Gaussian Process Regresion For Hydrometallurgy

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02 March, 2022

Overview

1. Problem Statement
2. Gaussian Processes
3. Optimization
4. Example on synthetic data
5. Future application

The Ideal Model

Ideally a hydromet processes would:

- be simple to model accurately
- have a low cost for collecting real data

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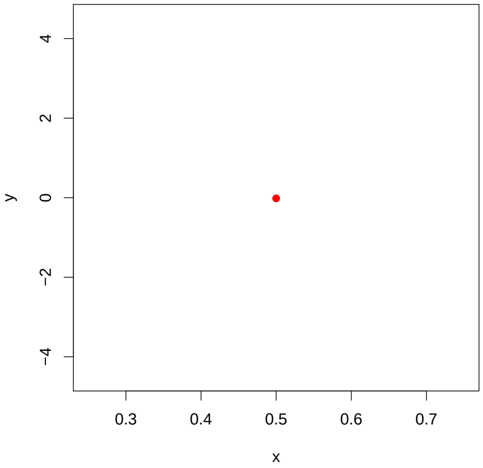
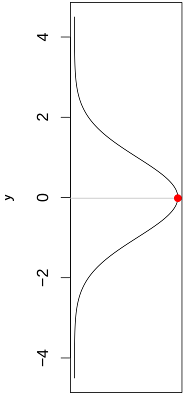
- flexible modeling which quantifies uncertainty of our data and predictions
- uncertainty quantification

Uncertainty: A Gaussian Distribution



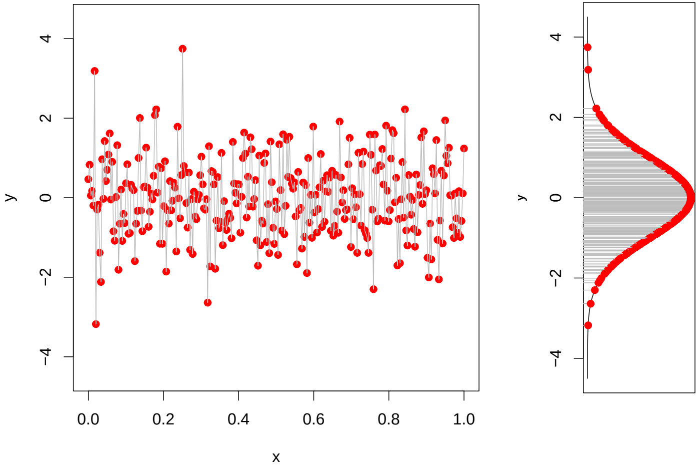


$$f(y) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{\frac{1}{2}(y-\mu)^2}{\sigma^2}}$$

Points independent but have a common:

- Mean (μ) of 0
- Standard deviation (σ) of 1

Multivariate Gaussian



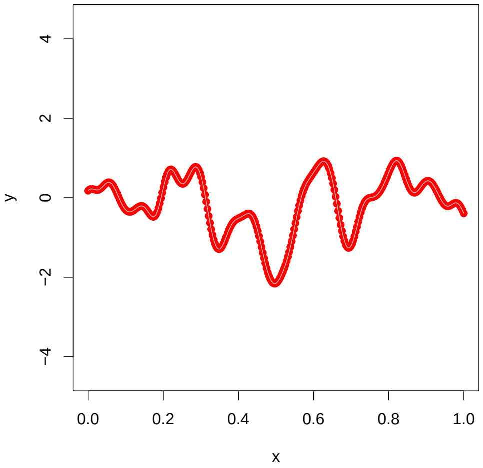
$$f(Y) = (2\pi\sigma^2)^{-\frac{n}{2}} e^{-\frac{\frac{1}{2}(Y-\mu)^T(Y-\mu)}{\sigma^2}}$$

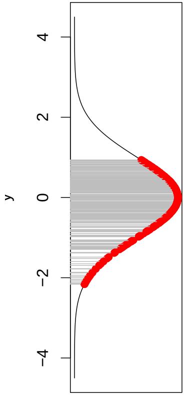
Points within a single vector *draw* are independent, vectors drawn are independent.

Points have a common:

- Mean (μ) of 0
- Standard deviation (σ) of 1

Multivariate Gaussian as a Random Function Generator





$$(2\pi\sigma^2)^{-\frac{n}{2}}|\Sigma|^{-\frac{1}{2}}e^{-\frac{\frac{1}{2}(Y-\mu)^T\Sigma^{-1}(Y-\mu)}{\sigma^2}}$$

Covariance or Correlation Matrix Σ - distance related?

