Working Title: Bayesian Optimization for the Optical Synchronization System at European XFEL

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***Abstract*—TODO**

I. Introduction

II. Fundamentals

Bayesian optimization (BO) is a very versatile and customizable method, depending on the underlying problem various strategies can be used for optimization. In this section the authors give an overview about the functionality of original BO.

A. Optical Synchronization System

B. Bayesian Optimization

The goal of BO is to globally optimize an unknown system represented by a Black Box (c. f. Figure 1). The transition from inputs to outputs is described by an unknown objective function $f : \mathcal{X} \longrightarrow \mathbb{R}$, where $\mathcal{X} \subseteq \mathbb{R}^d$ describes a compact set of input parameters. In order to ensure applicability of BO we need to impose restrictions on the transition function as shown in [1]: f is a member of a reproducing kernel Hilbert space (RKHS) $\mathcal{H}$ defined by a kernel function $k : \mathcal{X} \times \mathcal{X} \longrightarrow \mathbb{R}$ and has finite RKHS norm $\|f\|_{\mathcal{H}} \leq B$. In general, f is a non-convex function which is learned online by evaluating the objective at some inputs $y_{\mathrm{nf}} = f(\mathbf{x}), \mathbf{x} \in \mathcal{X}$. The kernel function determines the dependence between function values at different inputs $\mathrm{COV}(f(\boldsymbol{x}), f(\boldsymbol{x}')) = k(\boldsymbol{x}, \boldsymbol{x}')$. The function values themselves are in most cases not accessible, rather observations are made by measuring the output. The resulting measurement uncertainty can be modeled by additive noise $\epsilon \sim \mathcal{N}(\mathbf{0}, \sigma_{\mathrm{n}}^2 I_{\mathrm{d}})$ such that the observation is composed of the true function value and a small noise term

$$y = f(\mathbf{x}) + \epsilon. \tag{1}$$

The second component of BO is the Gaussian process model (GPM) used to model the objective function. ~~Therefore,~~ the set of n observations is defined by $\mathcal{O} = \{\mathbf{x}_i; y_i, i = 1 \ldots n\}$ and the input-output pairs are fed into the GPM. In the next step, the predictive distribution $p(f_*|\mathcal{O}, X_*)$ given the set of observations is determined for s test inputs $X_*^T = [x_{*,1}, \ldots, x_{*,s}]$, now the GPM provides intrinsic information about the approximation accuracy at every test point in form of a posterior distribution.

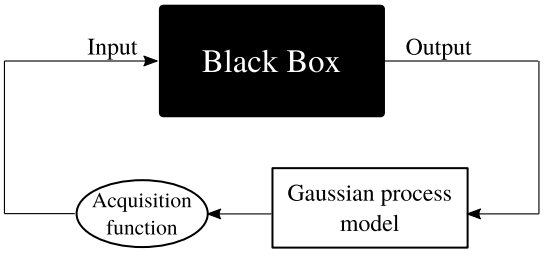

Fig. 1. Schematic illustration of Bayesian optimization

~~Eventually,~~ an acquisition function determines new promising inputs from the predictive distribution. A commonly~~~~ choice is expected improvement (EI) as initially described in [2], this acquisition function determines the ~~expected value~~ that the function at point $\mathbf{x}$ improves the so far best observation $f^*(\mathbf{x})$

$$EI(\mathbf{x}) := \mathbb{E}\left[\max(f^* - f(\mathbf{x}), 0)\right]. \tag{2}$$

~~Rewrite~~ the expression into integral form and using integration by parts ~~the expected improvement is given by~~

$$EI(\boldsymbol{x}) = (f_n^* - \mu(\boldsymbol{x})) \cdot \Phi_s(\lambda) + \sigma(\boldsymbol{x}) \cdot \phi_s(\lambda), \tag{3}$$

where $\lambda = \left(\frac{f_n^* - \mu(\boldsymbol{x})}{\sigma(\boldsymbol{x})}\right)$, ϕ_s denotes the standard normal probability density function (PDF), Φ_s represents the standard cumulative distribution function (CDF), and $\mu(\mathbf{x})$ and$\sigma(\mathbf{x})$ describes the posterior mean and standard deviation.

Two other widely used functions are upper confidence bound (UCB) $u(\mathbf{x})$ and lower confidence bound (LCB) $l(\mathbf{x})$ given by

$$\begin{aligned} u(\mathbf{x}) &= \mu(\mathbf{x}) + \beta\sigma(\mathbf{x}) \\ l(\mathbf{x}) &= \mu(\mathbf{x}) - \beta\sigma(\mathbf{x}). \end{aligned} \tag{4}$$

The ~~term~~ β acts as trade-off between exploration and exploitation. ~~While~~ exploration, points with a high uncertainty are going to be evaluated, whereas ~~while~~ exploitation the function ~~is~~ within a ~~well known~~ space optimized. UCB and LCB are later especially used to define safe inputs as described in Section III.

