Gaussian Processes for Regression: A Quick Introduction

- Motivation

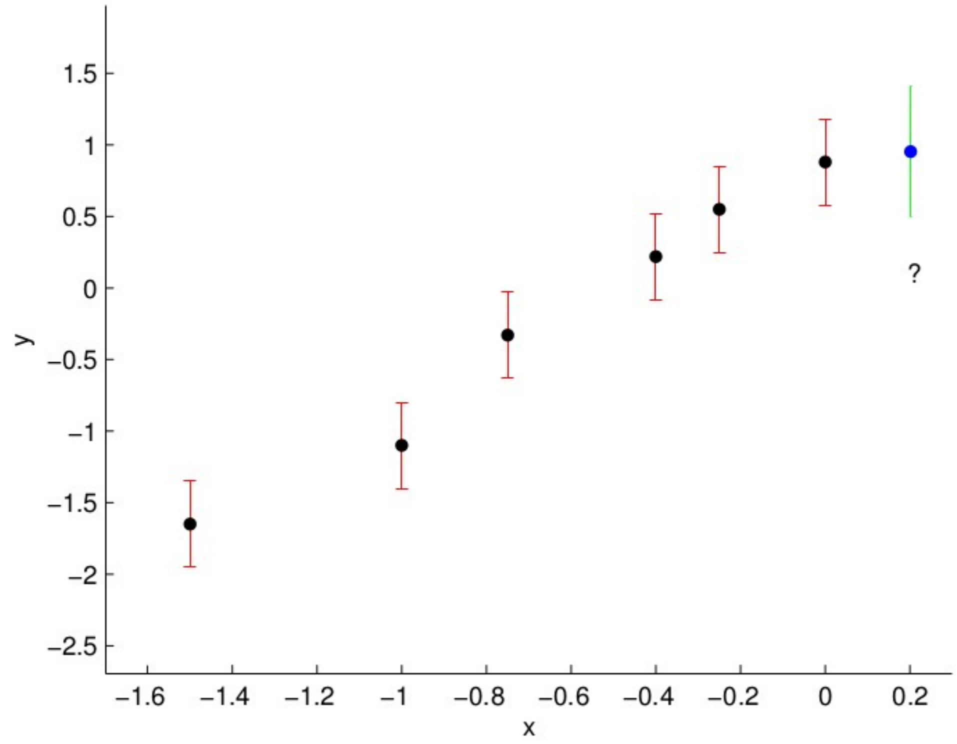

Figure 1: Given six noisy data points (error bars are indicated with vertical lines), we are interested in estimating a seventh at $x_* = 0.2$.

M. Ebden, “Gaussian Processes for Regression: A Quick Introduction”, 2008

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- Kernel Function and Covariance Matrix

$$k(x, x') = \sigma_f^2 \exp\left[\frac{-(x-x')^2}{2l^2}\right] + \sigma_n^2 \delta(x, x'),$$

$$K = \begin{bmatrix} k(x_1, x_1) & k(x_1, x_2) & \cdots & k(x_1, x_n) \\ k(x_2, x_1) & k(x_2, x_2) & \cdots & k(x_2, x_n) \\ \vdots & \vdots & \ddots & \vdots \\ k(x_n, x_1) & k(x_n, x_2) & \cdots & k(x_n, x_n) \end{bmatrix}$$

$$K_* = \begin{bmatrix} k(x_*, x_1) & k(x_*, x_2) & \cdots & k(x_*, x_n) \end{bmatrix} \qquad K_{**} = k(x_*, x_*).$$

- Prediction

$$y_* | \mathbf{y} \sim \mathcal{N}(K_* K^{-1} \mathbf{y},\; K_{**} - K_* K^{-1} K_*^{\mathrm{T}}).$$

