Gaussian Process Regression

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Gaussian Process Regression

Introduction

- Gaussian Process (GP) is a *non-parametric probabilistic* approach.
- GP extends the concept of Gaussian distribution of numbers to *functions*!

- A GP is defined by a mean function (often zero) and a *covariance function* or *kernel:*

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

Optimizable parameters

- $y = f(x)$ and y_* (prediction for new x_*) make a joint Gaussian distribution:

$$\begin{array}{r} \textit{cal} \\ \textit{val} \end{array} \begin{bmatrix} \mathbf{y} \\ y_* \end{bmatrix} \sim \mathcal{N}\left(\mathbf{0}, \begin{bmatrix} K & K_*^{\mathrm{T}} \\ K_* & K_{**} \end{bmatrix}\right)$$

Covariance matrices

- *Conditional* probability $p(y_*|y)$:

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

Best estimate: $\bar{y}_*$ *Uncertainty: s^2*

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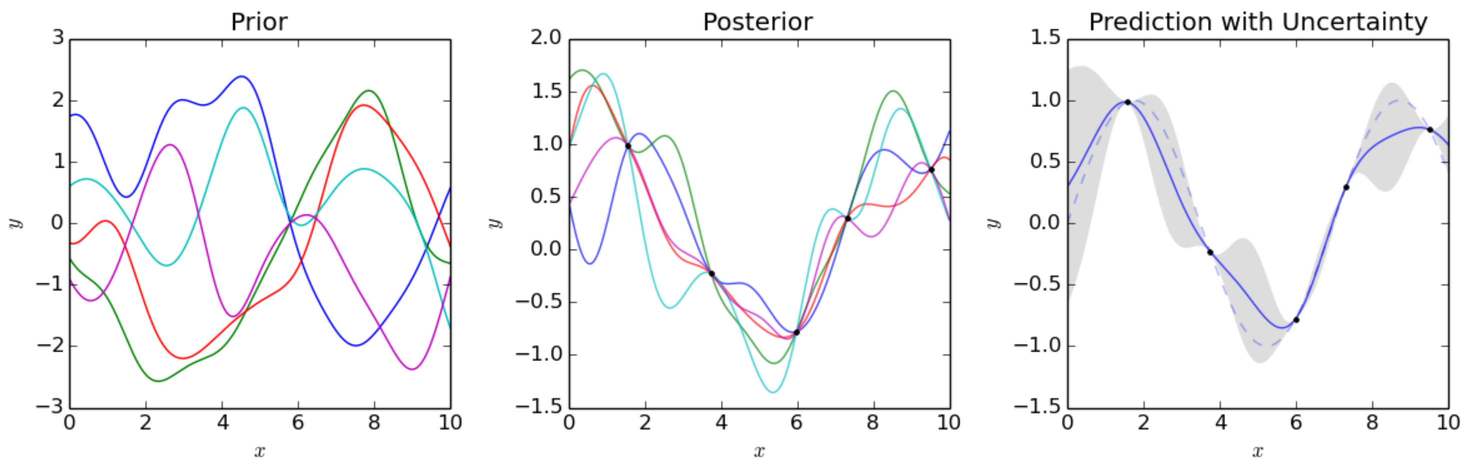
Introduction

GP begins with a prior distribution and updates this prior as new data are observed, producing the posterior distribution over functions.



Great demo: http://www.tmpl.fi/gp/

Gaussian Process Regression

Benefits

- Non-linear
- Kernel parameters automatically learned from data
- Different kernels can be combined together
- Automatic feature selection (ARD)
- Fully probabilistic predictions
- Fairly resistant to over-fitting

GPR on the Challenge data

Settings

- 207 redundant samples removed from calibration set
- Pre-processing: ***SG(1,15,2) + SNV***
- Kernel: ***Matérn v=5/2***
- Kernel Parameters optimized by maximizing marginal likelihood
- Inference method: ***Gaussian likelihood***

GPML *Matlab Code version 4.1*
(by Carl Edward Rasmussen and Hannes Nickisch)
http://www.gaussianprocess.org/gpml/

