

Gr-ResQ – Graphene Recipes for Synthesis of high-Quality materials
Week 2 - Bayesian Search

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We shall explore how to optimise a search over the parameter space using Bayesian methods. Click on the following link and open the notebook in Colab:

<https://github.com/ertekin-research-group/DOE-vs-Bayes/blob/main/bin/bayes.ipynb>

- *Question 1. In Part 1 – Imagine that you sample the objective function, but your measurements are noisy. What happens to your ability to learn the underlying function as the noise increases? Should you just pick your highest sampled point as the maximum?*

- *Question 2. In Part 2, make sure you understand what all the lines on the plots are. How well does the Gaussian Process Regressor work as a surrogate function? How does your answer change if you vary the noise from 0.01,0.1,1,10?*

- *Question 3. In Part 3, what does the sequence of plots in the bottom row show? How does the next data point get selected, from one plot to the next?*
