Bayesian optimal experimental design (BOED) is a principled framework for making efficient use of limited experimental resources. Unfortunately, its applicability is hampered by the difficulty of obtaining accurate estimates of the expected information gain (EIG) of an experiment. To address this, we introduce several classes of fast EIG estimators suited to the experiment design context by building on ideas from variational inference and mutual information estimation. We show theoretically and empirically that these estimators can provide significant gains in speed and accuracy over previous approaches. We demonstrate the practicality of our approach via a number of experiments, including an adaptive experiment with human participants.

1 INTRODUCTION

Tasks as seemingly diverse as designing a study to elucidate human cognition, selecting the next query point in an active learning loop, and designing online feedback surveys all constitute the same underlying problem: designing an experiment to optimize the information gathered. Bayesian optimal experimental design (BOED) forms a powerful mathematical abstraction for tackling such problems (Chaloner and Verdinelli, 1995; Lindley, 1956; Rainforth, 2017; Sebastiani and Wynn, 2000; Vincent and Rainforth, 2017) and has been successfully applied in numerous settings, including psychology (Myung et al., 2013), Bayesian optimisation (Hernández-Lobato et al., 2014), active learning (Golovin et al., 2010), bioinformatics (Vanlier et al., 2012), and neuroscience (Shababo et al., 2013).

Suppose we have parameters \( \theta \) that we wish to learn about and for which we have some prior beliefs \( p(\theta) \). These parameters might, for example, encapsulate characteristics of a participant in a psychology trial. In the BOED framework, we construct a predictive model \( p(y|\theta, d) \) for possible experimental outcomes \( y \), given a design \( d \) and a particular value of \( \theta \). Here \( d \) might represent a question posed to the participant and \( y \) the observed response. We now choose the design that optimizes the expected information gain (EIG) of running the experiment,

\[
\text{EIG}(d) \triangleq \mathbb{E}_{p(y|d)} [H(p(\theta)) - H(p(\theta|y,d))],
\]

where \( H(\cdot) \) represents the entropy of the distribution and \( p(\theta|y,d) \propto p(\theta)p(y|\theta,d) \) is the posterior resulting from running the experiment with design \( d \) and observing outcome \( y \). In other words, we seek the design that, in expectation over possible experimental outcomes, most reduces the entropy of the posterior for the target latent variables. If the predictive model is correct, this forms a design strategy that is optimal from an information-theoretic viewpoint (Lindley, 1972; Sebastiani and Wynn, 2000).

This BOED framework is particularly powerful in sequential contexts, where it allows the results of previous experiments to be used in guiding the designs for future experiments. For example, as we ask a participant a series of questions in a psychology trial, we can use the information gathered from previous responses to ask more pertinent questions in the future, that will, in turn, return more information. This ability to design experiments that are self-adaptive can substantially increase their efficiency: fewer iterations are required to uncover the same level of information, allowing one to reduce costs or recover better quality data from the resources available.

In practice, however, the BOED approach is often
hampered by the difficulty of obtaining fast and high-quality estimates of the EIG: it constitutes a nested expectation problem and so conventional Monte Carlo (MC) estimation methods cannot be applied (Rainforth et al., 2018). To address this, we introduce four efficient and widely-applicable variational methods for estimating the EIG.

We begin by exploiting an equivalence between the EIG and mutual information to develop variational lower and upper bounds on the EIG, building on Barber and Agakov (2003). Optimizing these bounds produces variational approximations that can in turn be used to estimate the EIG itself. Specifically, the lower bound estimator, \( \hat{\mu}_{\text{post}} \), utilizes amortized variational inference (Dayan et al., 1995; Rezende et al., 2014; Stuhlmüller et al., 2013), whilst the upper bound estimator, \( \hat{\mu}_{\text{marg}} \), employs a variational approximation to the marginal distribution as a proposal distribution in a NMC bound estimator, \( \hat{\mu}_{\text{VNMC}} \), allows one to trade-off resources between the fast learning of a biased estimator permitted by the variational approaches, and the ability of NMC estimators to reduce this bias.

Our methods benefit from advances in flexible families of amortized distributions using neural networks (Rezende and Mohamed, 2015; Tabak and Turner, 2013). For this reason we implemented our estimators in Pyro (Bingham et al., 2018), a universal probabilistic programming language (PPL) that provides first-class support for neural networks and variational methods. Providing these estimators as a library\(^1\) in a PPL greatly expands the space of potential applications and users (Ouyang et al., 2018).

To verify the practical utility of our estimators, we evaluate their speed and accuracy on experiment design problems inspired by applications from psychology and industrial research. In particular, we show that the asymptotic biases mentioned above are relatively small for a number of examples of practical importance. We go on to use our estimators to conduct adaptive experiments, sequentially applying BOED in a study with human participants recruited from Mechanical Turk. In summary, we find our new class of variational EIG estimators to provide a fast, flexible, and accurate solution to the core step of automated experiment design.

