GLASSES: Relieving The Myopia Of Bayesian Optimisation

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Abstract

We present GLASSES: Global optimisation with Look-Ahead through Stochastic Simulation and Expected-loss Search. The majority of global optimisation approaches in use are myopic, in only considering the impact of the next function value; the non-myopic approaches that do exist are able to consider only a handful of future evaluations. Our novel algorithm, GLASSES, permits the consideration of dozens of evaluations into the future. We show that the far-horizon planning thus enabled leads to substantive performance gains in empirical tests.

1 Introduction

Global optimisation is core to any complex problem where design and choice play a role. Within Machine Learning, such problems are found in the tuning of hyperparameters [14], sensor selection [5] or experimental design [10]. Most global optimisation techniques are myopic, in considering no more than a single step into the future. Relieving this myopia requires solving the *multi-step lookahead* problem: the global optimisation of an function by considering the significance of the next function evaluation on function evaluations (steps) further into the future. It is clear that a solution to the problem would offer performance gains. For example, consider the case in which we have a budget of two evaluations with which to optimise a function $f(x)$ over the domain $\mathcal{X} = [0, 1] \subset \mathbb{R}$. If we are strictly myopic, our first evaluation will likely be at $x = 1/2$, and our second then at only one of $x = 1/4$ and $x = 3/4$. This myopic strategy will thereby result in ignoring half of the domain $\mathcal{X}$, regardless of the second choice. If we adopt a two-step lookahead approach, we will select function evaluations that will be more evenly distributed across the domain by the time the budget is exhausted. We will consequently be better informed about f and its optimum.

There is a limited literature on the multi-step lookahead problem. [12] perform multi-step lookahead by optimising future evaluation locations, and sampling over future function values. This approach scales poorly with the number of future evaluations considered, and the authors present results for no more than two-step lookahead. [9] reframe the multi-step lookahead problem as a partially observed Markov decision process, and adopt a Monte Carlo tree search approach in solving it. Again, the scaling of the approach permits the authors to consider no more than six steps into the future.

There is a clear link between the multi-step lookahead problem and that considered in the literature as *batch* Bayesian optimisation. The two problems are distinct but related: the multi-step lookahead problem requires the challenging marginalisation over unknown future evaluation *locations*, in addition to the unknown future evaluation *values* also marginalised by batch approaches. Similarly to the state-of-the-art in multi-step lookahead, the batch literature provides only poor scaling with the number of evaluations. [6] present results for no more than six simultaneous function evaluations. [1, 2] use the surrogate model for f to generate 'fake' observations and avoid the marginalization step. This produce a large accumulation of errors that does not allow the use of these techniques for the collection of large batches.

We propose an algorithm, GLASSES, that provides scaling superior to existing alternatives.

1.1 Bayesian Optimisation with one step look-ahead

Let $f : \mathcal{X} \to \mathbb{R}$ be well behaved function defined on a compact subset $\mathcal{X} \subseteq \mathbb{R}^d$. We are interested in solving the global optimization problem of finding $\mathbf{x}_M = \arg\min_{\mathbf{x}\in\mathcal{X}} f(\mathbf{x})$. We assume that f is a *black-box* from which only perturbed evaluations of the type

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$y_i = f(\mathbf{x}_i) + \epsilon_i$, with $\epsilon_i \sim \mathcal{N}(0, \sigma^2)$, are available. The goal is to make a series of evaluations $\mathbf{x}_1, \dots, \mathbf{x}_n$ of f such that the the minimum of f is evaluated as soon as possible.

