

Gaussian Processes

- A non-parametric, Bayesian model
- Calculates the probability distribution over all possible function fitting the data.
- Prior can be specified by:

$$y \sim GP(\mu, \kappa)$$

• Here, μ is a mean of labels (y) and $\kappa = \kappa(x, x')$ is a covariance function.

Emulator

- We used George, a python module for Gaussian process regression.
- We first standardised the data.
- We set μ to be mean value of FoMs in training dataset and covariance to be a normalised exponential squared kernel:

$$\kappa(x,x') = \frac{1}{\sqrt{2\pi|C|}} \exp(-\frac{(x-x')^T C^{-1} (x-x')}{2})$$

- Here, C is a 6x6 identity matrix resulting in equal scale lengths in all dimensions.
- Then, we maximise the likelihood of the fitting function.
- Finally, we make predictions, reverse the standardisation and get the final predicted values of FoM.

Testing

- To test the robustness of emulator with used kernel, we chose some particular scenarios out of 36 scenarios as testing sample and remaining others to be training sample.
- We made predictions using different kernels.