Nevertheless, using this naive BO method we are facing several challenges for high-dimensional problems. A very intuitive problem is the significantly increased number of evaluations to find the optimum for higher dimensional problems. This can lead, depending on the time ~~effort~~ for one evaluation, to prohibitively high time consumption. In addition, the computational complexity of inferring f is cubic to the number of

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observations due to matrix inversion. ~~The~~ major limitation is ~~caused by~~ seeking for new promising inputs with a acquisition function $\alpha(\mathbf{x})$. New inputs are defined by

$$\mathbf{x}_{\text{new}} = \max_{\mathbf{x}\in\mathcal{X}} \alpha(\mathbf{x}), \tag{5}$$

which corresponds to ~~a~~ global optimization of a non-convex function across the whole input space. ~~In general,~~ this operation is feasible up to problem dimensionality $\dim(\mathcal{X}) = 10\ldots20$ [3]. One approach to solve these issues is to divide the overall optimization problem into several sub-problems which are solved successively. The LineBO [4] restricts the sub-problems to one-dimensional subspaces $\mathcal{L} = 1$ that can be efficiently optimized. The optimization of $\alpha(\mathbf{x})$ can now be achieved via, e. g. grid search. In order to reduce the total number of observations, a local Gaussian process (GP) can be used, which means that all observations are discarded after each subspace optimization. As [4] ~~mentioned,~~ using a local GP reduces the computational effort but also the convergence rate. Nevertheless, the overall optimization problem becomes tractable.

Another challenge deals with implicit constraints on the evaluation point and is system specific. Many systems like the one studied in this thesis consists of several subsystems with safety-critical properties. For example, if the in-loop jitter of the master laser oscillator (MLO) and master timing reference oscillator (MO) exceed a specific threshold, the MLO itself and all subsystems get unlocked. Restoring all subsystems of the accelerator into the locked state is very time-consuming and slows down the optimization significantly. Therefore, safety conditions are necessary to force the algorithm ~~choosing~~ new inputs solely from a safe set. The problem can be reformulated to

$$\min_{\boldsymbol{x}\in\mathcal{X}} f(\boldsymbol{x}) \qquad \text{s.t.} \qquad g(\boldsymbol{x}) \leq 0. \tag{6}$$

One approach to include constraints is shown in [5] and [6], in Section III the procedure will be extended.

III. Modified Safe Bayesian Optimization

Performing a sequential subspace BO solves the feasibility issues for high-dimensional problems. Furthermore, it opens the applicability of a safe BO algorithm as SafeOpt [6] which relies in its current formulation on a discretized domain. Nevertheless, there are still issues regarding the safety options, e. g. the choice of β or, if set constant, reasonable kernel function hyperparameters $\boldsymbol{\theta}$. Utilizing commonly kernels as squared exponential or Matérn, $\boldsymbol{\theta}$ is composed of the signal variance σ_{f}^2, the length scales vector $\boldsymbol{l}$ and the noise variance σ_{n}^2. Setting the length scales to small and the signal standard deviation to high values would preserve safeness with a high probability as this allows the function to vary faster, however, at the cost of convergence rate. Therefore, a new optimization strategy will be introduced, ~~whereby~~ the safety constraints still holds and even for conservatively chosen hyperparameters good convergence rates are achieved.

Algorithm 1 gives an overview ~~about~~ the new strategy. In contrast to the initial approach, this strategy rejects the

Algorithm 1: Modified Safety Options (MoSaOpt)

Input: Initial safe set $\mathcal{S}_0$,
acquisition function $\alpha(\boldsymbol{x})$,
safety threshold T,
confidence β,
GP Prior G_0,
initial hyperparameters $\boldsymbol{\theta}$