Assume that n points have been gathered so far, having a dataset $\mathcal{D}_0 = \{(\mathbf{x}_i, y_i)\}_{i=1}^N = (\mathbf{X}_0, \mathbf{Y}_0)$. Before collecting any new point, a surrogate probabilistic model for f is calculated. This is topically a Gaussian Process (GP) $p(f) = \mathcal{GP}(\mu; k)$ with mean function μ and a covariance function k, and whose parameters will be denoted by θ. Let $\mathcal{I}_0$ be the current available information: the conjunction of $\mathcal{D}_0$, the model parameters and the model likelihood type. Under Gaussian likelihoods, the predictive distribution for y_* at $\mathbf{x}_*$ is also Gaussian with mean posterior mean and variance

$$\mu(y_*|\mathcal{I}_0) = \mathbf{k}_\theta(\mathbf{x}_*)^\top [\mathbf{K}_\theta + \sigma^2 \mathbf{I}]^{-1} \mathbf{y},$$

and

$$\sigma^2(y_*|\mathcal{I}_0) = k_\theta(\mathbf{x}_*, \mathbf{x}_*) - \mathbf{k}_\theta(\mathbf{x}_*)^\top [\mathbf{K}_\theta + \sigma^2 \mathbf{I}]^{-1} \mathbf{k}_\theta(\mathbf{x}_*),$$

where $\mathbf{K}_\theta$ is the matrix such that $(\mathbf{K}_\theta)_{ij} = k_\theta(\mathbf{x}_i, \mathbf{x}_j)$, $\mathbf{k}_\theta(\mathbf{x}_*) = [k_\theta(\mathbf{x}_1, \mathbf{x}_*), \dots, k_\theta(\mathbf{x}_n, \mathbf{x}_*)]^\top$ [13].

Given the GP model, we now need to determine the best location to sample. Imagine that we only have one remaining evaluation before we need to report our inferred location about the minimum of f. Denote by $\eta = \min \mathbf{Y}_0$, the current best found value. We can define the loss of evaluating f this last time at $\mathbf{x}_*$ assuming it is returning y_* as

$$\lambda(y_*) \triangleq \begin{cases} y_*; & \text{if} \quad y_* \leq \eta \\ \eta; & \text{if} \quad y_* > \eta. \end{cases}$$

Note that the loss corresponds to the new observed minimum, $\min(\eta, y_*)$. The expectation of this loss is therefore given by

$$\Lambda_1(\mathbf{x}_*|\mathcal{I}_0) \triangleq \mathbb{E}[\min(y_*, \eta)] = \int \lambda(y_*) p(y_*|\mathbf{x}_*, \mathcal{I}_0) dy_*$$

where the subscript in Λ refers to the considered future evaluations, one in this case. Giving the properties of the GP, $\Lambda_1(\mathbf{x}_*|\mathcal{I}_0)$ can be computed in closed form for any $\mathbf{x}_* \in \mathcal{X}$. In particular, for Φ the usual Gaussian cumulative distribution function we have that

$$\begin{aligned} \Lambda_1(\mathbf{x}_*|\mathcal{I}_0) &\triangleq \eta \int_\eta^\infty \mathcal{N}(y_*; \mu, \sigma) dy_* \\ &+ \int_{-\infty}^\eta y_* \mathcal{N}(y_*; \mu, \sigma) dy_* \\ &= \eta + (\mu - \eta)\Phi(\eta; \mu, \sigma) - \sigma \mathcal{N}(\eta, \mu, \sigma), \end{aligned} \tag{1}$$

where we have abbreviated $\sigma(y_*|\mathcal{I}_0)$ as σ and $\mu(y_*|\mathcal{I}_0)$ as μ. Finally, the case of having one future evaluation we would select the point where $\Lambda_1(\mathbf{x}_*|\mathcal{I}_0)$ gives the minimum value, which can be obtained by any gradient descent algorithm [11].

[8] [7] [14] [3]

1.2 Looking many steps ahead: Challenge and contribution of this work

$$\begin{aligned} \Lambda_n(\mathbf{x}^\star|\mathcal{I}_0) &= \int \lambda(y_n) \prod_{j=1}^n p(y_j|\mathbf{x}_j, \mathcal{I}_{j-1}) p(\mathbf{x}_j|\mathcal{I}_{j-1}) \\ &\quad dy_* \dots dy_n d\mathbf{x}_2 \dots d\mathbf{x}_n \end{aligned}$$

2 The glasses Algorithm

2.1 Predicticting BO future steps

2.2 Computing the Expected Loss

Our goal is to compute $E_{p(\mathbf{y})}[\min(\mathbf{y}, \eta)]$ for $\mathbf{y} = \{y_1, \dots, y_n\}$ and $p_0(\mathbf{y}) \sim \mathcal{N}(\mathbf{y}; \mu, \Sigma)$. This approximates the n-steps ahead expected loss $\Lambda_n(\mathbf{x}_*)$. The goal of this section is to write $E_{p(\mathbf{y})}[\min(\mathbf{y}, \eta)]$ in a way that it is suitable to be computed by Expectation Propagation. Next proposition will do the work (I think).