2 BACKGROUND

The BOED framework is a model-based approach for choosing an experiment design \( d \) in a manner that optimizes the information gained about some parameters of interest \( \theta \). Given a prior \( p(\theta) \) and a predictive model \( p(y|\theta,d) \), where \( y \) is the outcome of the experiment, the information gained about \( \theta \) from running experiment \( d \) and observing \( y \) is the reduction in entropy from the prior to the posterior:

\[
\text{IG}(y, d) = H[p(\theta)] - H[p(\theta|y, d)]
\]

At the point of choosing \( d \), however, we are uncertain about the outcome. Thus in order to define a metric to assess the utility of the design \( d \) we take the expectation of IG(\( y, d \)) under the marginal distribution over outcomes \( p(y|d) = \mathbb{E}_{\theta} \left[ p(y|\theta,d) \right] \), that is

\[
\text{EIG}(d) \equiv \mathbb{E}_{p(y|d)} \left[ H[p(\theta)] - H[p(\theta|y, d)] \right]
\]

which is exactly the mutual information between \( \theta \) and \( y \) given \( d \). This can also be rewritten as

\[
\text{EIG}(d) = \mathbb{E}_{p(\theta|d)} \left[ \log \frac{p(y|\theta, d)}{p(y|d)} \right]
\]

which can be interpreted as the epistemic uncertainty in \( y \) averaged over the prior \( p(\theta) \).

The Bayesian optimal design is then defined by

\[
d^* \in \arg \max_{d \in D} \text{EIG}(d).
\]

---

\(^1\)Implementation will be made available at publication.
We now introduce our variational estimators for estimating the EIG. See Table 1 for a summary that also includes several baseline approaches that we discuss in Sec. 5. We note that while \( \hat{\mu}_{\text{post}} \) and \( \hat{\mu}_{\text{marg}} \) have not, to the best of our knowledge, been used in a BOED setting, \( \hat{\mu}_{\text{VNMC}} \) and \( \hat{\mu}_{m+t} \) represent novel estimators in their own right.

### 3.1 Variational Posterior \( \hat{\mu}_{\text{post}} \)

Suppose we approximate the integrand in (4) as \( q_p(\theta|y,d)/p(\theta) \) where \( q_p(\theta|y,d) \) is a variational approximation amortized over \( y \). Neglecting any error in estimating the outer expectation, the resulting EIG approximation is in fact a lower bound to EIG(\( d \)) (Barber and Agakov, 2003)

\[
\text{EIG}(d) = E_{p(y,\theta|d)} \left[ \log \frac{p(\theta|y,d)q_p(\theta|y,d)}{p(\theta)q_p(\theta|y,d)} \right] 
\]

\[
= E_{p(y,\theta|d)} \left[ \log \frac{q_p(\theta|y,d)}{p(\theta)} \right] 
\]

\[
+ E_{p(y|d)} \left[ KL \left( p(\theta|y,d)\|q_p(\theta|y,d) \right) \right] 
\]

\[
\geq E_{p(y,\theta|d)} \left[ \log \frac{q_p(\theta|y,d)}{p(\theta)} \right] \triangleq \mathcal{L}_{\text{post}}(d) \tag{12}
\]

where the bound is tight when \( q_p(\theta|y,d) = p(\theta|y,d) \). Analogously to variational inference settings, we can learn \( q_p(\theta|y,d) \) by introducing a family of variational distributions \( q_p(\theta|y,d,\phi) \) parameterized by \( \phi \) and then maximizing the bound with respect to \( \phi \)

\[
\phi^* = \arg \max_{\phi} E_{p(y,\theta|d)} \left[ \log \frac{q_p(\theta|y,d,\phi)}{p(\theta)} \right], \tag{13}
\]

\[
\text{EIG}(d) \approx \mathcal{L}_{\text{post}}(d; \phi^*). \tag{14}
\]

Provided that we can generate samples from the model, this maximization can be performed using stochastic gradient methods (Robbins and Monro, 1951) and the unbiased gradient estimates

\[
\nabla_\phi \mathcal{L}_{\text{post}}(d; \phi) \approx \frac{1}{S} \sum_{s=1}^{S} \nabla_\phi \log q_p(\theta_i|y_i,d,\phi), \tag{15}
\]

where \( y_i, \theta_i \) i.i.d. \( p(y,\theta|d) \), and we note that no reparameterization is required as \( p(y,\theta|d) \) is independent of \( \phi \). After \( K \) gradient steps we obtain an approximation of the variational parameters \( \phi_K \), which we use to compute a corresponding EIG estimate by constructing a MC estimator for \( \mathcal{L}_{\text{post}}(d; \phi) \), namely

\[
\hat{\mu}_{\text{post}}(d) \triangleq \frac{1}{N} \sum_{n=1}^{N} \log q_p(\theta_n|y_n,d,\phi_K) / p(\theta_n) \tag{16}
\]

where \( y_n, \theta_n \) i.i.d. \( p(y,\theta|d) \).

