Introduction to Machine Learning

Lecture 3: Regression

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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 (distributed computing)

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

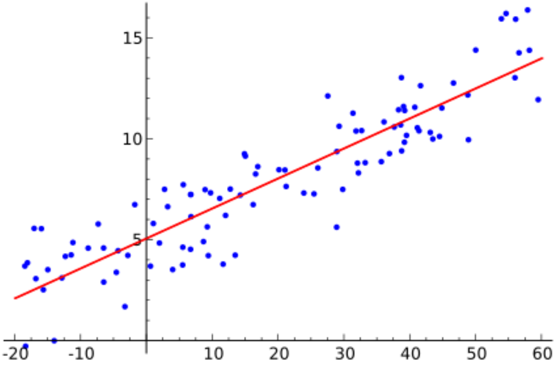
Regression in Machine Learning: Applications

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

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- Several ways to solve the problem
  - Closed-form expression (exact formula)
  - Optimization

Linear regression: Toy example

living area (m^2)	**# bedrooms**	price (1000's euros)
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General formulation:

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

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

Regression formulation

2 main ways to solve the linear least-squares problem:

$$\min_w \sum_i \left(w^T x^{(i)} - y^{(i)} \right)^2 \tag{1}$$

Method 1: Closed-form expression

$$w = \left(X^T X \right)^{-1} X^T Y$$

It can be compuationally expensive (matrix multiplication, matrix inversion, matrix multiplication, matrix-vector multiplication)

Method 2: Numerical optimization For example gradient descent algorithms, ...

Polynomial regression

Polynomial regression ≈ Kernel trick

Remind the kernel trick from the SVM lecture.

Example:

$$x = (x_1, x_2)$$

can become

$$\phi(x) = (1, x_1, x_2, x_1^2, x_2^2, x_1 x_2)$$

with a **second order kernel**.

Then we can find w solution of

$$\min_w \sum_i \left(w^T \phi\left(x^{(i)}\right) - y^{(i)}\right)^2 \tag{2}$$

Practical information

Variable standardization

Variables have various magnitudes. Example:

- Living area: Up to a few hundreds m^2
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Another option: Scale between 0 and 1

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

Overfitting and underfitting

Illustration on a generated example: Try to fit the function

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

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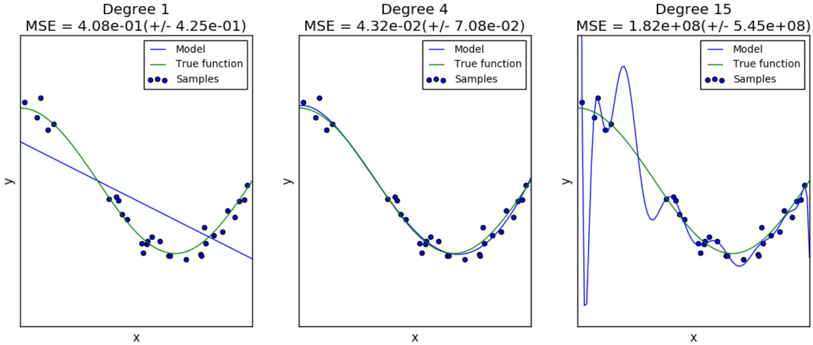

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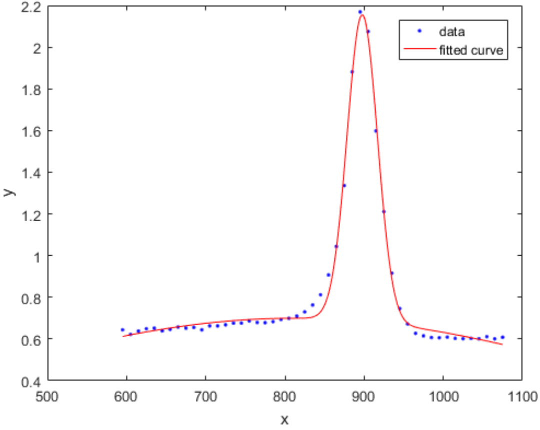
It can be done over several train/test splits.

Toy example: Fitting a distribution

Find A, x_0 and σ such that

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

best fits the data in terms of least-square error.



Regression with SVMs

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

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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)

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Note: We can use kernels as for SVM

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Thank you! Questions?