Theme: Curve Fitting

Mark van der Wilk

Department of Computing
Imperial College London

@markvanderwilk
m.vdwilk@imperial.ac.uk

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Overview

What is regression?

Regression as Minimising a Loss

A Statistical View on Regression

Conclusion

Curve Fitting (Regression) Examples

We will be considering *curve fitting* or *supervised learning*.

- Given a dataset of N examples of inputs and outputs...
- predict what the output will be for a new input.

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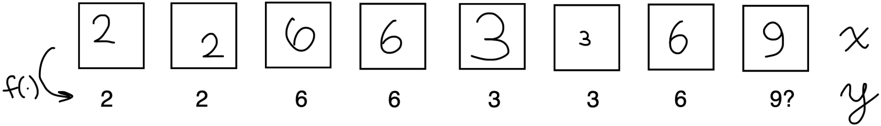
Image classification. Inputs $\in \mathbb{R}^D$, outputs $\in \mathbb{N}$:



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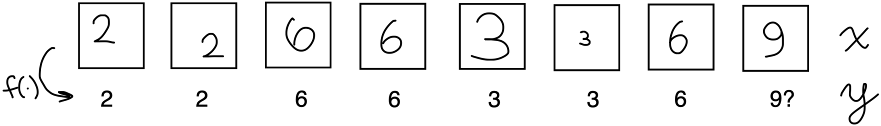


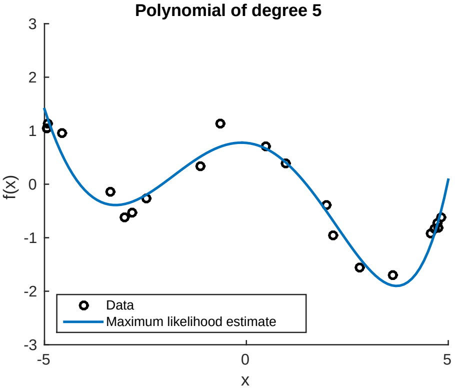
Translation. Inputs $\in \bigcup_{\ell=1}^{\infty} \mathbb{N}^{\ell}$, outputs $\in \bigcup_{k=1}^{\infty} \mathbb{N}^{k}$:

`Wiskunde is belangrijk.` $\rightarrow$ `Mathematics is important.`

Dutch English

Regression Example

Curve fitting in 1D. Inputs $\in \mathbb{R}$, outputs $\in \mathbb{R}$:



Curve fitting

"All the impressive achievements of deep learning amount to just curve fitting."
— Judea Pearl

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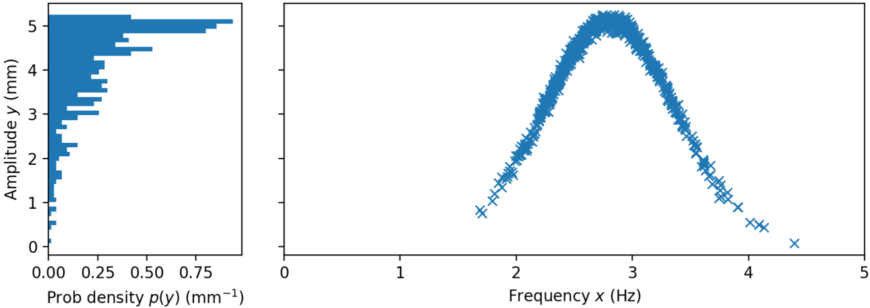


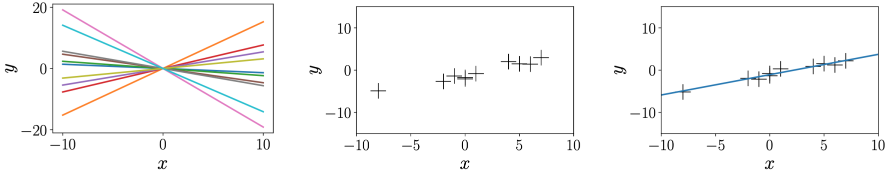
For some observed x, the world is generating data from $\pi(y|x)$.

We can choose two possible goals for regression:

- Loss view: Find a function $f(x)$ that goes "near" outputs y.
- Stats view: Match a statistical model $p(y|x, \boldsymbol{\theta})$ to $\pi(y|x)$.

Loss view: Good and bad functions

We now have many functions that we can choose from:



Left: example functions. Middle: Training set. Right: A good fit. Source: Mathematics for Machine Learning book.