We call this the variational posterior EIG estimator, or posterior estimator when the context is clear.

### 3.2 Variational Marginal \( \hat{\mu}_{\text{marg}} \)

In some scenarios, \( \theta \) may be high-dimensional, making it difficult to train a good variational posterior approximation. An alternative approach that can
be attractive in such cases is to instead introduce a marginal density approximation \( q_m(y|d) \) and approximate the integrand of (6) as \( \frac{p(y|\theta, d)}{q_m(y|d)} \). This yields an upper bound (Barber and Agakov, 2003)

\[
\text{EIG}(d) = \mathbb{E}_{p(y, \theta|d)} \left[ \log \frac{p(y|\theta, d)q_m(y|d)}{p(y|d)q_m(y|d)} \right]
\]

(17)

\[
= \mathbb{E}_{p(y, \theta|d)} \left[ \log \frac{p(y|\theta, d)}{q_m(y|d)} - \text{KL}(p(y|\theta, d)||q_m(y|d)) \right]
\]

\[
\leq \mathbb{E}_{p(y, \theta|d)} \left[ \log \frac{p(y|\theta, d)}{q_m(y|d)} \right] \equiv \mathcal{U}_{\text{marg}}(d),
\]

(18)

where the bound is tight when \( q_m(y|d) = p(y|d) \).

Analogously to \( \hat{\mu}_{\text{post}} \), a variational marginal estimator of the EIG, \( \hat{\mu}_{\text{marg}}(d) \), can be obtained by introducing a family of variational distributions, \( q_m(y|d, \psi) \), performing \( K \) stochastic gradient updates to approximately minimize \( \mathcal{U}_{\text{marg}}(d; \psi) \), and using the resulting variational parameters \( \psi_K \) to produce a Monte Carlo estimate for \( \mathcal{U}_{\text{marg}}(d; \psi_K) \)

\[
\hat{\mu}_{\text{marg}}(d) \triangleq \frac{1}{N} \sum_{n=1}^{N} \log \frac{p(y_n|\theta_n, d)}{q_m(y_n|d, \phi_K)},
\]

(19)

where we again draw \( y_n, \theta_n \overset{i.i.d.}{\sim} p(y, \theta|d) \). We highlight that the true value of \( \text{EIG}(d) \) necessarily lies between the expected values of \( \hat{\mu}_{\text{post}} \) and \( \hat{\mu}_{\text{marg}} \).

3.3 VARIATIONAL NMC \( \hat{\mu}_{\text{VNMC}} \)

Rather than using \( q_p(\theta|y, d) \) to form an estimate of the integrand of (4), we can instead sample \( \theta \sim q_p(\theta|y, d) \) and approximate the integrand of (6) as

\[
\log \frac{p(y|\theta, d)}{p(y|d)} \approx \log \frac{1}{K} \sum_{\ell=1}^{K} \frac{p(y|\theta^\ell, d)}{q_p(\theta^\ell|y, d)}
\]

(20)

Here the denominator is, in expectation, an IWAE bound (Burda et al., 2015) on \( p(y|d) \). By Jensen’s inequality, we thus have an upper bound on \( \text{EIG}(d) \)

\[
\text{EIG}(d) \leq \mathbb{E} \left[ \log \frac{p(y|\theta_0, d)}{\frac{1}{K} \sum_{\ell=1}^{K} \frac{p(y|\theta^\ell, d)}{q_p(\theta^\ell|y, d)}} \right] \equiv \mathcal{U}_{\text{VNMC}}(d, L)
\]

(21)

where the expectation is taken over \( y, \theta_{0:L} \sim p(y, \theta_0|d) \prod_{\ell=1}^{L} q_p(\theta^\ell|y, d) \).

Using this bound, we can train a variational approximation \( q_p(\theta|y, d, \psi) \) in an analogous manner as done in Sec. 3.1, except that we now perform minimization.\(^2\)

We can then use this to construct the NMC estimator \( \hat{\mu}_{\text{VNMC}}(d) \)

\[
\hat{\mu}_{\text{VNMC}}(d) \triangleq \frac{1}{N} \sum_{n=1}^{N} \log \frac{p(y_n|\theta_n, d)}{q_m(y_n|d, \psi_K)}
\]

(22)

where \( \theta_n \overset{i.i.d.}{\sim} p(\theta) \) and the full set of variational parameters is \( \psi_K = \{ \psi_n \} \).

Note though that, unlike for the previous bounds, because of the expectation over \( q_p(\theta|y, d) \), it is now important to reparameterize \( \theta \) when possible to avoid high variance gradients.

3.4 IMPLICIT LIKELIHOODS AND \( \hat{\mu}_{m+\ell} \)

So far we have assumed that we have an explicit likelihood model: one in which we can evaluate \( p(y|\theta, d) \) pointwise. Many models of interest are implicit likelihood models and lack this feature. For example, a model with a nuisance latent variable \( \psi \) (such as a random effects model) is an implicit likelihood model because \( p(y|\theta, d) = \mathbb{P}(p|\psi) [p(y|\theta, \psi, d) \] is not known in closed form but can still be sampled from directly.

