Gaussian Process Bayesian Optimization for the Design of a Precision Particle Physics Experiment

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on behalf of the Muon EDM Collaboration.

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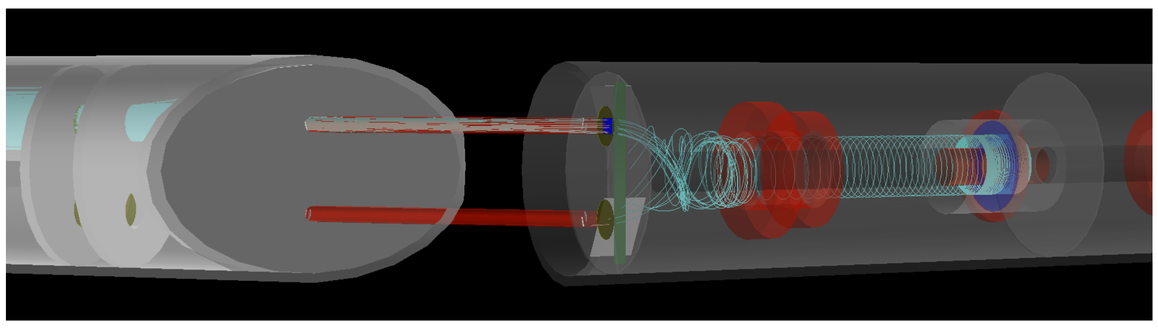
Overview

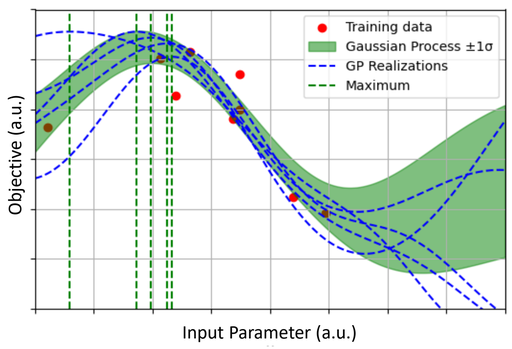
We present the optimization of the injection of muons into the **muon EDM experiment** at PSI – a precision particle physics experiment with the aim to measure the muon electric dipole moment to unprecedented precision [1].



The experiment can be simulated with expensive Monte-Carlo simulations using G4Beamline [2], but optimizing by sampling the entire configuration space of possible experimental configurations quickly becomes infeasible.

Gaussian processes are powerful tools for **regression tasks with uncertainty quantification.**

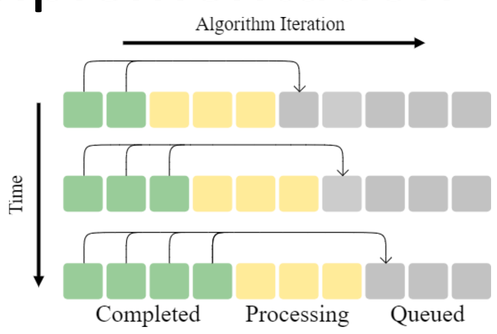
Bayesian optimization employs Gaussian processes as a surrogate model to **intelligently search for the global maximum.**



We apply the Thompson Sampling (TS) procedure following [3], allowing for a **batched implementation**. This involves sampling individual realizations of the GP and choosing the maximizer. We optimize the kernel hyperparameters via marginal likelihood.

Parallel processing implementation

Our algorithm supports execution across hundreds to thousands of cores in parallel. Instead of waiting for batch completions, we run n concurrent optimization steps. Each step is an independent process that reads and writes results to disk.



A local approximation

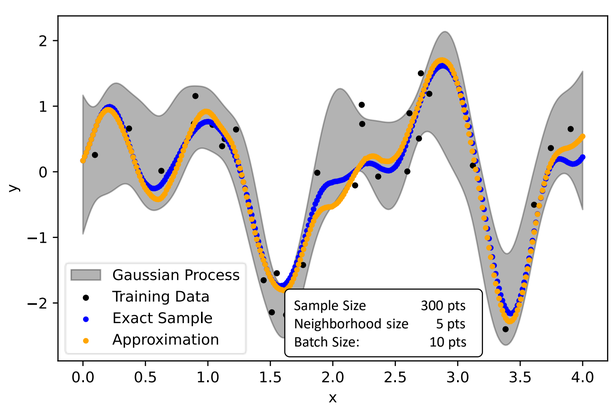
Sampling realizations of a GP scales poorly with the number of points, as the whole covariance matrix must be stored in memory. We therefore apply a local approximation and sample the GP sequentially in batches.

