COMS30035, Machine learning:

From regression to classification and neural networks:

Revising regression

(based on slides by Dima Damen)

Rui Ponte Costa

Department of Computer Science, SCEEM
University of Bristol

September 29, 2022

Textbooks

Chapter 3 of the Bishop book is directly relevant:

- Bishop, C. M., Pattern recognition and machine learning (2006). Available for free here.

- **Note:** this first part is a revision of what you should have covered in Data Science for CS last year; for more complete slides see here.

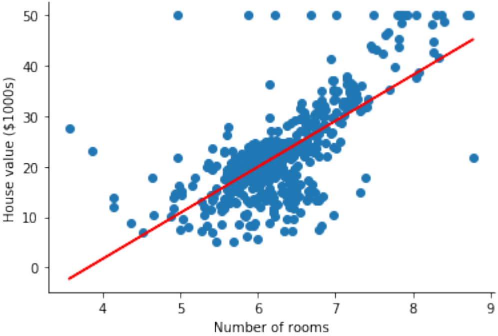
Agenda

- **Revising linear and nonlinear regression** [see extra slides; Chapter 3, Bishop]
  - Linear regression
  - Nonlinear regression
  - Probabilistic models
  - Maximum likelihood estimation
- Sequential Bayesian regression [Chapter 3, Bishop]
  - Bayesian formulation
  - Maximum a posteriori
  - Example
- Classification and neural networks [Chapter 5, Bishop]
  - Architectures (Parametric model)
  - The supervised case
  - Optimising nnets using backprop
  - Highly flexible model $\rightarrow$ overfitting: early stopping/drop-out.

Revisiting regression

- Goal: Finding a relationship between two variables (e.g. regress *house value* against *number of rooms*)

- Model: Linear relationship between *house value* and *number of rooms*?



Revisiting regression – deterministic model

Data: a set of data points $D = \{(x_1, y_1), (x_2, y_2), \cdots, (x_N, y_N)\}$ where x_i is the house value i and y_i is the number of rooms i.

Task: build a model that can predict the house value from the number of rooms

Model Type: parametric; assumes a polynomial relationship between house value and number of rooms

Model Complexity: assume the relationship is linear
house value $= a_0 + a_1 * \text{rooms}$

$$y_i = a_0 + a_1 x_i \tag{1}$$

Model Parameters: model has two parameters a_0 and a_1 which should be estimated.

- a_0 is the y-intercept
- a_1 is the slope of the line

Least Squares Solution - matrix form

- To find a solution to the parameters $\theta = \{a_0, a_1\}$ solve least squares problem which in matrix form, means to find $\mathbf{a}_{LS}$; [1]

$$\|\mathbf{y} - \mathbf{X}\,\mathbf{a}_{LS}\|^2 = 0 \tag{2}$$

$$\mathbf{a}_{LS} = (\mathbf{X}^T\mathbf{X})^{-1}\,\mathbf{X}^T\,\mathbf{y} \tag{3}$$

- Matrix formulation also allows least squares method to be extended to **polynomial fitting**
- For a polynomial of degree $p+1$ we use (note: $p > 1$ gives nonlinear regression)

$$y_i = a_0 + a_1 x_i + a_2 x_i^2 + \cdots + a_p\, x_i^p$$

[1] $\|\mathbf{A}\|^2 = \sqrt{\sum\sum |a_{ij}|^2}$ denotes the Frobenius norm, defined as the square root of the sum of the absolute squares of its elements. For a detailed derivation see this derivation - p8

Least Squares Solution

Example

Find the best least squares fit by a linear function to the data using $p = 1$

x	-1	0	1	2
y	0	1	3	9

$$\mathbf{y} = \begin{bmatrix} 0 \\ 1 \\ 3 \\ 9 \end{bmatrix} \quad \mathbf{X} = \begin{bmatrix} 1 & -1 \\ 1 & 0 \\ 1 & 1 \\ 1 & 2 \end{bmatrix} \quad \mathbf{X}^T\mathbf{X} = \begin{bmatrix} 1 & 1 & 1 & 1 \\ -1 & 0 & 1 & 2 \end{bmatrix} \begin{bmatrix} 1 & -1 \\ 1 & 0 \\ 1 & 1 \\ 1 & 2 \end{bmatrix} = \begin{bmatrix} 4 & 2 \\ 2 & 6 \end{bmatrix}$$

$$\mathbf{a}_{LS} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y} = \frac{1}{20} \begin{bmatrix} 6 & -2 \\ -2 & 4 \end{bmatrix} \begin{bmatrix} 1 & 1 & 1 & 1 \\ -1 & 0 & 1 & 2 \end{bmatrix} \begin{bmatrix} 0 \\ 1 \\ 3 \\ 9 \end{bmatrix} = \begin{bmatrix} 1.8 \\ 2.9 \end{bmatrix}$$