The variational posterior approach is applicable without modification in this setting, as both training \( \phi_K \) and evaluating \( \hat{\mu}_{\text{post}} \) only require drawing samples from \( p(y|\theta, d) \). This is an advantage over NMC, which requires evaluating \( p(y|\theta, d) \).

Although \( \hat{\mu}_{\text{marg}} \) is not directly applicable in this setting, it can be modified to accommodate implicit likelihoods. Specifically, we can utilize two approximate densities: \( q_m(y|d) \) for the marginal and \( q_p(\theta|y, d) \) for the likelihood. We then form the approximation

\[
\text{EIG}(d) \approx \mathcal{I}_{m+\ell}(d) \triangleq \mathbb{E}_{p(y, \theta|d)} \left[ \log \frac{q_p(\theta|y, d)}{q_m(y|d)} \right].
\]

(23)

We cannot use (23) to learn \( q_m(y|d) \) and \( q_p(\theta|y, d) \), as it is not a bound. Instead we maximize

\[
\mathcal{F}(d) \triangleq \mathbb{E}_{p(y, \theta|d)} \left[ \log q_m(y|d) + \log q_p(\theta|y, d) \right]
\]

yielding variational approximations \( q_m(y|d, \psi_K) \) and \( q_p(\theta|y, d, \lambda_K) \). These can then be used to define our fourth estimator

\[
\hat{\mu}_{m+\ell}(d) \triangleq \frac{1}{N} \sum_{n=1}^{N} \log \frac{q_p(y_n|\theta_n, d, \lambda_K)}{q_m(y_n|d, \psi_K)}
\]

(25)

where \( y_n \overset{i.i.d.}{\sim} p(y|\theta|d) \) and the full set of variational parameters is \( \psi_K = \{ \psi_K \} \).

We note that it is very challenging, and potentially impossible, to construct non-vacuous upper bounds in this implicit likelihood setting. This is because
EIG(d) can be arbitrarily large. For the explicit likelihood settings we are using, we can use information from the likelihood to form the bound $U_{\text{marg}}$ in (18). Without an explicit likelihood, one needs to deal with the negative conditional entropy term $E_{p(y, \theta|d)}[p(y|\theta, d)]$, which may be arbitrarily large.

3.5 USING ESTIMATORS FOR BOED

To use our EIG estimators to carry out BOED, we further need to consider the problem of optimizing for the design as per (8) and, in sequential settings, the inference required for $p(\theta|d_{1:t-1}, y_{1:t-1})$.

For the former problem, there are a variety of methods one can use such as grid search, Bayesian optimization (Snoek et al., 2012), or methods that adaptively allocate resources between different estimators (Amzal et al., 2006; Rainforth, 2017). Our estimators are compatible with all these approaches, with adaptive resource allocation methods able to control the number of samples used in the final (nested) MC estimates.

As for inference, we note that samples from $p(\theta|d_{1:t-1}, y_{1:t-1})$ are sufficient for subsequent design maximization—we do not need to know this density in closed form. Indeed, for $\mu_{\text{post}}$ and $\mu_{\text{marg}}$, it is never necessary to evaluate $p(\theta)$ in either the optimization of the variational parameters or the final MC estimates. For $\mu_{\text{post}}$, a $p(\theta)$ term does appear in the variational objective, but we can simply extract out $H[p(\theta)]$, which is a constant w.r.t. $d$ and $\phi$.

For $\mu_{\text{VNMC}}$ the problem is a little more complex due to the $p(y, \theta|d)$ term in the inner expectation. However, here we can note that

$$p(y, \theta|d, d_{1:t-1}, y_{1:t-1}) = \frac{p(\theta) \prod_{i=1}^N p(y_i|\theta, d_i)}{p(y_{1:t-1}|d_{1:t-1})}$$

where all terms in the numerator are known and the denominator is a constant with respect to the new design $d_t$ and the variational parameters $\phi_K$, so it can be safely ignored as was done for $\mu_{\text{post}}$. Overall, any inference scheme to sample $p(\theta|d_{1:t-1}, y_{1:t-1})$ is compatible with our approach.