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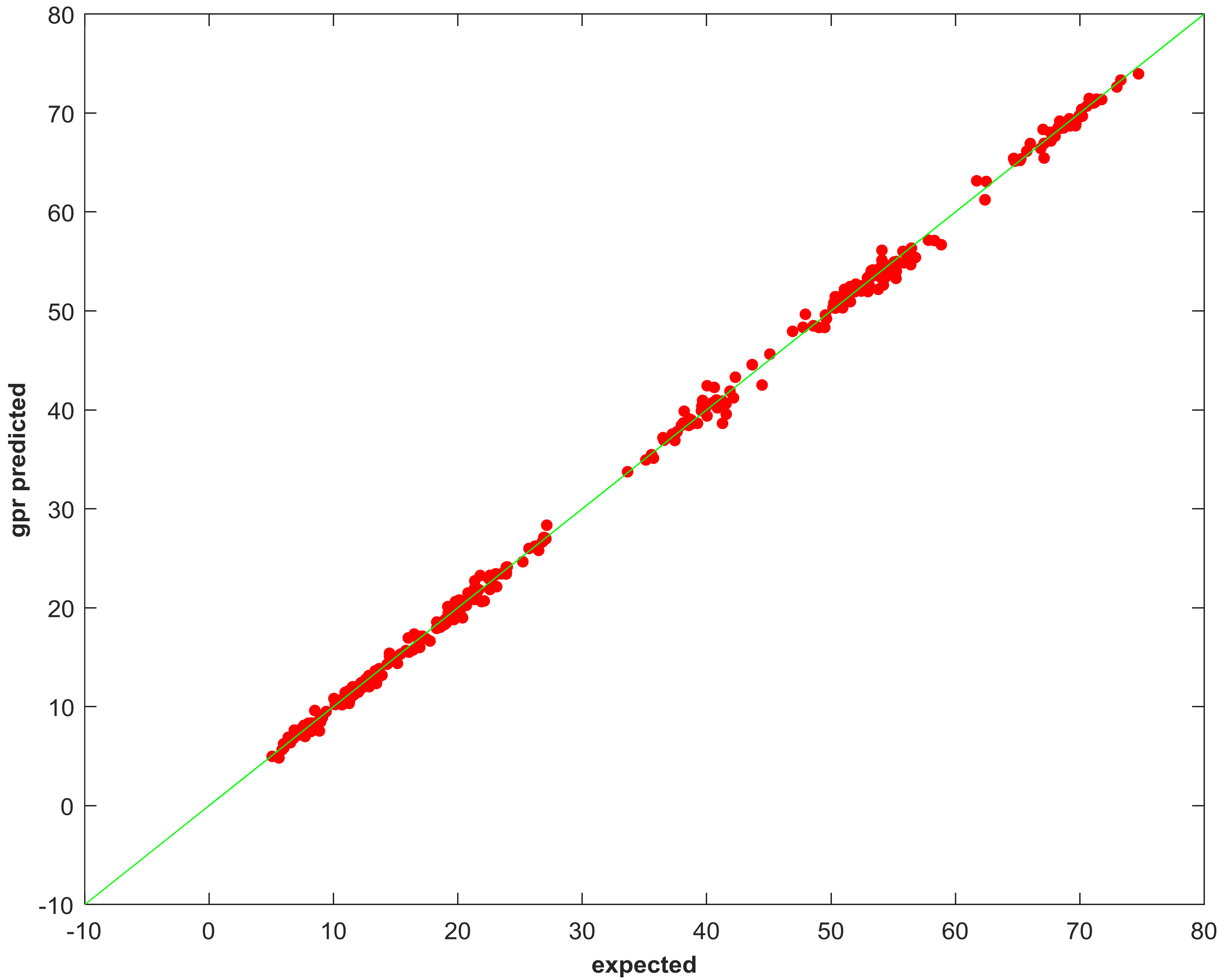
GPR on the Challenge data