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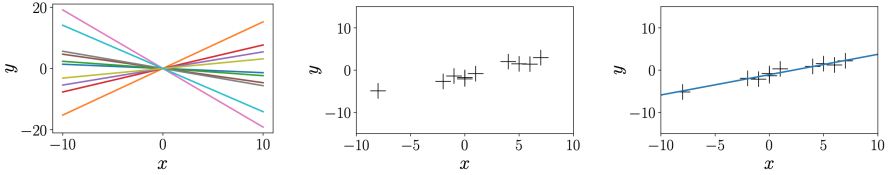

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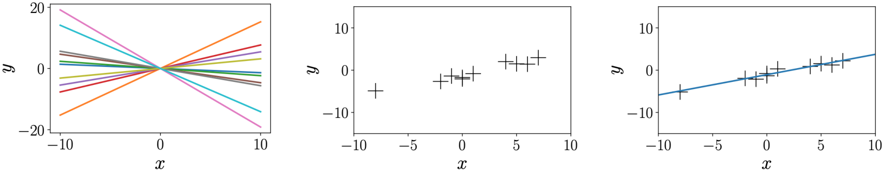

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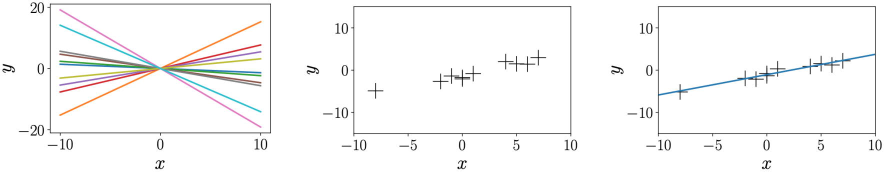

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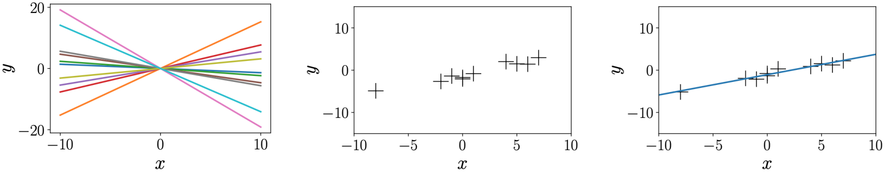

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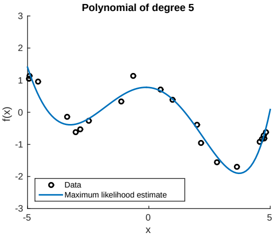
- Choose a good function, i.e. $\boldsymbol{\theta}^* = \operatorname{argmin}_{\boldsymbol{\theta}} L(\boldsymbol{\theta})$

Curve Fitting: Representing functions

Little question: How do we represent functions?



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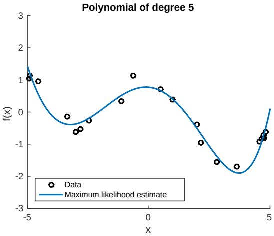

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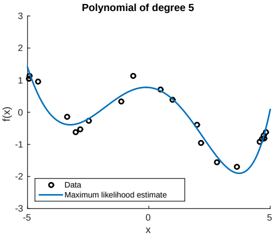

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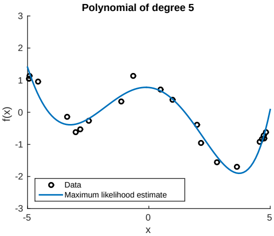

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For example, linear or polynomial functions:

$$f_{\boldsymbol{\theta}}(x) = a \cdot x + b\,, \qquad \boldsymbol{\theta} = \begin{bmatrix} a \\ b \end{bmatrix}, \tag{1}$$

$$f_{\boldsymbol{\theta}}(x) = a \cdot x^3 + b \cdot x^2 + c \cdot x + d\,, \qquad \boldsymbol{\theta} = \begin{bmatrix} a & b & c & d \end{bmatrix}^{\mathrm{T}}. \tag{2}$$

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Maximum Likelihood Estimation

Revision from `50008: Probability & Statistics`

- Model is a probability distribution on data: $p(y|\boldsymbol{\theta})$
- For an observed dataset (fixed), we can evaluate the probability assigned to it for different $\boldsymbol{\theta}$
- This defines the likelihood $\ell(\boldsymbol{\theta}) = p(y|\boldsymbol{\theta})$

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Maximum likelihood does:

$$\boldsymbol{\theta}^* = \operatorname*{argmax}_{\boldsymbol{\theta}} \ell(\boldsymbol{\theta}) = \operatorname*{argmax}_{\boldsymbol{\theta}} \log \ell(\boldsymbol{\theta}) \tag{3}$$

Likelihood for Linear Regression

Assume:

- Gaussian deviations from the function:

$$p(y_n|x_n, \boldsymbol{\theta}) = \mathcal{N}\left(y_n; f_{\boldsymbol{\theta}}(x_n), \sigma^2\right) \tag{4}$$

- Independent deviations between datapoints. So denoting $y \in \mathbb{R}^N$, $x \in \mathbb{R}^N$ for N datapoints, we get the likelihood:

$$p(y|x, \boldsymbol{\theta}) = \prod_{n=1}^{N} \mathcal{N}\left(y_n; f_{\boldsymbol{\theta}}(x_n), \sigma^2\right) \tag{5}$$

- You will show that this is equivalent to the loss view (exercises).

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- Parameterise functions as $f(\mathbf{x}_i, \boldsymbol{\theta})$
- Training the model means finding parameters $\boldsymbol{\theta}^*$, such that
  - $f(\boldsymbol{x}_i, \boldsymbol{\theta}^*) \approx y_i$ (loss is minimised)
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- Not discussed: How to find $\boldsymbol{\theta}^*$