4 CONVERGENCE RATES

We now investigate the convergence of our estimators, assuming for now that we fix $M = L$ for $\mu_{\text{VNMC}}$. We start by breaking the overall error down into three terms: a) variance in MC estimation of the bound; b) the gap between the bound and the tightest bound possible given the variational family; and c) the gap between the tightest possible bound and EIG(d). Then with variational EIG approximation $\mathcal{B}(d) \in \{L_{\text{post}}(d), U_{\text{marg}}(d), U_{\text{VNMC}}(d, L), T_{m+1}(d)\}$, optimal variational parameters $\phi^*$, learned variational parameters $\phi_K$ after $K$ stochastic gradient iterations, and MC estimator $\hat{\mu}(d, \phi_K)$, we have, by the triangle inequality,

$$\|\hat{\mu}(d, \phi_K) - \text{EIG}(d)\|_{L^2} \leq \|\hat{\mu}(d, \phi_K) - \mathcal{B}(d, \phi_K)\|_{L^2} + \|\mathcal{B}(d, \phi_K) - \mathcal{B}(d, \phi^*)\|_{L^2} + \|\mathcal{B}(d, \phi^*) - \text{EIG}(d)\|.$$  

where we have used the notation $\|X\|_{L^2} = \sqrt{\mathbb{E}[X^2]}$ to denote the $L^2$ norm of a random variable.

By the weak law of large numbers, (26a) scales as $N^{-1/2}$ and can thus be arbitrarily reduced by taking more MC samples. Provided that our stochastic gradient scheme converges, (26b) can be reduced by increasing the number of stochastic gradient steps $K$. However, (26c) is a constant that can only be reduced by expanding the variational family (or increasing $L$ for $\mu_{\text{VNMC}}$). These approaches thus converge to a biased estimate of the EIG(d), namely $\mathcal{B}(d, \phi^*)$.

As established by the following Theorem, if we set $N \propto K$, the rate of convergence to this biased estimate is $O(T^{-1/2})$, where $T$ represents the total computational cost, with $T = O(N + K)$.

**Theorem 1.** Let $\mathcal{X}$ be a measurable space, $\Phi$ a convex subset of a finite dimensional inner product space; let $X_1, X_2, \ldots$ be i.i.d. random variables taking values in $\mathcal{X}$ and $f : \mathcal{X} \times \Phi \to \mathbb{R}$ a measurable function. Let

$$\mu(\phi) \triangleq \mathbb{E}[f(X_1, \phi)] = \hat{\mu}_N(\phi) \triangleq \frac{1}{N} \sum_{n=1}^N f(X_i, \phi)$$

and suppose that $\sup_{\phi \in \Phi} \|f(X_1, \phi)\|_{L^2} < \infty$. Then

$$\sup_{\phi \in \Phi} \|\hat{\mu}_N(\phi) - \mu(\phi)\|_{L^2} = O(N^{-1/2}).$$

Now suppose Assumption 1 in Appendix A holds and that $\phi^*$ is the unique minimizer of $\mu$. Using $K$ iterations of the Polyak-Ruppert averaged stochastic gradient descent algorithm of Moulines and Bach (2011) with gradient estimator $\nabla \phi f(X_t, \phi)$ then

$$\|\mu(\phi_K) - \mu(\phi^*)\|_{L^2} = O(K^{-1/2})$$

and, combining with the first result,

$$\|\hat{\mu}_N(\phi_K) - \mu(\phi^*)\|_{L^2} = O(N^{-1/2} + K^{-1/2})$$

$$= O(T^{-1/2}) \text{ if } N \propto K.$$  

The proof, which is presented in Appendix A, relies on standard results from the theories of MC and stochastic optimization. We note that the assumptions required for the latter, though standard in the literature, are quite strong and may not always hold in practice. In particular, the convergence may often
be to a local optimum \(\phi^l\), rather than the global optimum \(\phi^*\), introducing an additional asymptotic bias term \(|\mathcal{B}(d, \phi^l) - \mathcal{B}(d, \phi^*)|\) into (26c).

Theorem 1 can be applied directly to \(\hat{\mu}_{\text{marg}}, -\hat{\mu}_{\text{post}}, \) and \(\hat{\mu}_{\text{VNMC}}\) (with fixed \(M = L\)), showing that they converge respectively to \(U_{\text{marg}}(d, \phi^*), -L_{\text{post}}(d, \phi^*), \) and \(U_{\text{VNMC}}(d, L, \phi^*)\) at a rate \(\mathcal{O}(T^{-1/2})\) if \(N \propto K\) and the assumptions are satisfied. For \(-\hat{\mu}_{m+\ell}\), we need to be a little more careful because the objective for training the variational parameters is distinct to \(-I_{m+\ell}\). Here we can instead apply the theorem separately for \(-E[\log q_m(y|d, \psi)]\) and \(-E[\log q_l(y|\theta, d, \lambda)]\), noting that the variational training and MC estimates for these are independent, yielding the same \(\mathcal{O}(T^{-1/2})\) convergence rate.

