Bayesian optimization (BO) has been used in many applications to optimize systems whose performance is expensive to evaluate, such as a robot’s walking motion (Antonova et al., 2017), deep brain stimulation (Grado et al., 2018), or machine learning model hyperparameters (Snoek et al., 2012). BO has also been generalized to situations where one can only obtain the performance of the system in the form of a binary output, corresponding, for example, to whether the system passes/fails a test (Tesch et al., 2013). Examples of binary Bayesian optimization (BBO) include testing whether a robot is able to successfully maneuver across a given environment, or the optimization of a model’s hyperparameters, by early-stopping the training of under-performing models while continuing others (Zhang et al., 2019). In these cases, the way the system is tested is critical in optimizing its performance. For example, if we ask a robot to move across an impossibly complex environment (e.g. filled with obstacles and pot-holes), it will always fail, leaving us none the wiser as to how to improve its performance.

A similar problem arises in preferential Bayesian optimization (PBO), where the performance of a system is evaluated via a set of comparisons between different parameter settings (Brochu et al., 2010). For example, PBO was used to improve the performance of hearing aid devices, by asking patients to evaluate which of two parameter settings they preferred, when listening to excerpts of music (Nielsen et al., 2014). In this example, the context (i.e. the audio stimuli) clearly plays a role in determining how much information is gained from subjects’ responses: an audio stimulus that was overly simple (e.g. a single monotone pitch) or random (e.g. white noise) would result in non-informative responses from subjects, impeding progress in optimizing the hearing device for most daily settings.

Here we show how to extend previous BO algorithms to deal with these two related problems, in which the measured performance of a system takes the form of a binary, context-dependent, output. We then show how this problem can be efficiently solved by applying a simple heuristic, where BO is used to maximize the system’s performance, while Bayesian active learning is used to choose a new context, such that the observed binary output (e.g. whether the system passed/failed a given test, or a comparison between two parameter settings) is maximally informative about the system’s performance. We show that our resulting algorithm per-
forms competitively on a range of benchmark problems. Further, we illustrate the relevance of our algorithm by applying it to a real-world problem, where the goal is to find the correct optical correction required to optimize a patient’s vision, based on their binary responses in a psychophysics task.

2 Problem statement

Consider a system, whose performance can be quantified by a function, \( g(x) \). For example, \( g(x) \) could represent the visual acuity (VA) of a patient fitted with glasses with optical parameters, \( x \). We are interested in solving the global optimization problem:

\[
x^* = \arg \max_{x \in \mathcal{X}} g(x),
\]

where \( \mathcal{X} \) is a bounded set denoted as the search space.

We consider the case where the performance of the system cannot be evaluated directly, but instead, can be assessed by observing whether it passes/fails a test in a given context, parameterized by \( s \). For example, we could test whether a subject (fitted with glasses with optical parameters, \( x \)) can correctly identify a visual stimulus, parameterized by \( s \), presented on-screen. The outcome of such a test is denoted by a binary variable, \( c \), with success probability given by:

\[
p(c = 1|x, s) = \Phi(f(s, x)),
\]

where \( \Phi \) is the normal cumulative distribution function, and \( f(s, x) \) is a function describing performance of the system with parameters \( x \) and given a context \( s \).

If we are to optimize the system based on observed binary outcomes, \( c \), the probability that the system passes a test in a given context, \( s \) (determined by \( f(s, x) \)) must be closely related to its overall performance, \( g(x) \). For simplicity, we begin by assuming that the same configuration, \( x^* \), maximizes performance in all contexts, such that:

\[
\forall s \in \mathcal{S}, \quad \arg \max_{x \in \mathcal{X}} g(x) = \arg \max_{x \in \mathcal{X}} f(s, x),
\]

where \( \mathcal{S} \) is a bounded set denoted as the context space. In our previous example, this would imply that the optical correction that maximizes VA also maximizes the subject’s performance in identifying a range of different visual stimuli, parameterized by \( s \). This condition will be true for a broad range of situations in which \( f(s, x) \) takes the form:

\[
f(s, x) = q(h(s)g(x) + b(s))
\]

where \( h(s) \) is non-negative for all \( s \), and \( q(\cdot) \) is a monotonically increasing one-dimensional function. Plugging this back into Eqn. 2, we have:

\[
p(c = 1|s, x) = \Phi[q(h(s)g(x) + b(s))].
\]

We can think of \( b(s) \) and \( h(s) \) as controlling the difficulty of the test. Without loss of generality, we can assume that \( g(x) \geq 0 \) for all \( x \). For large \( h(s) \) the probability of success will saturate close to 1 for all \( x \): i.e., the task is easy, so the system always passes the test. In contrast, when \( h(s) \) is close to zero, the system will perform close to baseline, with success probability \( \Phi(q(b(s))) \). In both these extreme cases, little information is gained about the parameters, \( x \), that optimize performance, since the success probability depends only weakly on \( g(x) \). Our goal, therefore, is to find a sampling rule that selects \( (s, x) \) on each trial so as to appropriately set the difficulty of the task, and efficiently optimize \( g(x) \) in a limited number of trials.

3 Contextual binary Bayesian optimization

3.1 Inference

As is standard in BO, we will build a surrogate model of \( f(s, x) \), by assuming a zero-mean Gaussian process (GP) prior, such that \( f \sim GP(0, k(\cdot, \cdot)) \), where \( k \) is a kernel function. When the observed outcome is binary, the posterior probability distribution over \( f \) cannot be written analytically but must be approximated. While a number of different approximations schemes exist, here we use the Laplace approximation, since it is standard and simple to implement (Rasmussen & Williams 2006). However, our approach could be applied to other approximation schemes such as expectation propagation (Minka 2001; Seeger 2002).

Ideally, the kernel should reflect prior knowledge about the objective, such as the fact that the optimum does not depend on the context. This can be done, for example, by assuming a multiplicative structure of the function of the form \( f(s, x) = h(s)g(x) \), which in practice can be incorporated by using a kernel that decomposes as: \( k(s, x, s', x') = k_1(s, s')k_2(x, x') \). Moreover, \( h \) should be constrained to be positive. In practice, we did not use this latter constraint in our experiments, as this would make the inference more difficult and it did not seem to impede performance.

3.2 Knowledge gradient acquisition rule

Having inferred a Bayesian model of the objective function, \( p(f|\mathcal{D}) \), the next step of any BO algorithm is to select new parameters, \( x \) and \( s \), to evaluate the objective. To do this, we extended the ‘knowledge gradient’ (KG) acquisition rule, developed previously for BO with continuous outputs (Frazier et al. 2009), to contextual BBO.