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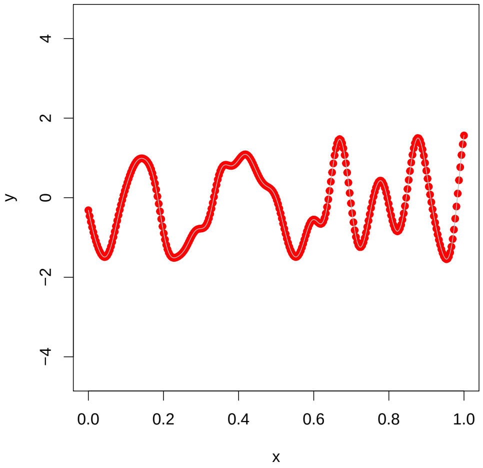

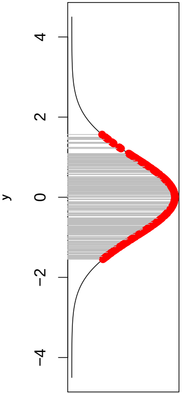

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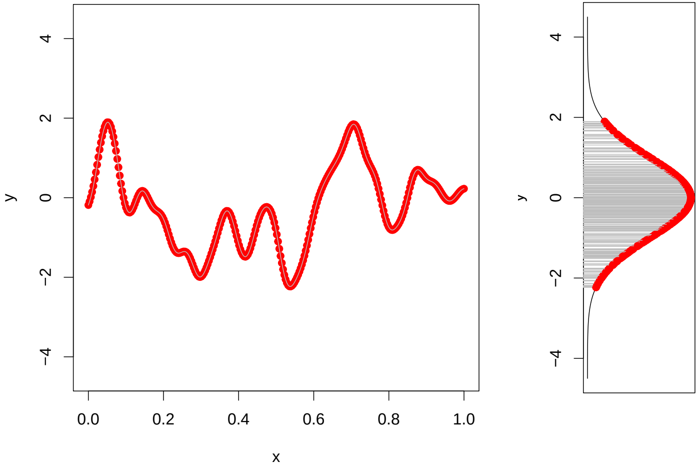

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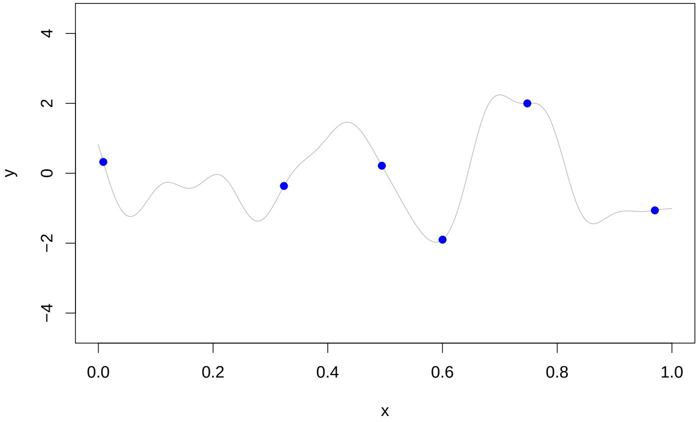
Incorporating Data



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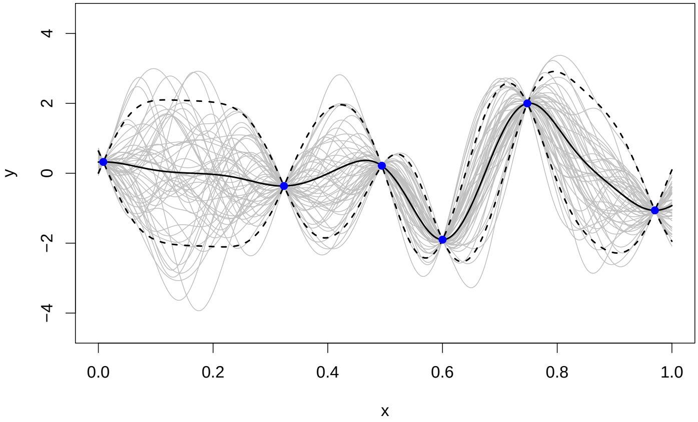