The key property of \(\hat{\mu}_{\text{VNMC}}\) is that in practice we need not set \(M = L\) and can remove the asymptotic bias by increasing \(M\) with \(N\). Specifically, using the NMC convergence results discussed in Sec. 2, if we set \(M \propto \sqrt{N}\), then \(\hat{\mu}_{\text{VNMC}}\) converges to EIG\((d)\) at a rate \(\mathcal{O}((NM)^{-1/3})\). This is much slower than the \(\mathcal{O}(K^{-1/2})\) convergence of \(\hat{\mu}_{\text{VNMC}}\) to \(U_{\text{VNMC}}(d, L, \phi^*)\) while \(M = L\) is held fixed. To exploit the faster convergence rate we can focus on training of the variational parameters until \(|U_{\text{VNMC}}(d, L, \phi^*) - \text{EIG}(d)|\) becomes the dominant error, before switching our computational efforts into increasing \(N\) and \(M\) to refine the NMC estimate. Note that the total cost of the \(\hat{\mu}_{\text{VNMC}}\) estimator is \(T = \mathcal{O}(KL + NM)\), where typically \(M \gg L\).

\(\hat{\mu}_{\text{VNMC}}\) can be interpreted as training an amortized importance sampling proposal for \(E_{\hat{p}(\theta)}[p(y|\theta, d)]\), then using this proposal to construct an NMC estimator. Consequently, one can think of stack the standard NMC approach as a particular case of \(\hat{\mu}_{\text{VNMC}}\) in which we naively take \(p(\theta)\) for this proposal.

5 RELATED WORK

Thus far the only alternative to our variational EIG estimators that we have considered is NMC. Here we discuss other alternatives that we benchmark against in our experiments; see Table 1 for a summary.

One established approach is to use a Laplace approximation to the posterior to make fast approximations of EIG (Lewi et al., 2009; Long et al., 2013)

\[
\hat{\mu}_{\text{laplace}}(d) = \frac{1}{N} \sum_{n=1}^{N} \left[ H[p(\theta)] - H[q(\theta|y_n, d)] \right]
\]

where \(q(\theta|y_n, d)\) is a Laplace approximation to \(p(\theta|y_n, d)\) that is computed once for each \(y_n \sim p(y|d)\).

Kleinegesse and Gutmann (2018) recently suggested an implicit likelihood approach that directly approximates the ratio \(r(d, \theta, y) = p(y|\theta, d)/p(y|d)\) using samples from \(p(y|\theta, d)\) and \(p(y|d)\) and the Likelihood-Free Inference by Ratio Estimation (LFIRE) method suggested by (Thomas et al., 2016), which is itself based around logistic regression. This yields the estimator

\[
\hat{\mu}_{\text{LFIRE}}(d) = \frac{1}{N} \sum_{n=1}^{N} \log \hat{r}(d, \theta_n, y_n)
\]

where \(\log \hat{r}(d, \theta_n, y_n)\) is estimated separately for each pairs of samples \(y_n, \theta_n\).

In principal one could also exploit the equivalence between EIG and MI and use other existing MI estimation methods, a number of which were recently summarized by Poole et al. (2018). Of particular note, Belghazi et al. (2018) use a bound on MI in the context of generative adversarial neural network training that is based on the Donsker-Varadhan (DV) representation of the KL divergence (Donsker and Varadhan, 1975). Specifically, they introduce a parametrized approximation \(T(y, \theta|d, \phi)\) to \(\log \frac{p(y|\theta|d)}{p(y|\theta|d, \phi)}\) and then optimize the lower bound

\[
L_{\text{DV}}(d) \triangleq E_{\hat{p}(\theta)}[T(y, \theta|d, \phi)] - \log \left( E_{\hat{p}(\theta)}[p(y|\theta|d, \phi)] \right)
\]

The estimator \(\hat{\mu}_{\text{DV}}\) is then produced in an analogous manner to \(\hat{\mu}_{\text{post}}\).

6 EXPERIMENTS

6.1 BENCHMARKING EXAMPLES

We begin by benchmarking our estimators against the aforementioned baselines on a selection of explicit and implicit likelihood models. For each experiment, we allowed a fixed computational budget; results are presented in Table 2 and fine details in Appendix B. We also note that additional experiments are presented in the supplementary materials.

A/B Test We consider a classical A/B test, commonly used in marketing and design applications. Here the experiment design is the choice of group sizes: \(n\) participants are split between groups A and B of size \(n_A\) and \(n - n_A\), respectively. For each participant we measure a continuous response \(y\). We consider a linear data analysis model

\[
\theta \sim N(0, \Sigma_\theta) \quad y|\theta, d \sim N(X_d\theta, I)
\]

where \(X_d\) is the \(n \times 2\) design matrix with \((1, 0)\) for the first \(n_A\) rows and \((0, 1)\) for the remainder. Since the posteriors for this model are Gaussian, the \(\hat{\mu}_{\text{laplace}}\) estimator is asymptotically exact and yields high qual-
Table 2: Squared bias and variance from 5 runs (averaged over designs) of EIG estimators applied to a number of benchmarking problems. We use $\mathcal{X}$ to denote that a method does not apply and $\ast$ when it is superseded by other methods. Bold indicates the estimator with the lowest empirical mean squared error (which equals the bias squared plus the variance) for the given example. Computational budgets were, from left to right, 10, 10, 60 and 10 seconds.