We first explain our binary KG algorithm for standard
BBO (i.e. with no contextual variable, s). As in standard KG, the reported solution of the optimization routine at iteration t is assumed to be the maximum of the posterior mean of the GP after observing data \( \mathcal{D}_t = \{ \{ x_1, c_1 \}, \{ x_2, c_2 \}, \ldots, \{ x_t, c_t \} \} \), that is:

\[
\mu_{t+1} = \arg \max_{x} \mathbb{E} [g(x)|\mathcal{D}_t]. \tag{6}
\]

The KG corresponds to the expected increase in \( \mu^* \) if we are allowed one additional observation, \( \{ x_{t+1}, c_{t+1} \} \):

\[
\text{KG}(x_{t+1}) = \sum_{c_{t+1}=0,1} p(c_{t+1}|x_{t+1}, \mathcal{D}_t) \mu^*_{t+1, x_{t+1}, c_{t+1}} - \mu^*_{t+1, x_{t+1}} \tag{7}
\]

where \( p(c_{t+1} = 1|x_{t+1}, \mathcal{D}_t) = \mathbb{E}_g[\Phi(g(x_{t+1}))|\mathcal{D}_t] \), and \( \mu^*_{t+1, x_{t+1}, c_{t+1}} \) is the maximum of the posterior mean after observing \( \{ \mathcal{D}_t, \{ x_{t+1}, c_{t+1} \} \} \). In supplementary B we show that the gradient of KG, required to maximize it efficiently, can be computed when using the Laplace approximation (see supplementary A) to approximate the GP posterior.

To extend the above KG acquisition function to contextual BBO, we simply add the context, s, to the system parameters, x, and replace \( g(x) \) with \( f(s, x) \). In this case, the maximization in Eqn 5 is performed only over the system parameters, x, given a fixed context, s0 (see supplementary C).

Computing the KG acquisition function is impractically slow for problems with moderately high dimensions, as its computation requires performing two nested optimizations: the optimization required for the Laplace approximation of the GP posterior (see supplementary C), and the maximization in Eqn 6. Thus, we looked for an alternative, that could scale to larger problems.

### 3.3 Sequential algorithm for choosing system parameters, x and context, s

In our set-up, the parameters, x, and s, play two very different roles. The system parameters x determine the system’s underlying performance, \( g(x) \), which we want to maximize. The context, s, determines how much information we gain about the system’s performance from binary observations, c. We therefore decided to choose x and s sequentially, using different heuristics: first, \( x_{t+1} \) was chosen using binary BO, so as to optimize the system’s performance; next, \( s_{t+1} \) was chosen using Bayesian active learning, to maximize the information we obtain from the binary observation, \( c_{t+1} \).

#### 3.3.1 Choosing x using Bayesian optimization

We tested two different acquisition rules for selecting \( x_{t+1} \): GP Upper Credible Bound (GP-UCB) (Srinivas et al., 2010), and Thompson Sampling (TS) (Thompson, 1933).

Thompson sampling (TS) involves choosing \( x_{t+1} \) by sampling from the distribution \( p(x^*|\mathcal{D}_t) \), where \( x^* \) is defined, for a given objective function, as \( x^* = \arg \max_{x} f(x, s) \) (note that, from Eqn 5, \( x^* \) is independent of s). In supplementary section C we describe how to efficiently sample from \( p(x^*|\mathcal{D}_t) \) in the context of GP classification and preference learning.

Second, we implemented a generalization of UCB to binary outputs, where \( x_{t+1} \) is chosen by maximising the following acquisition function:

\[
\alpha_{\text{UCB}}(x) = \mathbb{E}(\Phi(f(x, s))) + \beta \sqrt{\mathbb{V}(\Phi(f(x, s)))}, \tag{8}
\]

where a constant \( \beta \) (set to \( \beta = \Phi^{-1}(0.95) \)) sets the balance between exploitation (first term on right hand side) and exploration (second term on right hand side). See Fauvel & Chalk (2021) for details on how to analytically compute this acquisition function and its gradient.

#### 3.3.2 Choosing s using Bayesian active learning

After choosing the system parameters, \( x_{t+1} \), the next step is to select a context \( s_{t+1} \) such that the observation, \( c_{t+1} \) will be maximally informative about the underlying function \( f(\cdot, x_{t+1}) \). To do this, we used the Bayesian Active Learning by Disagreement (BALD) algorithm, developed by Houlsby et al. (2011).

For a given \( x_{t+1} \), the context \( s_{n+1} \) is chosen so as to maximize the mutual information between the observation \( c_{t+1} \) and the objective function \( f(\cdot, x_{t+1}) \),

\[
I(c_{t+1}, f|s_{t+1}, x_{t+1}) = H(c_{t+1}|s_{n+1}) - \mathbb{E}_f[H(c_{t+1}|x_{t+1}, s_{n+1}, f)], \tag{9}
\]

where \( H(c_{t+1}|x_{t+1}, s_{n+1}) \) is the total entropy of \( c_{t+1} \), and \( \mathbb{E}_f[H(c_{t+1}|x_{t+1}, s_{n+1}, f)] \) is the conditional entropy of c, given the latent function \( f(\cdot, x_{t+1}) \). (Note that all three terms are also conditioned on the observed data, \( \mathcal{D}_t \), which was removed from the equation for notational simplicity). This acquisition criterion can be efficiently approximated (Houlsby et al., 2011).

### 3.4 Preferential Bayesian optimization

We next considered how to extend our method to preferential optimization (PBO). In standard PBO, Bocian...
The functions in this scenario is straightforward. Likewise, our sequential acquisition rule can be generalized to this scenario by selecting the duel \((s, x, x')\) using PBO, and then choosing the context of the duel \(s\) using Bayesian active learning.

In our experiments, we selected system parameters using either: (i) the KernelSelfSparring (KSS) algorithm [Sui & Burdick, 2017], which is a simple extension of TS, described above, or (ii) the Maximally Uncertain Challenge (MUC) acquisition rule, described in [Fauvel & Chalk, 2021]. Contextual parameters, \(s\), were then selected using Bayesian active learning by disagreement (BALD; see previous section).

### 4 Experiments with synthetic test functions

To evaluate the performance of our method, we ran optimization experiments on a set of 34 functions from a widely used virtual library for optimization experiments [Surjanovic & Bingham, 2021]. The functions in this library exhibit a diversity of behaviors that occur in real-life optimization problems.