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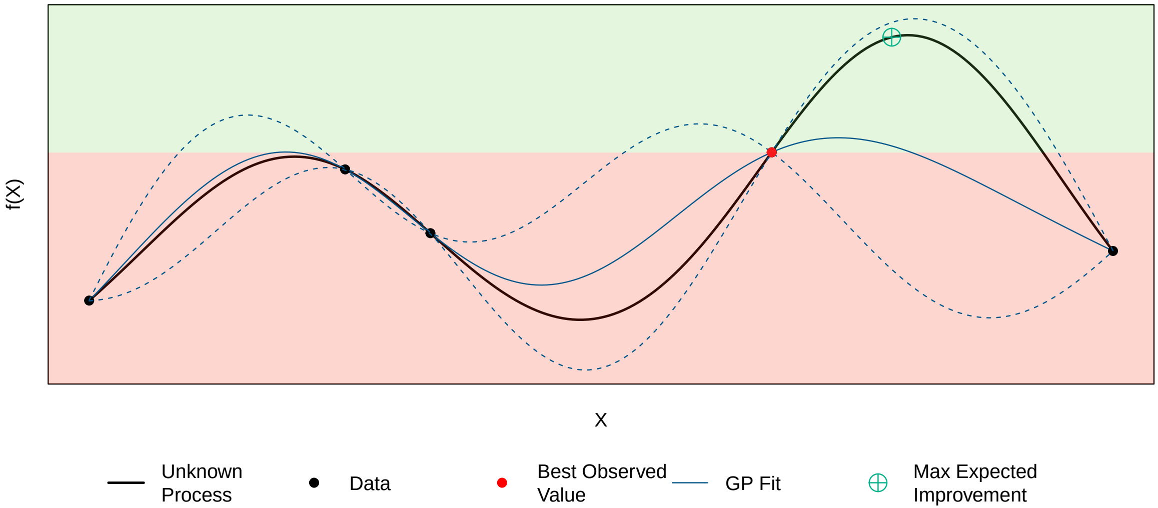
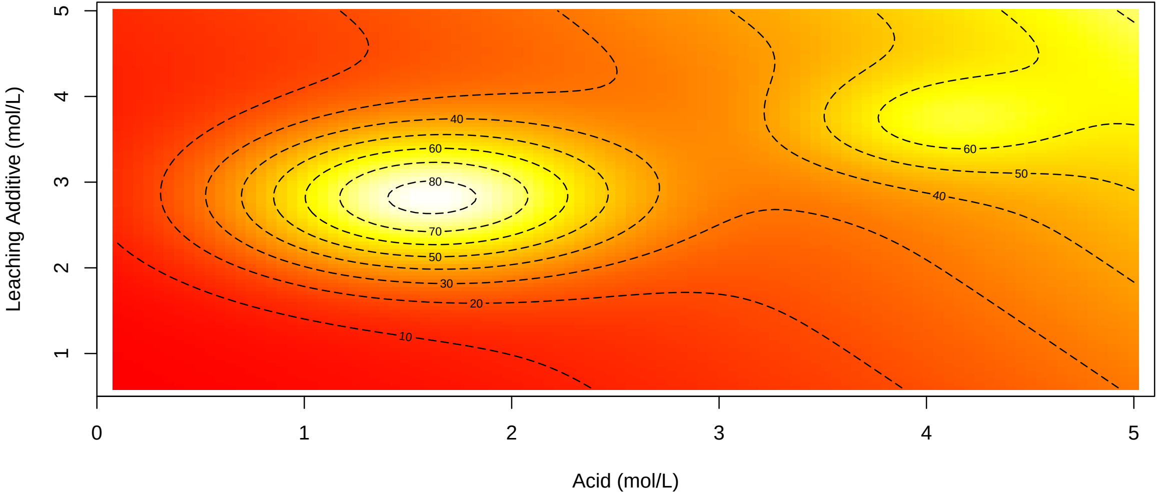
Properties of this fit?