|                      | A/B Test |                      |                      |                      |                      |                      |
|----------------------|----------|----------------------|----------------------|----------------------|----------------------|----------------------|
|                      | $\mu_{\text{post}}$ | $9.90 \times 10^{-3}$ | 8.09 $\times 10^{-3}$ | 3.91 $\times 10^{-2}$ | 4.95 $\times 10^{-2}$ | 2.21 $\times 10^{-2}$ | 2.70 $\times 10^{-2}$ | 1.07 $\times 10^{-4}$ | 4.48 $\times 10^{-5}$ |
|                      | $\mu_{\text{marg}}$ | 7.60 $\times 10^{-2}$ | 8.51 $\times 10^{-3}$ | 1.69 $\times 10^{-4}$ | 2.97 $\times 10^{-4}$ | $\ast$ | $\ast$ | $\ast$ | $\ast$ |
|                      | $\mu_{\text{NM}}$ | 5.24 $\times 10^{-3}$ | 4.40 $\times 10^{-3}$ | 4.77 $\times 10^{-3}$ | 9.50 $\times 10^{-3}$ | $\ast$ | $\ast$ | $\ast$ | $\ast$ |
|                      | $\mu_{\text{in+}}$ | $\ast$ | $\ast$ | $\ast$ | $\ast$ | 3.05 $\times 10^{-3}$ | 7.72 $\times 10^{-5}$ | 3.75 $\times 10^{-6}$ | 2.83 $\times 10^{-5}$ |
|                      | $\mu_{\text{NM}}$ | 5.65 $\times 10^{0}$ | 6.59 $\times 10^{-1}$ | 4.07 $\times 10^{-2}$ | 2.12 $\times 10^{-2}$ | $\ast$ | $\ast$ | $\ast$ | $\ast$ |
|                      | $\mu_{\text{plae}}$ | 2.39 $\times 10^{-4}$ | 1.11 $\times 10^{-3}$ | 1.19 $\times 10^{-1}$ | 7.70 $\times 10^{-2}$ | $\ast$ | $\ast$ | $\ast$ | $\ast$ |
|                      | $\mu_{\text{LFIRE}}$ | 1.57 $\times 10^{0}$ | 7.51 $\times 10^{-1}$ | 1.22 $\times 10^{-1}$ | 1.37 $\times 10^{-2}$ | 9.66 $\times 10^{-2}$ | 7.69 $\times 10^{-2}$ | $\ast$ | $\ast$ |
|                      | $\mu_{\text{DV}}$ | 2.51 $\times 10^{0}$ | 2.85 $\times 10^{-2}$ | 7.83 $\times 10^{-2}$ | 5.57 $\times 10^{-3}$ | 7.19 $\times 10^{-3}$ | 6.76 $\times 10^{-4}$ | 1.24 $\times 10^{-5}$ | 1.93 $\times 10^{-5}$ |

Figure 1: EIG curves for the Location Finding example, with estimators run until variance is negligible and iterates of $\phi$ are stable to highlight the asymptotic bias of EIG estimates. All our estimators also perform well: they outperform NMC and other previously proposed methods by a large margin.

**Location Finding** We consider searching for an unknown location, such as a participant’s economic utility indifference, using random responses that are both censored and corrupted with non-uniform noise. Let $d \in \mathbb{R}$ and $y = f(\eta)$ where $\eta \mid d \sim N(d - \theta, \sigma_\theta^2 (1 + |d|))$ and $\theta \sim N(\mu_\theta, \sigma_\theta^2)$ and $f$ is the composition of a sigmoid transformation $\mathbb{R} \rightarrow (0, 1)$ followed by clamping $(0, 1) \rightarrow [\epsilon, 1 - \epsilon]$. In this case we can make the marginal estimator asymptotically exact by using an $f$-transformed Gaussian for $q_m(y | d)$. The posterior and Laplace methods are both asymptotically biased (see Figure 1) and in this case both make the same (Gaussian) distributional assumption. The posterior method, however, produces better EIG estimates.

**Mixed Effects Regression** We consider BOED for a mixed effects regression model with a non-linear linking function that will also serve as the basis for the adaptive experiment we run in Sec. 6.3. This class of models is commonly used for analyzing data in a variety of scientific disciplines, where including nuisance variables can be a critical component of the model. In our adaptive experiment, the nuisance variables—i.e. the random effects—are used to account for the variability of individual human participants. Because of the presence of nuisance variables these implicit likelihood models represent a significant challenge for BOED. A simplified version of the model we use is specified as follows

$$\theta \sim N(0, \Sigma_\theta) \quad \text{[fixed effects]}$$

$$\psi_i \sim N(0, \Sigma_\psi) \quad \text{[random effects]}$$

$$\eta(\theta, \psi_i, d) \sim N(X_d \theta + X_d \psi_i, \sigma_\eta^2)$$

$$y = f(\eta) \quad \text{[link function]}$$

where $X_d$ is the design matrix and there are random effects $\psi_i$ for each participant (see Appendix B.3 for a complete description). Encouragingly, we find that our variational estimators outperform the LFIRE and DV baselines on this model and exhibit low errors even though they both make suboptimal distributional assumptions about the posterior/marginal.