For each objective function, we inferred the hyperparameters for three different kernels (squared exponential, Matérn 3/2 and Matérn 5/2) using maximum likelihood estimation with 1000 randomly chosen samples. We then determined for each function the kernel that best described the function by measuring the root-mean-squared error on 3000 points. The benchmark functions are listed in supplementary H. In all cases, we used the Laplace approximation to approximate the posterior over the objective, \(p(f|\mathcal{D})\).

We introduced a scalar context variable \(s \in [0, 1]\), so that for a test function \(g\) the response of a system query is 1 with probability \(P(s, x) = \Phi(sg(x))\) and 0 otherwise.

To take the context variable into account when building the GP surrogate model, we used the following kernel: for a base kernel \(k\) determined using the aforementioned procedure, we used: \(k_s((x, s), (x', s')) = ss'k(x, x')\).

To compare the different algorithms, we used the stratified analysis method proposed by Dewancker et al. (2016). Briefly, for each benchmark function, we performed pairwise comparisons between acquisition functions using the Mann-Whitney U test at \(\alpha = 5 \times 10^{-4}\) significance on the best value found at the end of the optimization sequence. This determines a partial ranking based on the number of wins.

Ties are then broken by running the same procedure, but based on the Area Under Curve, which is related to the speed at which the algorithm reaches the optimum. This generates a new partial ranking, based on which a Borda score ([Dwork et al., 2001] is attributed to each acquisition function (the Borda score of a candidate is the number of candidates with a lower rank). Then, rankings from different benchmarks are aggregated by summing the Borda scores to establish a global ranking. This can be seen as a weighted vote from each benchmark function.

### 4.1 Binary Bayesian optimization in adaptive contexts

We then ran optimizations on each function for 40 different random number generator seeds, on 60 iterations. The initial number of random samples was set to 5.

We termed the sequential acquisition rules in the binary feedback scenario TS with active learning by disagreement (TS-ALD) and GP-UCB with active learning by disagreement (UCB-ALD). We termed the generalization of KSS and MUC to the contextual scenario KSS-ALD and MUC-ALD.

We compared the different acquisition rules: the contextual binary knowledge gradient (cBKG), UCB-ALD and TS-ALD, with the following controls:

- Fully random, in which \((s, x)\) was chosen at random at each iteration,
- \(x\) chosen using TS and \(s\) chosen randomly,
- \(x\) chosen using UCB and \(s\) chosen randomly,
- \((s, x)\) selected using BALD.

To avoid saturation effects when transforming the benchmark functions through the non-linearity, we scaled the functions so that they have mean 0 and variance 1. Examples of regret curves are presented in figure [1] and the results of the stratified analysis are summarized in table [4]. More detailed results showing...
pairwise comparisons between acquisition functions are presented in table S1.

UCB-ALD and TS-ALD show superior performance compared to cBKG [1], despite the fact that, compared to cBKG, where \( x \) and \( s \) are jointly selected, these sequential decision strategies induce an adaptivity gap (Jiang et al., 2019). Here, we used the Laplace approximation, given that Expectation Propagation (EP) is known to improve performance compared to the Laplace approximation and that the gradient of cBKG with EP seems intractable, this suggests that TS-ALD and UCB-ALD are better acquisition functions in general. The three heuristics outperformed the different controls.

Table 1: Comparison of acquisition functions on benchmarks. UCB-ALD largely outperforms the other rules. Importantly, the sequential acquisition rules (TS-ALD and UCB-ALD) outperform cBKG.

| Acquisition rule         | Rank | Borda score |
|--------------------------|------|-------------|
| UCB-ALD                  | 1    | 144         |
| TS-ALD                   | 2    | 83          |
| cBKG                     | 3    | 59          |
| UCB (random context)     | 4    | 46          |
| BALD                     | 5    | 35          |
| TS (random context)      | 6    | 19          |
| Random                   | 7    | 10          |

4.2 Preferential Bayesian optimization in adaptive contexts

We then evaluated the performance of our sequential acquisition rules in their generalization to the case of preferential judgments: KSS-ALD and MUC-ALD. Given the limited performance of BKG in the previous experiments and the fact that the preferential version of Knowledge Gradient is impractically slow, we did not evaluate this acquisition function.

We then ran optimizations on each test function for 40 different random number generator seeds, on 60 iterations. We compared KSS-ALD and MUC-ALD to the following controls:

- Fully random, in which \((s, x_1, x_2)\) was chosen at random at each iteration,
- \(x\) chosen using KSS and \(s\) chosen randomly,
- \(x\) chosen using MUC and \(s\) chosen randomly,
- \((s, x_1, x_2)\) selected using BALD.

Examples of regret curves are shown in figure 2 and the results of the stratified analysis are summarized in figure 2. More detailed results showing pairwise comparisons between acquisition functions are presented in table S2. Again, adaptive selection of the context leads to superior performance compared to controls.

Table 2: Comparison of acquisition functions on benchmarks. The sequential acquisition rules outperform the controls. MUC-ALD is the most efficient acquisition function.

| Acquisition rule           | Rank | Borda score |
|----------------------------|------|-------------|
| MUC-ALD                    | 1    | 99          |
| KSS-ALD                    | 2    | 37          |
| Kernel Self-Sparring       | 3    | 22          |
| BALD                       | 4    | 9           |
| Random                     | 5    | 5           |

5 Application: adaptive optimization in psychometric measurements

To illustrate the relevance of our algorithm, we considered the problem of optimizing the parameters of a lens to improve a patient’s vision based on their responses in a visual task.

Different types of visual defects typically result in different types of error (myopia results in ‘spherical refractive error’, \( S \); astigmatism results in ‘cylindrical refractive error’, \( C \)). These errors induce image blur, but can be corrected by optimizing different optical parameters of a patient’s lenses. However, patients’ visual performance are typically assessed indirectly, for example by testing their performance in a visual task (e.g. asking patients to identify a letter, presented onscreen). Clearly, the task used to test patients’ visual performance will play a critical role in optimizing their vision. If the task is too easy/difficult (e.g. the letters presented onscreen are too small/large) then patients will always succeed/fail, and little information will be gained as to how to optimize their optics. In the following, we show our contextual BO algorithm can be used to address this problem.

5.1 Model of patients’ responses

A simple formula relates the spherico-cylindrical error (measured in diopters \((\delta)\)) to image blur \( \beta \) (Raasch, 1995; Blendowske, 2015):

\[
\beta = \sqrt{\frac{1}{2}(S^2 + (S + C)^2)}
\]  

We are thus trying to find the parameters of the optics \( x = (S, C) \) that minimize \( \beta \), or equivalently, minimize visual acuity (VA), defined as the log of the minimum angle of resolution (MAR, measured in minutes of
Contextual Bayesian optimization with binary outputs

Figure 1: Results across three different objective functions and different methods in binary BO with adaptive contexts. Solid lines correspond to the mean value of the inferred maximum across the 40 repetitions. Shaded areas correspond to standard error on the mean. Either cBKG, UCB-ALD, or TS-ALD outperform the other acquisition rules, however, there is a lot of variability from one experiment to another. The cBKG acquisition rule tends to be less robust than the sequential heuristics.

