

1 We thank the reviewers for their insightful comments. First, we want to highlight that the main contribution of this paper
 2 is a novel and efficient realization of general multi-step lookahead BO, which has *never been successfully attempted*
 3 before. This is a long-standing and notoriously hard problem (see, e.g., [22]) and we now filled in the gap. The
 4 generality of our approach with differentiable, multi-step trees allows swapping in different utility functions to get
 5 different nonmyopic BO policies, or to solve an entirely different problem such as Bayesian quadrature. We will first
 6 address some common issues, then individual ones.

7 **Number of samples** (branching factor m_i): Indeed this part could benefit from further analysis. From our results,
 8 we see even one sample (i.e., multi-path) produced reasonable results. We attempted to systematically study how m_i
 9 would change the performance, only to realize it was much more complicated than we thought. First, more samples
 10 means higher approximation accuracy, however, it also increases the dimension of the optimization dramatically, which
 11 makes it harder to optimize; poorer optimization could counter the benefit of higher accuracy. Second, even if we
 12 could optimize it perfectly, would it necessarily be better to have a more accurate approximation? In theory, yes, but in
 13 practice, given that “all models are wrong” and hence more lookahead may hurt (see [33]), it is not necessary that more
 14 accurate approximation of a “wrong” expected utility will lead to better results – perhaps a rough estimate is all we
 15 need in practice. That said, we are not arguing against lookahead policies, but merely pointing out that some seemingly
 16 simple questions may not be so simple. In-depth analysis could merit a standalone paper.

17 **Sec. 4:** We realize that adding this dense section makes the paper more challenging to read. However, it presents
 18 essential techniques that make our method efficient. We will improve the clarity of the presentation.

19 **R1:** Proposition 1 is simply saying $\max_{x,y} f(x,y) = \max_x \max_y f(x,y)$, which is a key idea for one-shot optimization.
 20 We assume the decision variable of the current step to be $x = x_1, y = y_1$.

21 **R3: Theoretical guarantees:** In expectation, full-lookahead (i.e., the optimal policy) is guaranteed to be better than
 22 greedy by definition. In general, it can be very challenging to prove or disprove k -step rolling horizon is always better
 23 than 1-step in expectation. Note all recent contributions to nonmyopic BO are also lacking in this regard [22, 11, 18, 15].

24 **Higher speedups on GPU:** this is inaccurate, we intended to say “speed” is higher.

25 **R5: Warm-start:** As we noted, the joint objective is a highly compli-
 26 cated high-dimensional function (up to around one thousand dimensions),
 27 and how to optimize it is critical. We use a perturbed version of the so-
 28 lution from the previous iteration to initialize the optimization, inspired
 29 by the conjecture that the surface would not change too much and there
 30 should be a nearby optimum. We did experiment without warm-start, for
 31 example, the average GAP of 3-step on the synthetic functions is about

	EI	2-path	3-path
branin	<i>0.993</i>	0.997	<i>0.989</i>
rosenbrock2	<i>0.972</i>	0.984	<i>0.968</i>
hartmann3	1.000	1.000	1.000
hartmann6	0.974	0.976	<i>0.975</i>
levy2	0.987	<i>0.982</i>	<i>0.970</i>

32 0.63, which is much worse than with warm-start (0.747, see Table 2 of the paper) (note that this is still much better
 33 than EI). We found warm-starting to result in very large improvements. Further study is needed to fully understand its
 34 effectiveness. **Gaussian-Hermite (GH) vs. MC quadrature:** We used GH in our experiments only to follow previous

35 work on nonmyopic BO (see e.g., [18, 32]), and it’s also a well-established quadrature rule for 1d integral against a
 36 Gaussian. We did experiment with quasi-MC (Sobol) for multi-step and multi-path, for multi-step GH tends to be better,
 37 but for multi-path we did not observe considerable differences. We will present both results in the camera-ready version.

38 **Relation to prior work:** The derivation of the optimal policy is simply an instantiation of the well-known Bellman
 39 equation, and it has been derived in several previous papers in various formats, including [18, 22, 15]. We are not
 40 inventing multi-step lookahead, but providing a novel and efficient solution technique with promising empirical results.

41 **Omitted entries:** Fig. 4(a) plots the last two rows of Table 2, and the omitted entries are actually complementary. We
 42 arranged it this way only to avoid oversized table and cluttered plot. We can add everything back to reduce confusion.

43 **Outperform all baselines:** Here baseline means EI, ETS and 12.EI.s; 12-ENO is a variant of our method. We will
 44 clearly delineate our methods vs baselines in the camera-ready. **Selection of benchmarks:** We fully adopted the

45 benchmarks used in [15], and we also argue that nonmyopic methods have significant advantage over myopic methods
 46 on “hard” function, but not worse on “easy” ones. To address your concern, we arbitrarily chose some commonly used
 47 “easy” benchmarks and ran EI, 2-path, 3-path for 100 repeats. Results are shown in the above table. We can see the

48 tested multi-step variants are never significantly worse than EI. We are happy to add the results of all 31 benchmarks in
 49 [15] to the camera-ready version. **Zeroth-order initialization:** Thanks for your interesting suggestion, we can certainly
 50 try using DIRECT, CMA-ES or even BO to initialize the optimization. **Emphasis on Bo/GPyTorch:** We stress that

51 one-shot optimization is not tied to any underlying implementation framework. However, one of our contributions is
 52 a generic implementation that was facilitated to a large degree by the abstractions, efficient inference methods, and
 53 auto-differentiation capabilities in Bo/GPyTorch.

54 Again, we appreciate all the concerns raised by the reviewers and will certainly add relevant details to the camera-ready
 55 version to address them. However, most of the main points are actually deep questions that deserve future research. Our
 56 contributions are fundamental and provide a versatile framework that enables studying these important questions.