Proposition 1 *It holds that*

$$\begin{aligned} \mathbb{E}[\min(\boldsymbol{y}, \eta)] &= \eta \int_{\mathbb{R}^n} \prod_{i=1}^n h_i(\boldsymbol{y}) \mathcal{N}(\boldsymbol{y}; \mu, \Sigma) d\boldsymbol{y} \\ &+ \sum_{j=1}^n \int_{\mathbb{R}^n} y_j \prod_{i=1}^n t_{j,i}(\boldsymbol{y}) \mathcal{N}(\boldsymbol{y}; \mu, \Sigma) d\boldsymbol{y} \end{aligned}$$

where $h_i(\boldsymbol{y}) = \mathbb{I}\{y_i > \eta\}$ *and*

$$t_{j,i}(\boldsymbol{y}) = \begin{cases} \mathbb{I}\{y_j \leq \eta\} & \textit{if} \quad i{=}j \\ \\ \mathbb{I}\{0 \leq y_i - y_j\} & \textit{otherwise.} \end{cases}$$

All the elements in (1) can be rewritten in a way that can be computed using EP but the work in [4].

- The second term is a Gaussian probability on unbounded polyhedron in which the limits are aligned with the axis.
- The first term requires some more processing but it is still computable under the assumptions in [4]. Let $\mathbf{w}_j$ the jth canonical vector. Then we have that

$$\begin{aligned} \int_{\mathbb{R}^n} y_j \prod_{i=1}^n t_{j,i}(\mathbf{y}) \mathcal{N}(\mathbf{y}; \mu, \Sigma) d\mathbf{y} &= \mathbf{w}^T \int_{\mathbb{R}^n} \mathbf{y} \prod_{i=1}^n t_{j,i}(\mathbf{y}) \mathcal{N}(\mathbf{y}; \mu \\ &= \mathbf{w}^T E[\mathbf{y}] z_j \end{aligned}$$

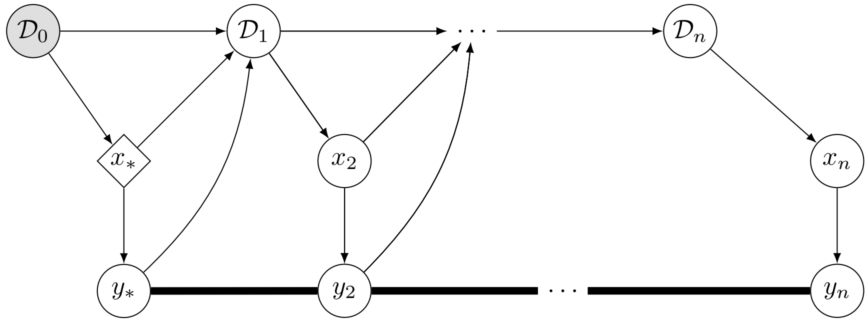

Figure 1: A Bayesian network describing the n-step lookahead problem. The shaded node ($\mathcal{D}_0$) is known, and the diamond node (x_*) is the current decision variable. All y nodes are correlated with one another under the GP model.

where the expectation is calculated over the normalized distribution over P_j, the one EP approximates with $q(\mathbf{y})$, and for z_j being the normalizing constant

$$z_j = \int_{\mathbb{R}^n} \prod_{i=1}^{n} t_{j,i}(\mathbf{y}) \mathcal{N}(\mathbf{y}; \mu, \Sigma) d\mathbf{y}$$

Because EP does moments matching, both the normalizing constant and the expectation are available.

2.3 Algorithm

3 Results

4 Conclusions

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Algorithm 1 Decision process of the GLASSES algorithm.