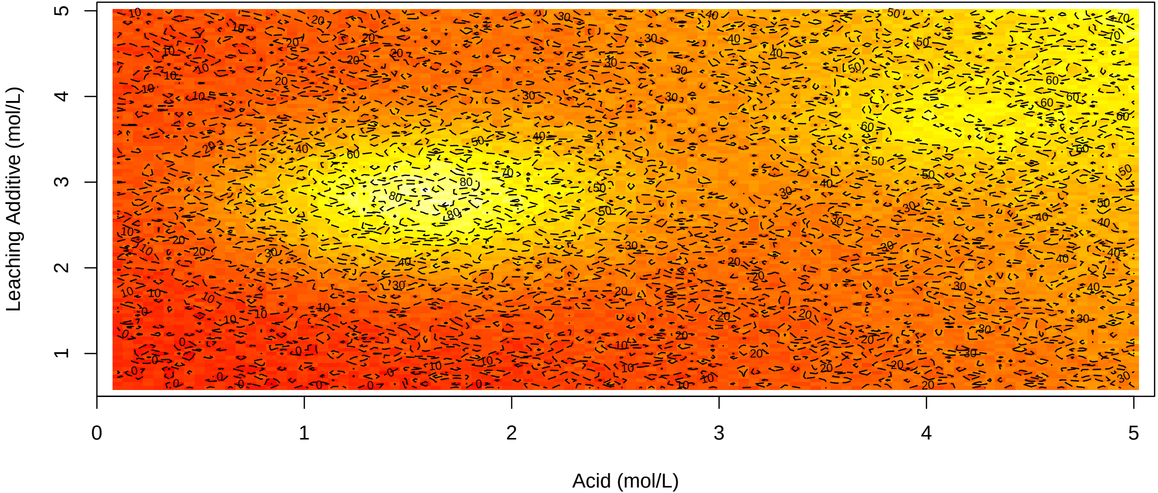
Optimization: Expected Improvement



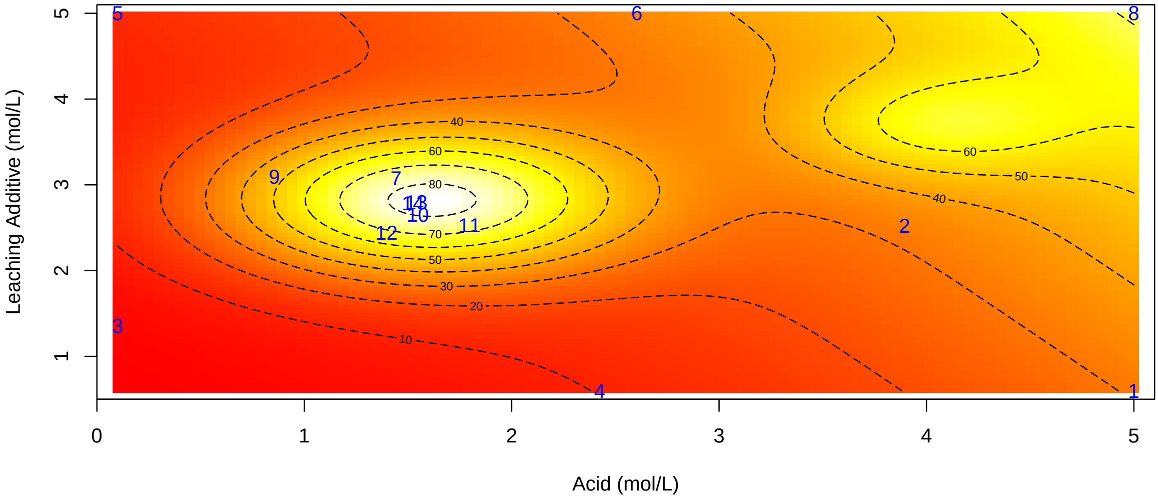
Application: TREE Recovery(%) for Simulated Leaching Process



Application: Simulated Leaching Process

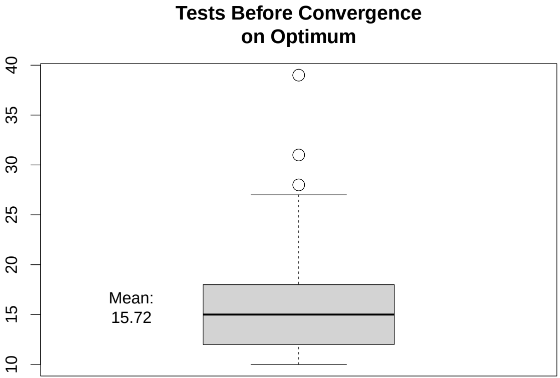


Optimization



Average Behavior

- Monte Carlo Experiment of 100 repitions
- Mean number of experiments to convergence: 15.72



Summary

- GPs are a flexible regression method
- Just like a normal distribution, GPs have an inherent quantification of uncertainty
- GP Functional uncertainty can be used for *active learning* experimental designs
- The complexity and uncertainty of hydrometallurgical processes provides a motivation for the utility of such methods.

"All models are wrong, but some are useful" -George Box

Additional Applications

GP flexibility and uncertainty quantification allows for

- Emulation and calibration of computer simulations with long computation time (dissertation work)
- Experimental design where points are specifically added to reduce prediction variance
- Modeling data where noise is a function of X

Thank You!!

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Acknowledgement

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