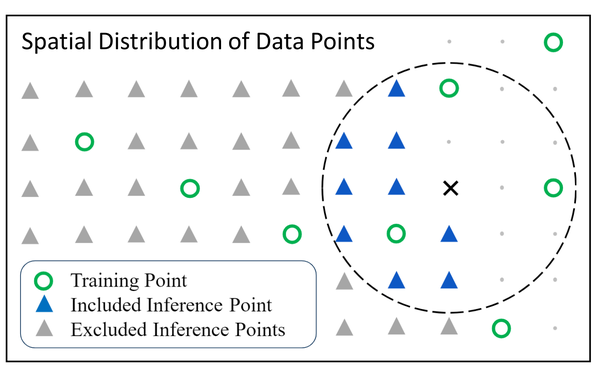
For each new batch of inference points, we consider only the inference points in a local neighborhood. This reduces the memory size significantly. This is equivalent to truncating entries with a covariance less than a threshold ε.

$$k(x,y) = \exp\left(-\frac{|x-y|^2}{4l^2}\right) > \varepsilon \quad \Longleftrightarrow \quad |x-y| < -2l\sqrt{\log(\varepsilon)}$$

Covariance Threshold — Local Approximation

One can show that the approximation error due to this is $O(M\varepsilon)$, where M is the number of batches of inference points.