We consider a simple model of subjects performing an n-alternatives forced-choice visual task, such as identifying a letter on a screen. The size of the letter, \( s \) (measured in log of the visual angle, in minutes of arc), determines the difficulty of this task. For a given optical correction \( x \), the probability of correct response is well described by a psychometric function (see e.g. Fülep et al. (2019) or Tokutake et al. (2011)):

\[
P(c = 1|s) = \gamma + (1 - \gamma)\Phi(a(s)x + b(s)),
\]

where \( \gamma \) is the chance probability of success, \( a \) and \( b \) are the slope and intercept of the psychometric curve. For \( \gamma \) large enough, we have \( P(c = 1|s) \approx \Phi(a(s)x + b(s)) \). Since in practice, with a letter chart, \( \gamma = \frac{n}{26} \), we will make this simplifying assumption in building our surrogate model.

We put a GP prior on \( f \), with zero mean and kernel \( k_\psi \) defined as:

\[
k_\psi((s, x), (s', x')) = \theta s s' + k(x, x')
\]

This kernel reflects the structure of the function \( f \) (see equation 14) with the assumption \( \gamma \approx 0 \) (see supplementary E).

We used a squared exponential kernel as \( k \). To minimize the effect of kernel hyperparameters, we simulated the response to 1000 random pairs \((s, x)\) and inferred the kernel hyperparameters using maximum likelihood estimation. The hyperparameters were then kept constant during the experiments.

5.3 Results

We repeated the simulated experiment 20 times for 260 iterations, for 8 different slopes values (evenly spaced between 1.0 logMAR$^{-1}$ and 8.0 logMAR$^{-1}$).
Tristan Fauvel, Matthew Chalk

Figure 2: Results across three different objective functions in preferential BO with adaptive contexts. Solid lines correspond to the mean value of the inferred maximum across the 40 repetitions. Shaded areas correspond to standard error on the mean. Sequential acquisition rules (KSS-ALD and MUC-ALD) consistently outperform the others.

The search space was $X = [-4\delta, 4\delta] \times [-4\delta, 4\delta]$ and the context space $S = [-1, 2]$ logMAR. Regret curves in the experiments where the slope of the psychometric function was set at 5.0 logMAR$^{-1}$ are shown on figure 3, and the results of the stratified analysis are summarized in table 3.

Both UCB-ALD and TS-ALD led to rapid and consistent improvement of the VA closed to its optimal value of logMAR = 0. UCB-ALD is the best performing algorithm (see table 3), with a mean VA at the end of the optimization sequence of $2.48 \times 10^{-2}$ logMAR in the case of a slope of 5.0 logMAR$^{-1}$ (s.e.m. = 8.22). At the end of the optimization sequence, the average spherical correction error of $2.74 \times 10^{-2} \delta$ (s.e.m. = 5.36 $\times 10^{-2}$). Note that this is closed to the precision that can be achieved nowadays (0.01$\delta$). The average cylindrical correction error is $1.53 \times 10^{-1} \delta$ (s.e.m. = 8.22 $\times 10^{-2}$).

However, when using random sampling, the optimization consistently failed (figure 3). Overall, the results are consistent with the one obtained on the synthetic benchmarks (table 3).

Here, we considered that the objective is a black box. However, for a specific application in a clinical setting, parameterizing the objective using domain knowledge would likely lead to faster and more robust improvement (see e.g. Cox & De Vries (2017)).

6 Discussion

6.1 Summary of contributions

In this paper, we introduced a new framework for binary and preferential BO: BO in adaptive contexts, in which the experimenter can choose the context where each function evaluation is performed. We proposed an acquisition function to jointly select the optimization variable and the context and showed how to generalize existing acquisition functions to this framework by combining them with Bayesian active learning. We show on synthetic benchmarks that the proposed algorithms outperform controls where the context (TS, UCB, random) or the correction (BALD, random) are not adaptively selected.

| Acquisition rule       | Rank | Borda score |
|------------------------|------|-------------|
| UCB-ALD                | 1    | 35          |
| TS-ALD                 | 2    | 26          |
| UCB (random context)   | 3    | 15          |
| BALD                   | 4    | 8           |
| TS (random context)    | 5    | 3           |
| Random                 | 6    | 0           |

Table 3: Comparison of acquisition functions on the refractive error correction experiment with 8 different slopes (evenly spaced between between 1.0 logMAR$^{-1}$ and 8.0 logMAR$^{-1}$). The two heuristics combining BO and active learning (UCB-ALD and MUC-ALD) outperform the controls where the context (TS, UCB, random) or the correction (BALD, random) are not adaptively selected.

Here, we considered that the objective is a black box. However, for a specific application in a clinical setting, parameterizing the objective using domain knowledge would likely lead to faster and more robust improvement (see e.g. Cox & De Vries (2017)).

6.2 Related work

In the bandit setting, contextual GP bandit [Krause & Ong, 2011] extends the GP bandit framework to
Contextual Bayesian optimization with binary outputs

Figure 3: A. Psychometric curves for various refractive errors corresponding to different visual acuities, with a slope of the psychometric function set at 5.0 logMAR\(^{-1}\). The baseline corresponds to the chance level in the n-alternatives forced-choice task (here, n = 26). VA of 20/20 corresponds to logMAR = 0. B. Visual acuity with the inferred best parameters throughout the optimization. The lines correspond to the average over 60 repetitions, whereas the shaded areas correspond to standard error on the mean. UCB-ALD and TS-ALD both lead to faster convergence towards optimal correction (logMAR = 0) compared to controls where the context (TS, UCB, random) or the correction (BALD, random) are not adaptively selected.

6.3 Code availability

Matlab implementation available at [https://disclose_upon_release](https://disclose_upon_release).

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A The Laplace approximation for Gaussian process classification

The following description of Laplace approximation for Gaussian process classification is given for completeness. It is required in order to understand the computation of the gradient of the Binary Knowledge Gradient. We follow the reasoning presented in Rasmussen & Williams (2006) as well as Bishop (2006), to which we refer the reader for further details.

In Gaussian process classification, we assume that observations $c$ at points $X = [x_1, \ldots, x_t]$ are Bernoulli random variables with parameters $\mu_c(X) = \pi(f(X))$, where $f$ is a latent function, and and $\pi$ is an inverse link function. We choose the convention where $c$ is either 0 or 1.

