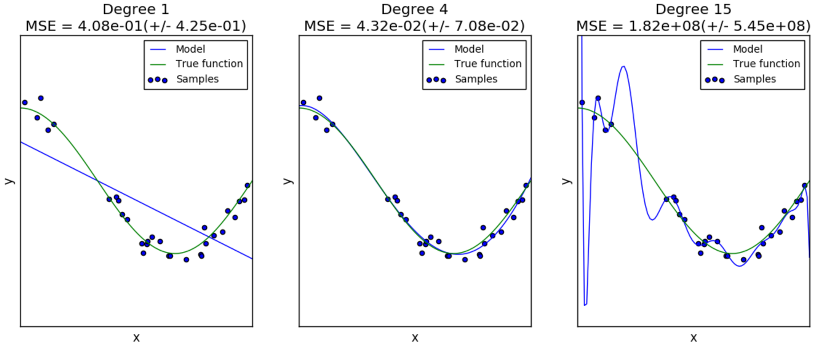
for $x \in [0, 1]$, with a polynomial regression

Overfitting and underfitting

Illustration on a generated example: Try to fit the function

$$y = f(x) = \cos\left(\frac{3\pi}{2}x\right) + \text{noise}$$

for $x \in [0, 1]$, with a polynomial regression



Parameter selection

As for classification models, parameter selection plays a key role in the regression performance:

- Degree of the polynomial
- Regularization parameter

Parameter selection

As for classification models, parameter selection plays a key role in the regression performance:

- Degree of the polynomial
- Regularization parameter

Optimal parameters can be chosen with cross-validation over a grid:

Parameter selection

As for classification models, parameter selection plays a key role in the regression performance:

- Degree of the polynomial
- Regularization parameter

Optimal parameters can be chosen with cross-validation over a grid:

- Split the data into train/test

Parameter selection

As for classification models, parameter selection plays a key role in the regression performance:

- Degree of the polynomial
- Regularization parameter

Optimal parameters can be chosen with cross-validation over a grid:

- Split the data into train/test
- Choose a degree $d \in \{1, \ldots, 20\}$

Parameter selection

As for classification models, parameter selection plays a key role in the regression performance:

- Degree of the polynomial
- Regularization parameter

Optimal parameters can be chosen with cross-validation over a grid:

- Split the data into train/test
- Choose a degree $d \in \{1, \ldots, 20\}$
- Train on the train set with this degree

Parameter selection

As for classification models, parameter selection plays a key role in the regression performance:

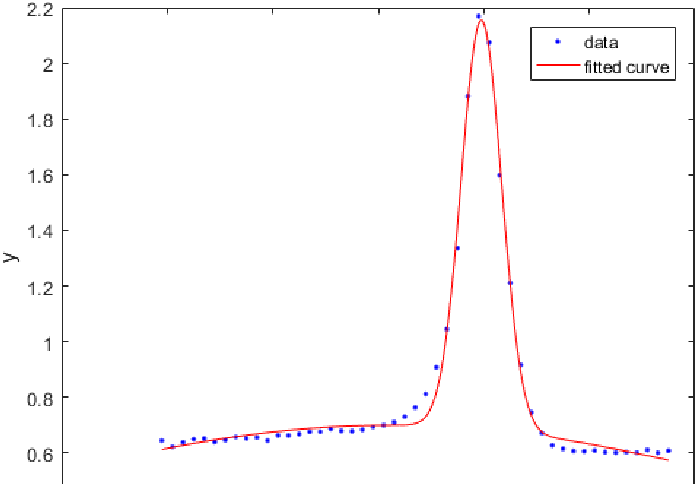
- Degree of the polynomial
- Regularization parameter

Optimal parameters can be chosen with cross-validation over a grid:

- Split the data into train/test
- Choose a degree $d \in \{1, \ldots, 20\}$
- Train on the train set with this degree
- Test the model on the test set

Fitting a distribution

$$\hat{y} = f(x) = Ae^{\dfrac{(x - x_0)^2}{2\sigma^2}}$$



Alternatives to least squares

It is possible to use a different loss function ℓ. Remember, we had

$$\ell\left(\hat{y}, y\right) = \left(\hat{y} - y\right)^2$$

Alternatives to least squares

It is possible to use a different loss function ℓ. Remember, we had

$$\ell\left(\hat{y}, y\right) = \left(\hat{y} - y\right)^2$$

We can use **support vector machines for regression** (SVR):

- If **within the margin** (*i.e.* $-\epsilon \leq \hat{y} - y \leq +\epsilon$) then **no penalty**
- linear or quadratic **penalty outside the margin**

(see flip-chart for illustration)

This loss function is called ϵ-insensitive.

Alternatives to least squares

It is possible to use a different loss function ℓ. Remember, we had

$$\ell\left(\hat{y}, y\right) = \left(\hat{y} - y\right)^2$$

We can use **support vector machines for regression** (SVR):

- If **within the margin** (*i.e.* $-\epsilon \leq \hat{y} - y \leq +\epsilon$) then **no penalty**
- linear or quadratic **penalty outside the margin**

(see flip-chart for illustration)

This loss function is called ϵ-insensitive.

Note: We can use kernels as for SVM

Thank you! Questions?