$$y = 1.8 + 2.9x$$

Regression with probabilistic models

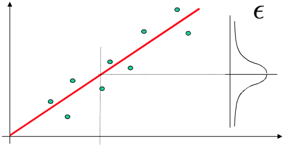
Probabilistic models are a core part of ML, as they allow us to also capture the uncertainty the model has about the data, which is critical for real world applications. For simplicity, lets drop a_0 from the previous model and add a random variable ϵ that captures the uncertainty

$$\text{house price} = a_1 \times \text{number of rooms} + \epsilon$$

We can assume, for example, that ϵ is given by $\mathcal{N}(\mu = 0, \sigma^2)$ which gives the likelihood

$$p(D|\theta) = \prod_{i=1}^{N} p(\text{price}_i|\text{rooms}_i, \theta) = \prod_{i=1}^{N} \frac{1}{\sqrt{2\pi\sigma}} e^{-\frac{1}{2}\frac{(\text{price}_i - a_1 \text{rooms}_i)^2}{\sigma^2}}$$

This model has two parameters: the slope a_1 and variance σ [2]



[2] Note that here $\mu = a_0$ which, for simplicity, we assume to be zero.

Maximum Likelihood Estimation

- Similar to building deterministic models, probabilistic model parameters need to be tuned/trained
- **Maximum-likelihood estimation (MLE)** is a method of estimating the parameters of a probabilistic model.
- Assume $\boldsymbol{\theta}$ is a vector of all parameters of the probabilistic model. (e.g. $\boldsymbol{\theta} = \{a_1, \sigma\}$).
- **MLE** is an extremum estimator[3] obtained by maximising an objective function of $\boldsymbol{\theta}$

[3] "Extremum estimators are a wide class of estimators for parametric models that are calculated through maximization (or minimization) of a certain objective function, which depends on the data." wikipedia.org

Maximum Likelihood Estimation

Definition

Assume $f(\theta)$ is an objective function to be optimised (e.g. maximised), the *arg max* corresponds to the value of θ that attains the maximum value of the objective function *f*

$$\hat{\theta} = \textit{arg max}_{\theta} f(\theta)$$

- Tuning the parameter is then equal to finding the maximum argument *arg max*

Maximum Likelihood Estimation - General

- Maximum Likelihood Estimation (MLE) is a common method for solving such problems

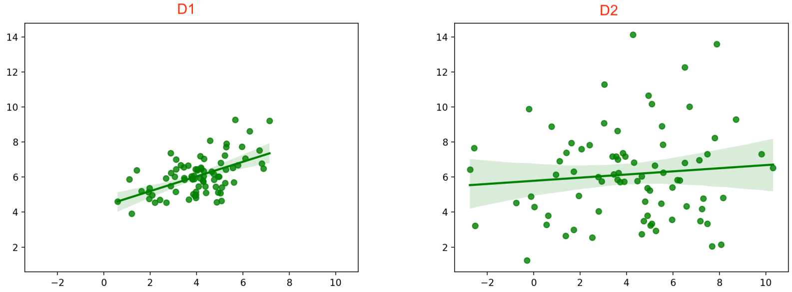
$$
\begin{aligned}
\theta_{MLE} &= arg\,max_{\theta}\, p(D|\theta) \\
&= arg\,max_{\theta}\, \ln p(D|\theta) \\
&= arg\,min_{\theta}\, -\ln p(D|\theta)
\end{aligned}
$$

MLE Recipe

1. Determine θ, D and expression for likelihood $p(D|\theta)$
2. Take the natural logarithm of the likelihood
3. Take the derivative of $\ln p(D|\theta)$ w.r.t. θ. If θ is a multi-dimensional vector, take partial derivatives
4. Set derivative(s) to 0 and solve for θ

Data Modelling - Deterministic vs Probabilistic

- **Probabilistic Models** can tell us more
- We could use the same MLE recipe to find σ_{ML}. This would tell us how uncertain our model is about the data D.
- For example: if we apply this method to two datasets (D_1 and D_2) what would the parameters $\theta = \{a_1, \sigma\}$ be?



$$a_{1\,ML}^{D_1} > a_{1\,ML}^{D_2} \text{ [slope] and } \sigma_{ML}^{D_1} < \sigma_{ML}^{D_2} \text{ [uncertainty}^4\text{]}$$

[4] The uncertainty (σ) is represented by the light green bar in the plots. Test it yourself.

Quiz time!

Go to Blackboard unit page » Quizzes » Lecture 3.1

[Should take you less than 5 minutes]