The predictive distribution at point $x$ is given by:

$$p(c = 1|x, D) = \int p(c = 1|f(x))p(f(x)|D)df(x). \quad (S1)$$

Since this integral is analytically intractable, we approximate $p(f(x)|D)$ with a Gaussian distribution. Indeed, for a a random normally distributed random variable $z$:

$$\int \Phi(z)N(z|\mu, \sigma^2)dz = \Phi\left(\frac{\mu}{\sqrt{1 + \sigma^2}}\right). \quad (S2)$$

A convenient way to do so is to note that:

$$p(f(x)|D) = \int p(f(x)|f)p(f|D)df,$$  

where $f$ is the vector of latent values at training points $X$. From the formula for Gaussian process posteriors, we have:

$$p(f(x)|f) = N\left(f(x)|k^\top K^{-1}f, k(x, x) - k^\top K^{-1}k\right), \quad (S4)$$

where $K = k(X, X)$ and $k = k(X, x)$.

The second term in the integral $p(f|D)$ is the posterior distribution of the latent value function at training points. By approximating it with a Gaussian distribution, then we could compute the integral in $S3$ which would give us a Gaussian approximation for $p(f(x)|D)$. This approximation would in turn allow us to compute $S1$.

A.1 Principle of the Laplace approximation

We start by finding a Gaussian approximation of $p(f|D)$. In general, for a random variable $z$ whose probability density function is $p(z) = \frac{f(z)}{Z}$, we can use a second a second order Taylor expansion around the mode $z_0$ of the distribution (where the gradient vanishes) so that:

$$\ln f(z) \sim \ln f(z_0) - \frac{1}{2}(z - z_0)^\top H(z - z_0), \quad (S5)$$

where $H$ is the negative of the Hessian of $f$ at $z_0$.

Taking the exponential and computing the appropriate normalization coefficients, we have:

$$p(z) \sim \frac{|H|^{1/2}}{(2\pi)^{D/2}} \exp\left(-\frac{1}{2}(z - z_0)^\top H(z - z_0)\right) = N(z|z_0, H^{-1}) \quad (S6)$$
A.2 Gaussian approximation of the posterior

In order to find a Gaussian approximation of \( p(f|D) \), we thus need to compute its mode and its Hessian. By using Bayes’ rule, we have:

\[
\ln p(f|D) = \ln p(f) + \ln p(D|f). \tag{S7}
\]

The prior term is:

\[
\ln p(f) = -\frac{1}{2} f^\top K^{-1} f - \frac{t}{2} \ln(2\pi) - \frac{1}{2} \ln |K|. \tag{S8}
\]

The likelihood term is:

\[
\ln p(D|f) = \ln \left( \prod_{i=1}^{t} \pi(f_i)^{c_i} (1 - \pi(f_i))^{1-c_i} \right) = \sum_{i=1}^{t} \ln \left( \pi(f_i)^{c_i} (1 - \pi(f_i))^{1-c_i} \right). \tag{S9}
\]

So the gradient of the log-posterior is:

\[
\nabla_f \ln p(f|D) = \nabla_f \ln p(D|f) - K^{-1} f, \tag{S10}
\]

whereas the Hessian is:

\[
\nabla^2_f \ln p(f|D) = \nabla^2_f \ln p(D|f) - K^{-1}, \tag{S11}
\]

where \( \nabla^2 \) refers to the Hessian matrix.

We introduce \( W = -\nabla^2_f \ln p(D|f) \), which is a diagonal matrix since conditionally on \( f \), observations are independent.

\[
\frac{\partial \ln p(c_i|f_i)}{\partial f_i} = \frac{\pi'(f_i)(c_i - \pi(f_i))}{\pi(f_i)(1 - \pi(f_i))}. \tag{S12}
\]

In the case where the link function is the cumulative normal distribution:

\[
\frac{\partial \ln p(c_i|f_i)}{\partial f_i} = \frac{(2c_i - 1)\phi(f_i)}{\Phi((2c_i - 1)f_i)}, \tag{S13}
\]

and

\[
\frac{\partial^2 \ln p(c_i|f_i)}{\partial f_i^2} = -\frac{\phi(f_i)^2}{\Phi((2c_i - 1)f_i)^2} - \frac{(2c_i - 1)f_i\phi(f_i)}{\Phi((2c_i - 1)f_i)}. \tag{S14}
\]

The mode \( f_0 \) satisfies the condition \( \nabla_f \ln p(f|D) = 0 \), so \( f_0 = K \nabla_f \ln p(D|f) \). The mode is usually found using the Newton-Raphson method.

The approximate posterior distribution is:

\[
p(f|D) = N(f_0, (K^{-1} + W)^{-1}). \tag{S15}
\]

A.3 Approximate predictive distribution

By combining equation with equation \([S15]\) we get:

\[
\mathbb{E}_f[f(x)|D] = k^\top K^{-1} f_0, \tag{S16}
\]

and:

\[
\nabla_f[f(x)|D] = k(x,x) - k^\top (K + W^{-1})^{-1} k. \tag{S17}
\]
B Gradient of the knowledge gradient

The knowledge gradient is defined as:

\[ \text{KG}(x) = \mathbb{E}_{c \sim p(c|\mathcal{D})}(\mu_{n+1}^* - \mu_n^{|\mathcal{D}, x_{n+1} = x}), \]  

(S18)

where \( \mu_{n+1}^* \) is the maximum of the posterior mean after observing \( (\mathcal{D}, (x, c)) \), and \( \mu_n^* \) is the maximum of the posterior mean after observing \( \mathcal{D} = (X, c_{1 \ldots n}) \).