Output: $\boldsymbol{x}^*$

for $i \leftarrow 1$ **to** n **do**
  if *exploration* **then**
    $\mathcal{S}_i \leftarrow \mathcal{S}_{i-1} \bigcup \{\boldsymbol{x} \in \mathcal{X} | u_(\boldsymbol{x}) \leq T\}$
    $\mathcal{G}_i \leftarrow \partial\mathcal{S}_i$
    $\mathcal{M}_i \leftarrow \{\boldsymbol{x} \in \mathcal{S}_i | l_(\boldsymbol{x}) \leq \min_{i=1:|\mathcal{O}|}(y_i)\}$
    $\boldsymbol{x}_i \leftarrow \arg\max_{\boldsymbol{x}\in\mathcal{G}_i}(w(\boldsymbol{x}))$
  else if *exploitation* **then**
    $\mathcal{M}_i \leftarrow \{\boldsymbol{x} \in \mathcal{S}_i | l_(\boldsymbol{x}) \leq \min_{i=1:|\mathcal{O}|}(y_i)\}$
    $\boldsymbol{\theta}_{\text{opt}} = \arg\max_{\boldsymbol{\theta}}(p(\boldsymbol{y}|X, \boldsymbol{\theta}))$
    $\boldsymbol{x}_i \leftarrow \arg\max_{\boldsymbol{x}\in\mathcal{M}_i}(\alpha(\boldsymbol{x}))$
  end
  $y_i \leftarrow f(\boldsymbol{x}_i) + \epsilon$
  $G_i \leftarrow G_{i-1} \bigcup \{\boldsymbol{x}_i, y_i\}$
end
$\boldsymbol{x}^* \leftarrow \arg\min_{\boldsymbol{x}_i\in\mathcal{O}} y_i$

trade-off between exploitation and exploration, instead, both ~~states~~ occurs subsequently. ~~Initially, the algorithm relies in exploration state, once switched to exploitation, exploration can never entered again.~~ Due to the fact that there exist no information about the location of the minimum the whole reachable set $\mathcal{R} = \{\boldsymbol{x} \in \mathcal{X} | f(\boldsymbol{x}) \leq T\}$ (T denotes the safety threshold that should never be exceeded) must be observed either.

In exploration state, the overall process remains as described in [5][6], whereby the definition of the safe set and minimizer set are adjusted for a minimization problem. The expanders are restricted to the boundary of the safe set, where the inputs with the largest gain of information are located. The exploration function

$$w(\boldsymbol{x}) = u(\boldsymbol{x}) - l(\boldsymbol{x}) = 2\beta\sigma(\boldsymbol{x}) \tag{7}$$

selects the expander with the highest uncertainty. Thus, the expansion of $\mathcal{S}$ is maximized and $\mathcal{R}$ is observed within the least possible number of steps. In exploitation state, the safe set is locked and only the minimizer set will be updated. With the gathered observations the hyperparameters are optimized via maximum likelihood estimation. Finally, a acquisition function, e. g. EI, is used to perform the optimization step with the fitted GPM.

The optimization of the hyperparameters

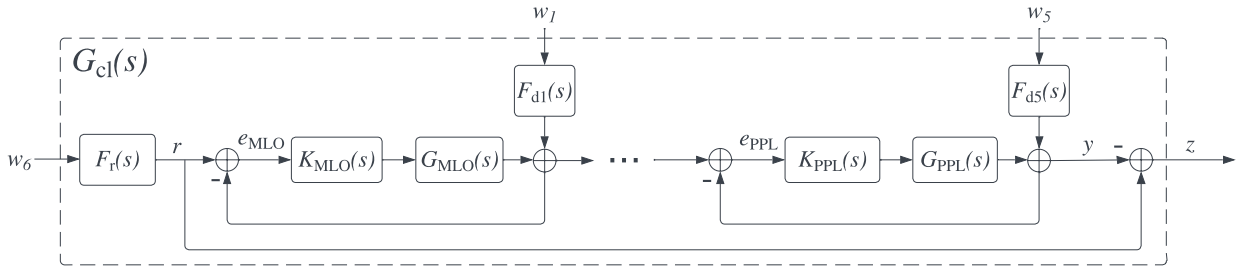

Fig. 2. Block diagram of the optical synchronization system for the simulation.

IV. Results

In this section different BO methods equipped with safe options are compared with respect the convergence rate and solution quality. In addition, this comparison is extended to non Bayesian algorithms Nelder-Mead [7] and set membership global optimization (SMGO-δ) [8]. In the second part the tuning of the optical synchronization system is described.

A. Comparison of BO Methods and Alternative Optimization Approaches

The comparison of the algorithms is based on a simulated system as illustrated in Figure 2, the filters $F_r(s)$ and $F_{d1} \dots F_{d5}$ colorize the additive white Gaussian noise (AWGN) signals $w_1 \dots w_6$ such that the signals have the same frequency behavior as the real noise source. The performance quantity is given by the RMS norm of performance output z. Using the fact that the input signals are AWGN with power spectral density (PSD) $S(\omega) = 1$, the optimization corresponds to a $\mathcal{H}_2$ minimization of the closed loop transfer function $G_{\mathrm{cl}}(s)$ as it follows from Parseval's theorem.

B. Tuning the Optical Sychronization System

V. Conclusion

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