Input: dataset $\mathcal{D}_0 = \{(\mathbf{x}_0, y_0)\}$, number of remaining evaluations (n).
Fit a GP with kernel k to $\mathcal{D}_0$.
Select $\mathbf{x}_{1*}, \dots, \mathbf{x}_{r*}$ representer points of the loss.
for $j = 1$ **to** r **do**
  Take s samples from a conditional n-DPP of kernel k given $\mathbf{x}_{j*}$.
  Approximate the expected loss at $\mathbf{x}_j^*$ for the s samples computing $E[\min(\mathbf{y}, \eta)]$.
  Average the expected loss for the s samples and obtain $\tilde{\Lambda}_n(\mathbf{x}_j^*)$.
end for
Approximate $\Lambda_n(\mathbf{x}_*)$ fitting a GP_2 to $\{(\mathbf{x}_{j*}, \tilde{\Lambda}_n(\mathbf{x}_{j*})\}_{j=1}^r$ with posterior mean μ_2.
Returns: New location at $\arg\min_{x \in \mathcal{X}} \{\mu_2(\mathbf{x})\}$.

Supplementary materials for: 'GLASSES: Relieving The Myopia Of Bayesian Optimisation"

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S1 Proofs

Proof 1 *Denote by*

$$
\begin{aligned}
E_{p(\boldsymbol{y})}[\min(\boldsymbol{y},\eta)] &= \int_{\mathbb{R}^n} \min(\boldsymbol{y},\eta)\mathcal{N}(\boldsymbol{y};\mu,\Sigma)d\boldsymbol{y} \\
&= \int_{\mathbb{R}^n-(\eta,\infty)^n} \min(\boldsymbol{y})\mathcal{N}(\boldsymbol{y};\mu,\Sigma)d\boldsymbol{y} + \int_{(\eta,\infty)^n} \eta\mathcal{N}(\boldsymbol{y};\mu,\Sigma)d\boldsymbol{y}
\end{aligned}
$$

The first term can be written as follows:

$$
\int_{\mathbb{R}^n-(\eta,\infty)^n} \min(\boldsymbol{y})\mathcal{N}(\boldsymbol{y};\mu,\Sigma)d\boldsymbol{y} = \sum_{j=1}^{n}\int_{P_j} y_j\mathcal{N}(\boldsymbol{y};\mu,\Sigma)d\boldsymbol{y}
$$

where $P_j := \{\boldsymbol{y} \in \mathbb{R}^n - (\eta,\infty)^n : y_j \leq y_i,\ \forall i \neq j\}$. *We can do this because the regions* P_j *are disjoint and it holds that* $\cup_{j=1}^n P_j = \mathbb{R}^n - (\eta,\infty)^n$. *Also, note that the* $\min(\boldsymbol{y})$ *can be replaced within the integrals since within each* P_j *it holds that* $\min(\boldsymbol{y}) = y_j$. *Rewriting the integral in terms of indicator functions we have that*

$$
\sum_{j=1}^{n}\int_{P_j} y_j\mathcal{N}(\boldsymbol{y};\mu,\Sigma)d\boldsymbol{y} = \sum_{j=1}^{n}\int_{\mathbb{R}^n} y_j \prod_{i=1}^{n} t_{j,i}(\boldsymbol{y})\mathcal{N}(\boldsymbol{y};\mu,\Sigma)d\boldsymbol{y} \tag{S.1}
$$

where $t_{j,i}(y) = \mathbb{I}\{y_i \leq \eta\}$ *if* $j = i$ *and* $t_{j,i}(y) = \mathbb{I}\{y_j \leq y_i\}$ *otherwise.*

The second term can be written as

$$
\int_{(\eta,\infty)^n} \eta\mathcal{N}(\boldsymbol{y};\mu,\Sigma)d\boldsymbol{y} = \eta\int_{\mathbb{R}^n} \prod_{i=1}^{n} h_i(\boldsymbol{y})\mathcal{N}(\boldsymbol{y};\mu,\Sigma)d\boldsymbol{y} \tag{S.1}
$$

where $h_i(\boldsymbol{y}) = \mathbb{I}\{y_i > \eta\}$. *Merge (S.1) and (1) to conclude the proof.*