With binary outputs, the knowledge gradient can be expressed as:

\[ \text{KG}(x) = \mu_c(x)(\mu_{1,n+1}^* - \mu_{0,n+1}^*) + (1 - \mu_c(x))(\mu_{0,n+1}^* - \mu_{n+1}^*), \]  

(S19)

where \( \mu_c(x) = \mathbb{E}_f[\Phi(f(x))|\mathcal{D}], \) and \( \mu_{1,n+1}^* \) (resp. \( \mu_{0,n+1}^* \)) is the maximum of the posterior mean after observing \( (\mathcal{D}, (x, 1)) \) (resp. \( (\mathcal{D}, (x, 0)) \)). That is:

\[ \mu_{c,n+1}^* = \max_{x' \in X} \mathbb{E}_f[f(x')|\mathcal{D} \cup (x, c)]. \]  

(S20)

The gradient of the knowledge-gradient is given by:

\[ \nabla \text{KG}(x) = \nabla \mu_c(x)(\mu_{1,n+1}^* - \mu_{0,n+1}^*) + \mu_c(x)\nabla \mu_{n+1}^* + (1 - \mu_c(x))\nabla \mu_{n+1}^*. \]  

(S21)

To compute the gradients of \( \mu_{1,n+1}^* \) and \( \mu_{0,n+1}^* \), inspired by \cite{Wu2016}, we use the envelope theorem \cite{Milgrom2002}, which states that, under sufficient regularity conditions, the gradient with respect to \( x \) of a maximum of a collection of functions of \( x \) is given simply by first finding the maximum \( x^* \) in this collection, and then differentiating this single function with respect to \( x \), keeping \( x^* \) fixed. Here, we have an infinite collection of functions \( \mathbb{E}_f[f(x')|\mathcal{D} \cup (x, c)] \) indexed by \( x' \).

**Theorem 1.** Corollary 4 of the envelope theorem in \cite{Milgrom2002} Let \( X \) denote the choice set and \( t \) be a parameter in \([0, 1]\) (the theorem generalizes to normed vector spaces). Let \( f : X \times [0,1] \to \mathbb{R} \) be an objective function parameterized by \( t \). We define:

\[ V(t) = \sup_{x \in X'} f(x, t), \]  

(S22)

\[ X^*(t) = \{ x \in X, f(x, t) = V(t) \}. \]  

(S23)

Suppose that \( X \) is a nonempty compact space, \( f(x, t) \) is upper semicontinuous in \( x \), and \( \frac{\partial f}{\partial t}(x, t) \) is continuous in \( (x, t) \). Then:

\[ \forall t \in [0,1], V'(t+) = \max_{x \in X^*(t)} \frac{\partial f}{\partial t}(x, t), \]  

(S24)

\[ \forall t \in (0,1], V'(t-) = \min_{x \in X^*(t)} \frac{\partial f}{\partial t}(x, t). \]  

(S25)

\( V \) is differentiable at any \( t \in (0,1) \) if and only if \( \left\{ \frac{\partial f}{\partial t}(x, t) | x \in X^*(t) \right\} \) is a singleton, and in that case \( \forall x \in X^*(t), V'(t) = \frac{\partial f}{\partial t}(x, t) \).

As a consequence, by writing \( x^* = \arg \max_{x \in X} \mathbb{E}_f[f(x')|\mathcal{D} \cup (x, c)] \), we get:

\[ \nabla_x \mu_{c,n+1}^* = \nabla \mathbb{E}_f[f(x^*)|\mathcal{D} \cup (x, c)]. \]  

(S26)

From the Laplace approximation, we have:

\[ \mathbb{E}_f[f(x^*)|\mathcal{D} \cup (x, c)] = k^\top \nabla y \log p(c|y), \]  

(S27)

where \( y \) corresponds to the inferred latent values of the training data, \( c = c_{1 \ldots n+1} \), and \( k = k((X, x), x^*) \).

So that:
\[ \nabla_x \mathbb{E}[f(x^*)|\mathcal{D} \cup (x, c)] = (\nabla_x k^\top) \nabla_y \log p(c|y) + k^\top \nabla_x \nabla_y \log p(c|y) \]
\[ = (\nabla_x k^\top) \nabla_y \log p(c|y) + k^\top (\nabla_y^2 \log p(c|y)) \nabla_x y \]
\[ = (\nabla_x k^\top) \nabla_y \log p(c|y) - k^\top W \nabla_x y, \]  
\[(S28)\]

where \( W = -\nabla_y^2 \log p(c|y) \).

From the Laplace approximation, we have \( y = K \nabla_y \log p(c|y) \), where \( K = k((X, x), (X, x)) \).

By differentiating this self-consistent equation,
\[ \nabla_x y = (\nabla_x K) \nabla_y \log p(c|y) + K (\nabla_y^2 \log p(c|y)) \nabla_x y \]
\[ = (\nabla_x K) \nabla_y \log p(c|y) - KW \nabla_x y. \]  
\[(S29)\]

By rearranging:
\[ \nabla_x y = (I + KW)^{-1} \nabla_x K \nabla_y \log p(c|y). \]  
\[(S30)\]

### C Contextual binary knowledge gradient

With binary outputs and contexts, the knowledge gradient can be expressed as:
\[ KG(s, x) = \mu_c(s, x) \mu_{t+1,1}^* + (1 - \mu_c(s, x)) \mu_{t+1,0}^* - \mu_t^*, \]  
\[(S31)\]

where \( \mu_c(s, x) = P(c = 1|s, x, \mathcal{D}_t) = \mathbb{E}_f[\Phi(f(s, x))|\mathcal{D}_t] \) is the predictive class distribution, and \( \mu_{t+1,1}^* \) (resp. \( \mu_{t+1,0}^* \)) is the maximum of the posterior mean for an arbitrary context \( s_0 \) after observing \((\mathcal{D}_t \cup (x, 1)) \) (resp. \( (\mathcal{D}_t \cup (x, 0)) \)). That is:
\[ \mu_{t+1,c}^* = \max_{x' \in \mathcal{X}} \mathbb{E}_f[f(s_0, x')|\mathcal{D}_t \cup (s_0, x, c)]. \]  
\[(S32)\]

Note that the term \( \mu_t^* \) in Eqn \( S31 \) can be neglected, since it does not depend on \( (s, x) \).

Importantly, if the kernel reflects the assumption that the maximum of the objective \( f \) does not depend on the context \( s \), then \( \mu_{t+1,c}^* \) can be computed for an arbitrary value of \( s_0 \). Indeed, following the Laplace approximation (supplementary A), with latent values \( f_0 \):
\[ \mathbb{E}_f[f(s, x)|\mathcal{D}] = k((s, x), (S, X))^\top K^{-1} f_0, \]  
\[(S33)\]

where \((S, X)\) corresponds to training points. Consider for example the case where \( f(s, x) = h(s)g(x) \), the kernel reflecting this structure is of the form \( k((s, x), (s', x')) = k_h(s, s')k_g(x, x') \). In that case, the posterior mean factorizes and it is clear that we can take the maximum with respect to \( x \) independently of \( s \).
### D Supplementary results

|       | A          | B          |
|-------|------------|------------|
|       | Random     | Random     |
| TS    | 0.00       | 0.00       |
| BALD  | 0.00       | 0.00       |
| UCB   | 0.00       | 0.00       |
| cBKG  | 0.00       | 0.00       |
| TS-ALD| 0.00       | 0.00       |
| UCB-ALD| 0.00    | 0.00       |