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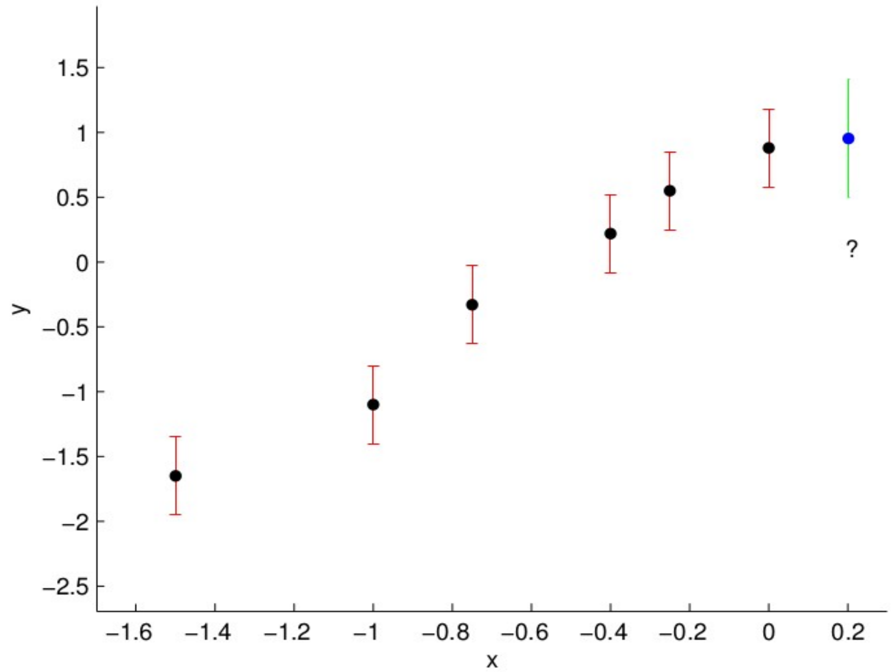
- Example



$$\mathbf{x} = \begin{bmatrix} -1.50 & -1.00 & -0.75 & -0.40 & -0.25 & 0.00 \end{bmatrix}.$$

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- Calculate Covariance Matrix

$$K = \begin{bmatrix} \color{red}{1.70} & 1.42 & 1.21 & 0.87 & 0.72 & 0.51 \\ 1.42 & \color{red}{1.70} & 1.56 & 1.34 & 1.21 & 0.97 \\ 1.21 & 1.56 & \color{red}{1.70} & 1.51 & 1.42 & 1.21 \\ 0.87 & 1.34 & 1.51 & \color{red}{1.70} & 1.59 & 1.48 \\ 0.72 & 1.21 & 1.42 & 1.59 & \color{red}{1.70} & 1.56 \\ 0.51 & 0.97 & 1.21 & 1.48 & 1.56 & \color{red}{1.70} \end{bmatrix}.$$

$$K_* = \begin{bmatrix} 0.38 & 0.79 & 1.03 & 1.35 & 1.46 & 1.58 \end{bmatrix}.$$

$$K_{**} = 1.70$$

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- Prediction and Result

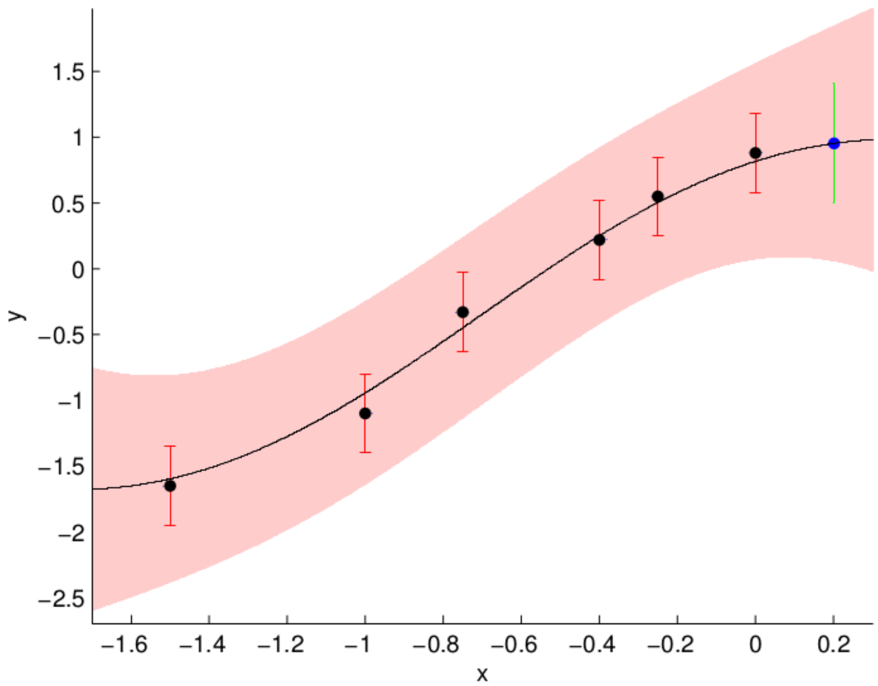

Figure 2: The solid line indicates an estimation of y_* for 1,000 values of x_*. Pointwise 95% confidence intervals are shaded.

$$\overline{y}_* \pm 1.96\sqrt{\mathrm{var}(y_*)}, \text{ giving a } 95\%$$

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- Practical Writing Python Code

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