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GPry: Fast Bayesian inference using Gaussian Processes

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In modern physics, with an increasing number of experiments, more available data will open a window towards testing new, increasingly complex-to-compute theories. Often, comparing this data against theory requires expensive computations arising from the sheer size of the dataset as well as numerical simulations required to go from theory to observables.
This in turn makes Bayesian inference using such codes prohibitively expensive, as typical sampling algorithms like Markov chain Monte Carlo usually take many tens of thousands of evaluations of the likelihood/posterior distribution, hence requiring a large amount of theory-simulations. Likelihood-free approaches circumventing this problem have lately gained some attention, however these come with their own set of challenges like managing biases and often require methods which need to be tailored to the problem at hand. With our Python package "GPry"we introduce a new tool which keeps the simplicity and robustness of likelihood-based inference, while drastically reducing the number of samples that are needed to get an MC sample of the posterior. This approach is based on interpolating the posterior distribution with a suitable Gaussian process and a deterministic, sequential acquisition of likelihood samples inspired by Bayesian optimization. To enable parallelization of the algorithm, we have also developed a batch acquisition procedure which allows the likelihood function to be evaluated in parallel. We also avoid a common problem in many similar approaches where vanishing posterior values or errors in the analysis chain cannot be correctly interpreted by supplementing the Gaussian process with a support vector machine classifier to define a finite region of interest. We show the performance of the algorithm on both test distributions as well as cosmological and binary inspiral problems.

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