Figure S1: Detailed results of performance comparison between acquisition functions in contextual Binary Bayesian optimization. Each entry $(i,j)$ corresponds to the fraction of benchmarks functions for which $i$ beats $j$ according to the Mann-Whitney $U$ test at $\alpha = 5 \times 10^{-4}$ significance based either on the best value found (A) or the Area Under the Curve (B).
Figure S2: Detailed results of performance comparison between acquisition functions in contextual Preferential Bayesian optimization. Each entry \((i,j)\) corresponds to the fraction of benchmarks functions for which \(i\) beats \(j\) according to the Mann-Whitney U test at \(\alpha = 5 \times 10^{-4}\) significance based either on the best value found (\(A\)) or the Area Under the Curve (\(B\)).
E  Kernel derivation for the psychophysics experiment

For lens parameters, $x$, the response of the patient is determined by:

$$ P(c = 1|s, x) = \gamma + (1 - \gamma)\Phi(a(x)s + b(x)) \quad (S34) $$

For $\gamma$ large enough, we have $P(c = 1|s) \approx \Phi(a(x)s + b(x))$. Since in practice, with a letter chart, $\gamma^{-1} = n = 26$, we will make this simplifying assumption in building our surrogate model.

We put a GP prior on $f$, with zero mean and kernel $k_\psi$ defined as:

$$ k_\psi((s, x), (s', x')) = \theta_{ss'} + k(x, x') \quad (S35) $$

This kernel reflects the structure of the function $f$ (see equation 14) with the assumption $\gamma \approx 0$. Indeed, we have:

$$ \text{Cov}(f(s, x), f(s', x')) = \text{Cov}(a(x)s + b(x), a(x')s' + b(x')) 
\quad = ss'\text{Cov}(a(x)s + b(x), a(x')s' + b(x')) 
\quad + (s + s')\text{Cov}(a(x), b(x')) + \text{Cov}(b(x), b(x')) \quad (S36) $$

We put GP priors on functions $a$ and $b$, with kernels $k_1$ and $k_2$ respectively. Since $a(x)$ and $b(x)$ are a priori independent conditionally on $x$, the second term on the right-hand side vanishes, so that:

$$ \text{Cov}(f(s, x), f(s', x')) = ss'k_1(x, x') + k_2(x, x') \quad (S37) $$

Since we assumed the slope to be constant at value $\sqrt{\theta}$, this further simplifies to:

$$ \text{Cov}(f(s, x), f(s', x')) = \theta_{ss'} + k(x, x') \quad (S38) $$

F  Visual acuity as a function of the correction parameters

Figure S3: **A.** Visual acuity as a function of the correction parameters $S$ (spherical correction) and $C$ (cylindrical correction) in diopters ($\delta$). The slope of the psychometric curve is kept fixed at 5.0 logMAR$^{-1}$. **B.** Probability of correct response in a 26-alternatives forced choice task for a stimulus of visual angle $1'$. In blue regions, the subject will always perform at chance level, independently of the correction parameters, so responses will be uninformative.
**G Sampling from GP classification models**

Acquisition rules based on Thompson sampling rely on samples from the posterior distribution over the maximum:

$$p(x^\star | \mathcal{D}) = p(f(x^\star) = \max_{x \in \mathcal{X}} f(x) | \mathcal{D})$$  \hfill (S39)

Hernández-Lobato et al. (2014) proposed the following sampling scheme: draw a sample from the posterior distribution $p(f | \mathcal{D})$, then return the maximum of the sample. One could iteratively construct the sample $f$ while it is being optimized but, as noted by Hernández-Lobato et al. (2014), this would have a cost $O(m^3)$, where $m$ is the number of evaluations of the function necessary to find the maximum. Although this is doable in practice, Hernández-Lobato et al. (2014) suggested a more efficient procedure by sampling a finite-dimensional approximation to $f$, based on a finite-dimensional approximation to the kernel $k(x, x') \sim \phi(x)^\top \phi(x')$ (Lázaro-Gredilla et al. 2010). In GP classification and preference learning, this approximate sampling cannot be directly applied. In the following section, we will explain how to apply existing approximate sampling methods to the case of GP classification models.

**G.1 Kernel approximation**

The sampling methods mentioned above consist in approximating a stationary kernel $k$ by means of the inner product of features $\phi$ such that: $k(x, x') \sim \phi(x)^\top \phi(x')$. Recently, a method was proposed by Solin & Särkkä (2020), which aims at making the approximation as good as possible for a given rank (see Riutort-Mayol et al. (2020) for details about the practical implementation). In this method, the kernel is approximated using a series expansion in terms of eigenfunctions of the Laplace operator on a rectangular domain $\Omega = [-L_1, L_1] \times \cdots \times [-L_d, L_d]$ (the search space is usually rectangular in Bayesian optimization).

In preference learning, a specific difficulty arises. Indeed, the base kernel used to model the value function may be shift-invariant, the preference kernel, however, is not in general. This inexact hypothesis introduced in the sampling algorithm, leads to samples that are not consistent with the anti-symmetric property of a preference function, i.e. $f(x, x') = -f(x', x)$, (see e.g. figure 4.1 in Gonzalez et al. (2017) where this inexact stationarity hypothesis is introduced).

However, assume that we have a finite dimensional approximation to the base kernel $k(x, x') \sim \phi(x)^\top \phi(x')$, it is easy to see that we can approximate the preference kernel by $k_{\text{pref}}((x_i, x_j), (x_k, x_l)) \sim \phi_{\text{pref}}(x_i, x_j)^\top \phi_{\text{pref}}(x_k, x_l)$, with:

$$\phi_{\text{pref}}(x_i, x_j) = \phi(x_i) - \phi(x_j)$$  \hfill (S40)

By construction, the corresponding sample is anti-symmetric.