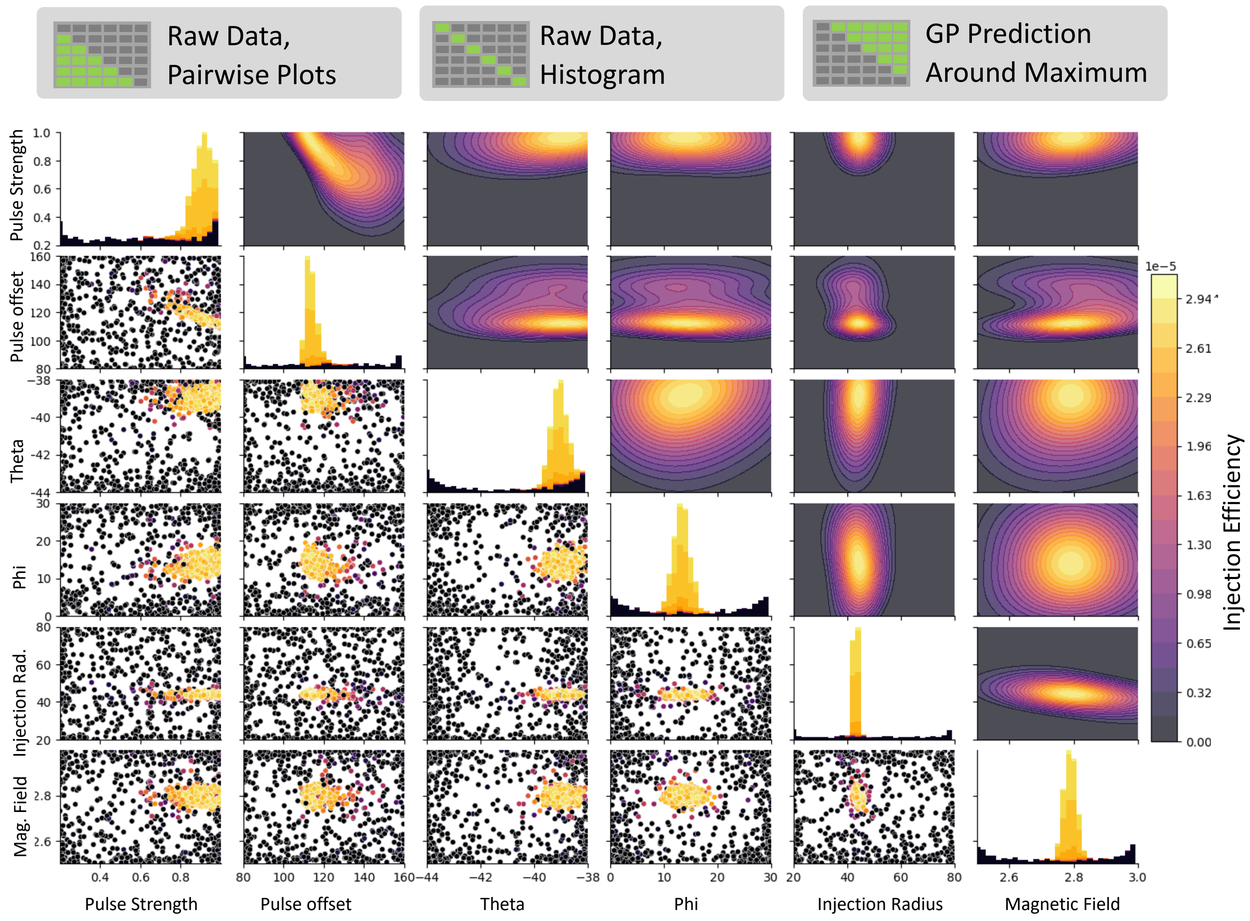




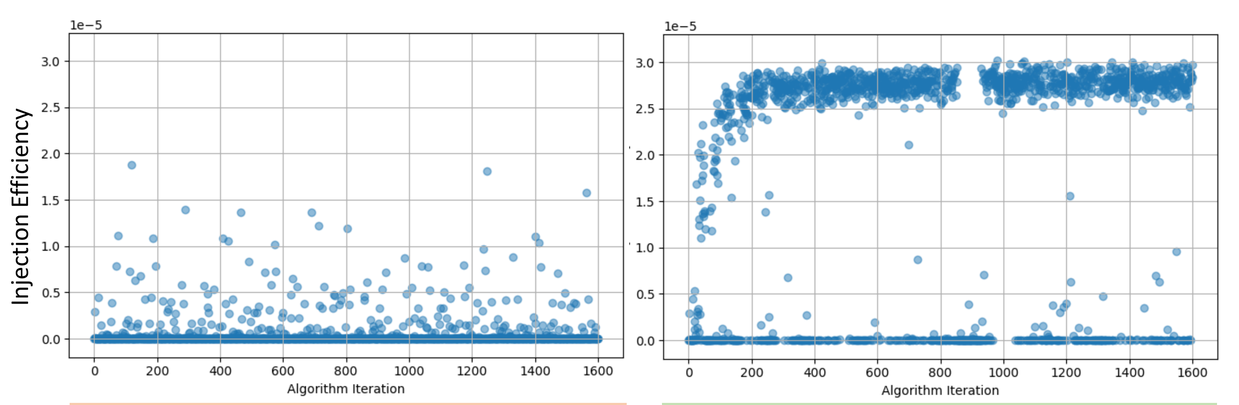
Optimization results

We present both the raw data, and the Gaussian Process prediction in the figure below, presented as pairwise plots of two parameters at a time.

Raw Data, Pairwise Plots | Raw Data, Histogram | GP Prediction Around Maximum



We compare our algorithm against a quasi-random search. We find significant performance benefits with the same number of simulations.



Raw Data, Sobol Sampling | Raw Data, Bayesian Optimization

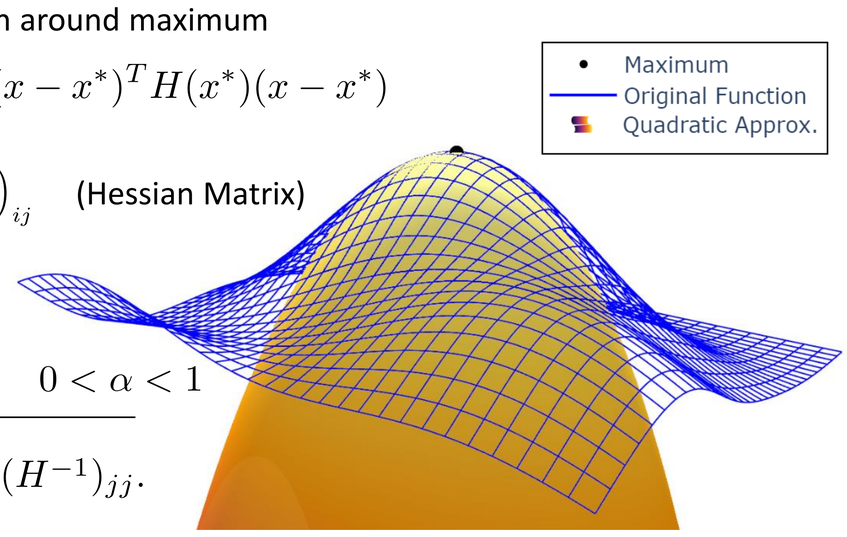
Estimating tolerances for parameters

We use the Gaussian process fit to determine the tolerance of our experimental parameters. We apply a quadratic approximation and can derive the parameter tolerance analytically.

Quadratic Approximation around maximum

$$f(x) \approx f(x^*) + \frac{1}{2}(x-x^*)^T H(x^*)(x-x^*)$$

$$H(x^*) = \left(\frac{\partial^2 f}{\partial x_i \partial x_j}(x^*)\right)_{ij}$$ (Hessian Matrix)



Parameter tolerance for

$$f(x^* \pm \delta x) = \alpha f(x^*) \quad 0 < \alpha < 1$$

$$||\delta x_j|| = \sqrt{\frac{2(1-\alpha)}{f(x^*)}(H^{-1})_{jj}}.$$

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References

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[3] S. R. Chowdhury and A. Gopalan, "On kernelized multi-armed bandits," in Proceedings of the 34th International Conference on Machine Learning (ICML 2017), PMLR, 2017.

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