Internal validation



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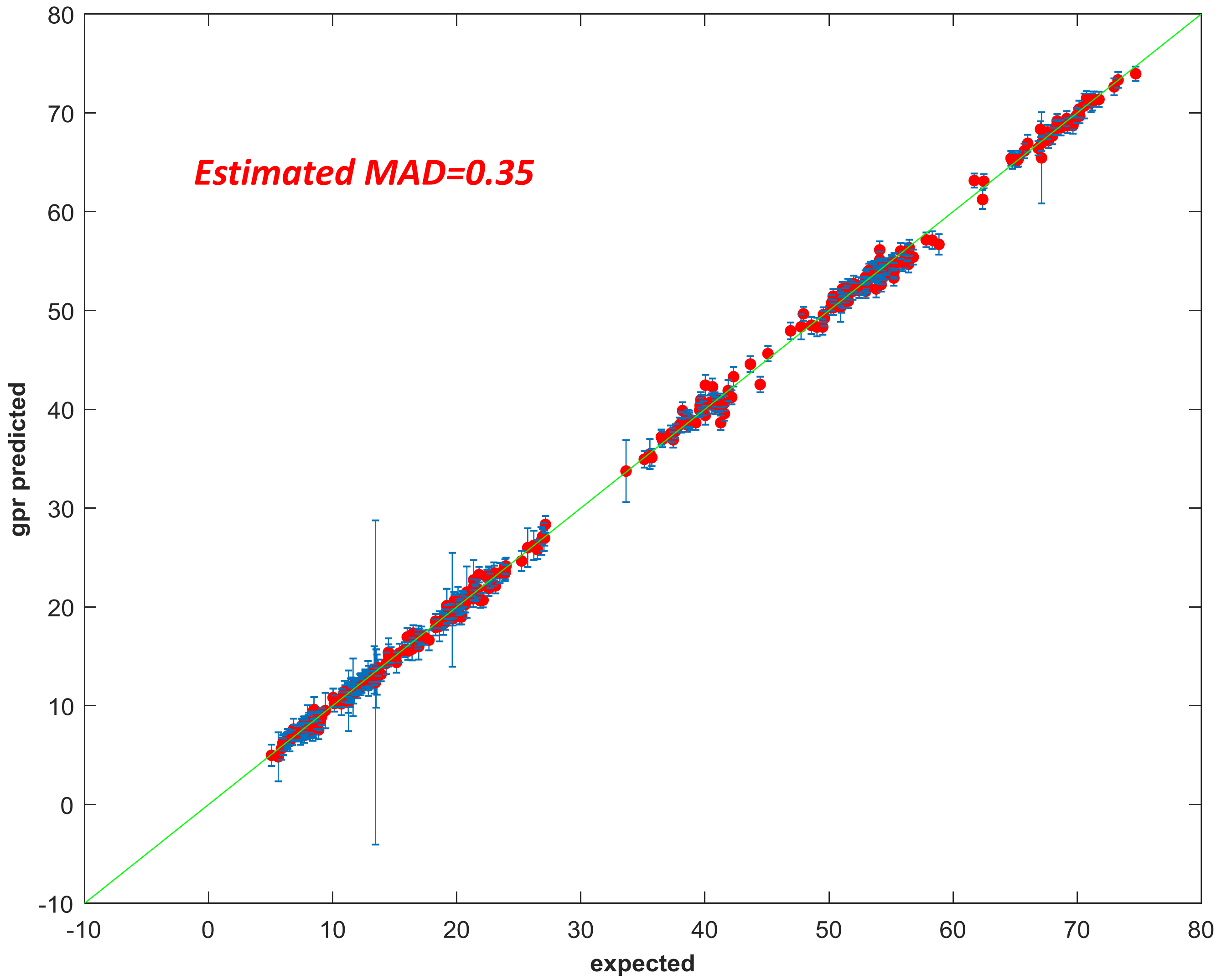
GPR on the Challenge data

Internal validation



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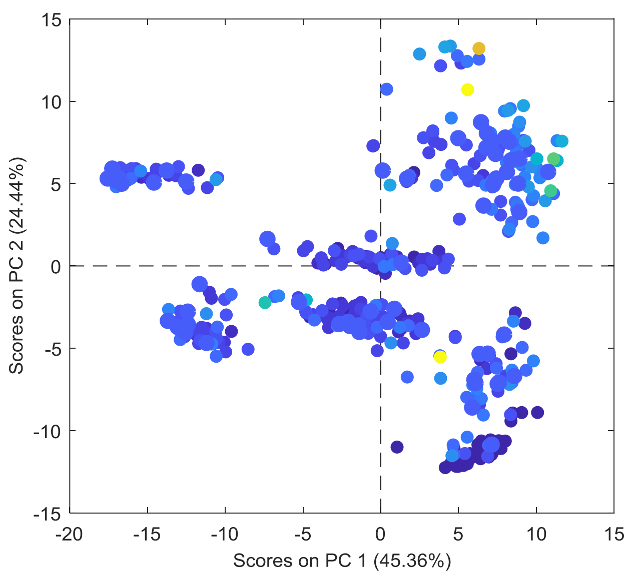
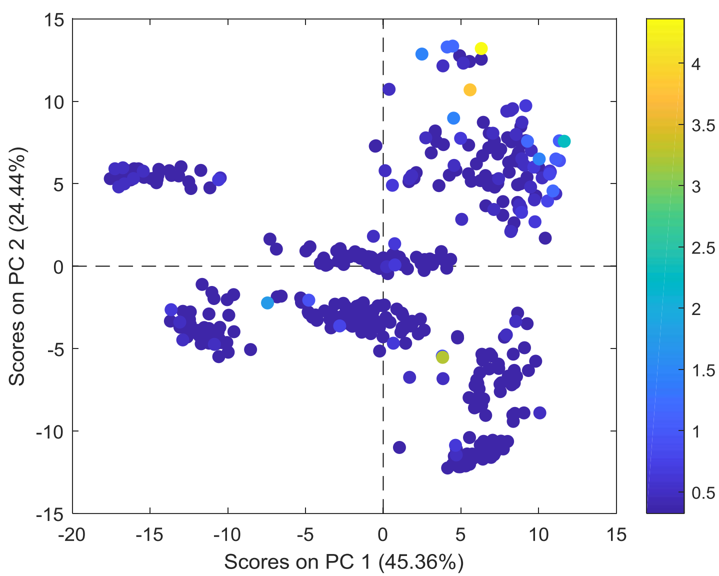
GPR on the Challenge data

Validation set

Nearest neighbour distance



GPR estimated standard deviation



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