**G.2 Weight-space approximation with non-Gaussian likelihoods**

The most widely used method for approximate sampling from GP in Bayesian optimization is the weight-space approximation. Assume that we have a finite-dimensional approximation to the kernel $k(x, x') \sim \phi(x)^\top \phi(x')$. The features $\phi(x)$ can be used to approximate the Gaussian process posterior with a Bayesian linear model: $f(x) \sim \phi(x)^\top \omega$, where (Lázaro-Gredilla et al. 2010):

$$\omega \sim \mathcal{N}\left( (\Phi^\top \Phi + \sigma^2 I)^{-1} \Phi^\top y, (\Phi^\top \Phi + \sigma^2 I)^{-1} \sigma^2 \right)$$  \hfill (S41)

In the case of non-Gaussian likelihoods, naively replacing $y$ in [S41] by the latent values inferred by the Laplace approximation (see [A]) or Expectation Propagation would not take into account the correlated heteroscedastic noise on the latent function values at training points. To the extent of our knowledge, the process of weight-space approximate sampling has not been rigorously introduced for latent GP models. Here, we suggest to use a sampling process in two steps. First, samples $y$ are drawn from the posterior distribution over the latent variables at training points: $\mathcal{N}(\mu, \Sigma)$, then $\omega$ is sampled from $\omega \sim \mathcal{N}\left( (\Phi^\top \Phi + \sigma^2 I)^{-1} \Phi^\top y, (\Phi^\top \Phi + \sigma^2 I)^{-1} \sigma^2 \right)$, where $\sigma$ is a small constant used for regularization.

To see why this sampling scheme is correct, note that: $p(f(x) | \mathcal{D}) = \int p(f(x) | X, y)p(y | \mathcal{D}) dy$. So given latent values sampled from $p(y | \mathcal{D})$, an approximate sample $f$ can be drawn from $p(f(x) | X, y)$ using the method of Hernández-Lobato et al. (2014).
However, the degeneracy, i.e., low-rankness of the GP approximation, causes the estimate to grow over-confident when the number of observed points exceeds the degrees of freedom of the approximation. This results in ill-behaved approximations, and, in particular, underestimated variance, in regions far away from the data points. This phenomenon is known as variance starvation (Wang et al., 2017; Mutný & Krause, 2018; Calandriello et al., 2019).

G.3 Decoupled-bases approximate sampling

Recently Wilson et al. (2020a) proposed an efficient way to sample from GP posteriors that avoids variance starvation. The original sampling method was devised for exact GP with Gaussian noise and sparse GP, where the GP is computed based on a set of inducing points that explain the data, however, it can easily be generalized to non-Gaussian likelihood with a latent function (Wilson et al., 2020b).

Briefly, this method is based on a corollary of Matheron’s rule. For a Gaussian process \( f \sim \mathcal{GP}(0, k) \), the latent process conditioned on latent values \((X, y)\) admits, in distribution, the representation:

\[
\begin{align*}
(f \mid y)(\cdot) &= f(\cdot) + k(\cdot, x) K^{-1} (y - f(X)) \\
&\approx \sum_{i=1}^{l} \omega_i \phi_i(\cdot) + \sum_{j=1}^{m} v_j k(\cdot, x_j),
\end{align*}
\]

(S42)

This corollary defines an approximation to the Gaussian process conditioned on \((X, y)\), where the stationary prior is approximated with a Bayesian linear model (weight-space prior), and the approximate posterior is obtained by adding an exact update (function-space update):

\[
(f \mid y)(\cdot) \approx \sum_{i=1}^{l} \omega_i \phi_i(\cdot) + \sum_{j=1}^{m} v_j k(\cdot, x_j),
\]

(S43)

where \( v = K^{-1} (y - \Phi \omega) \), and \( \omega \) is sampled from \( \mathcal{N}(0, I) \). This method is termed decoupled-bases decomposition of the GP.

To sample from the posterior latent function, we thus sample \( \omega \) from \( \mathcal{N}(0, I) \) and compute the corresponding weight-space prior, then sample \( y \) from \( \mathcal{N}(\mu_f(X), \Sigma_f(X, X)) \) and compute the corresponding function-space update.
## H Benchmarks

| Name                  | D | Kernel   | Space                      |
|-----------------------|---|----------|----------------------------|
| Ackley                | 2 | Matérn 3/2 | $[-32.768, 32.768]^2$     |
| Beale                 | 2 | SE-ARD   | $[-4.5, 4.5]^2$           |
| Bohachevsky           | 2 | SE-ARD   | $[-100, 100]^2$           |
| Three-Hump Camel      | 2 | Matérn 5/2 | $[-5, 5]^2$               |
| Six-Hump Camel        | 2 | SE-ARD   | $[-3, 3] \times [-2, 2]$  |
| Colville              | 4 | Matérn 5/2 | $[-10, 10]^4$           |
| Cross-in-Tray         | 2 | Matérn 5/2 | $[-10, 10]^2$           |
| Dixon-Price           | 2 | Matérn 5/2 | $[-5, 5]^2$               |
| Drop-Wave             | 2 | Matérn 3/2 | $[-5.12, 5.12]^2$        |
| Eggholder             | 2 | SE-ARD   | $[-512, 512]^2$           |
| Forrester et al (2008)| 1 | SE-ARD   | $[0, 1]$                  |
| Goldstein-Price       | 2 | SE-ARD   | $[-2, 2]^2$               |
| Griewank              | 2 | SE-ARD   | $[-600, 600]^2$           |
| Hartmann 3-D          | 3 | SE-ARD   | $[0, 1]^3$                |
| Hartmann 4D           | 4 | SE-ARD   | $[0, 1]^4$                |
| Hartmann 6D           | 6 | SE-ARD   | $[0, 1]^6$                |
| Holder                | 2 | SE-ARD   | $[-10, 10]^2$             |
| Langer                | 2 | Matérn 3/2 | $[0, 10]^2$              |
| Levy                  | 2 | SE-ARD   | $[-10, 10]^2$             |
| Levy N.13             | 2 | Matérn 5/2 | $[-10, 10]^2$            |
| Perm 0,d,β            | 2 | SE-ARD   | $[-2, 2]^2$               |
| Perm d,β              | 2 | SE-ARD   | $[-2, 2]^2$               |
| Powell                | 4 | SE-ARD   | $[-4, 5]^4$               |
| Rosenbrock            | 2 | SE-ARD   | $[-2.048, 2.048]^2$       |
| Rotated Hyper-Ellipsoid | 2 | Matérn 3/2 | $[-65.536, 65.536]^2$   |
| Schaffer n4           | 2 | Matérn 3/2 | $[-100, 100]^2$        |
| Schwefel              | 2 | SE-ARD   | $[-500, 500]^2$          |
| Shekel                | 4 | SE-ARD   | $[0, 10]^4$               |
| Schubert              | 2 | Matérn 3/2 | $[0, 10]^2$             |
| Sphere                | 2 | SE-ARD   | $[-5.12, 5.12]^2$        |
| Sum Squares           | 2 | SE-ARD   | $[-10, 10]^2$             |
| Trid                  | 2 | SE-ARD   | $[-4, 4]^2$               |
| Ursem Waves           | 2 | SE-ARD   | $[-1.2, 1.2] \times [-0.9, 1.2]$ |

Table S1: Benchmark functions in Bayesian optimization experiments.