**Extrapolation** We consider designing experiments to reduce posterior uncertainty in the model prediction at another point in design space—a point that we cannot experiment on directly. For this example, we take $\psi \sim N(\mu_\psi, \Sigma_\psi)$ and

$$\theta | \psi \sim \text{Bernoulli}(\logit^{-1}(X_{\theta} \psi))$$

$$y | \psi, d \sim \text{Bernoulli}(\logit^{-1}(X_d \psi))$$

where $X_\theta = \begin{bmatrix} 1 & -\frac{1}{2} \end{bmatrix}$ and $X_d = \begin{bmatrix} -1 & d \end{bmatrix}$ for $d \in \mathbb{R}$. Interestingly, this model admits efficient sampling of $y, \theta \sim p(y, \theta | d)$ but not $y \sim p(y | \theta, d)$. Therefore, whilst the posterior, marginal + likelihood and DV methods are all applicable, LFIRE is not. We see that the marginal + likelihood method exhibits the lowest mean squared error.
Convergence in fixed budget (shown by the dashed lines). We conjecture that the next we consider the convergence in real-time when increasing $K$ and keeping $N$ fixed. (c) Convergence in time when setting $N = K$ and increasing both (dashed lines represent theoretical rates). (d) Final RMSE with $N + K = 5000$ fixed, for different $K$. Each graph shows the mean of 100 runs with shading representing a 90% confidence interval in the mean. Time is measured in seconds.

6.2 CONVERGENCE RATES

We now investigate the empirical convergence characteristics of our estimators using the A/B Test example (for which there is no asymptotic bias). We start by considering the convergence of $\mu_{\text{post}}$ and $\mu_{\text{marg}}$ for a particular design and examine the effect of allocating our computational budget in different ways and of increasing our overall budget. The results are shown in Figure 2.

We first consider the convergence in $N$ after a taking a fixed number of $K$ updates to the variational parameters. As shown in Figure 2a, the RMSE initially decreases as we increase $N$, before plateauing due to the bias in the estimator. We also see that $\mu_{\text{post}}$ substantially outperforms $\mu_{\text{marg}}$.

Next consider the convergence in real-time when $N$ is held fixed and we increase $K$. We see in Figure 2b that, as expected, the errors decrease with time and that when a small value of $N = 5$ is taken, we again see a plateauing effect, with the variance of the final MC estimator now becoming the limiting factor.

In Figure 2c we take $N = K$ and increase both, obtaining the predicted convergence rate $O(T^{-1/2})$ (shown by the dashed lines). We conjecture that the better performance of $\mu_{\text{post}}$ is likely due to $\theta$ being lower dimensional (dim = 2) than $y$ (dim = 10).

In Figure 2d, we instead fix $T = N + K$ to investigate the optimal trade-off between optimization and MC error: it appears the range of $K/T$ between 0.4 and 0.9 gives the lowest RMSE.

Finally, we show how $\hat{\mu}_{\text{VNMC}}$ can improve over NMC by using an improved variational proposal for estimating $p(y|d)$. In Figure 3, we plot the EIG estimates obtained by first running $K$ steps of stochastic gradient with $L = 1$ to learn $q_p(\theta|y, d)$, before increasing $M$ and $N$. These estimates converge to the true EIG as $N \to \infty$ when we set $M = \sqrt{N}$. We see that spending some of our time budget training $q_m(\theta|y, d)$ leads to noticeable improvements in the estimation, but also that it is important to increase $N$ and $M$: the starting points for the curves are $M = 10, N = 100$. The initial rapid improvement is because in this region $N, M \ll K$ and so increases in $N$ and $M$ represent a much better overall trade-off. Further, we see that, rather than plateauing like $\mu_{\text{post}}$ and $\mu_{\text{marg}}$, $\hat{\mu}_{\text{VNMC}}$ continues to improve after this initial period, albeit at a slower $O(T^{-1/3})$ rate.

6.3 ADAPTIVE EXPERIMENT WITH PEOPLE

To demonstrate that our variational estimators are useful in practice we now describe an application of sequential BOED to a psychology experiment with real participants using the previously introduced mixed effects regression model. It is very common for psychologists to be interested in understanding which features of a stimulus lead to certain responses in people; for instance, which features of a face lead to
people judging it as friendly? In this setting there are both fixed effects for the various stimulus features common to all participants, and random effects capturing individual preferences and idiosyncratic use of response scales. Hence, this data is usually modeled with mixed effects regression models; as discussed above, this yields a challenging experiment design problem with an implicit likelihood.

Specifically, we conduct an adaptive experiment with human participants recruited from Amazon Mechanical Turk. Each participant is presented with a sequence of 10 pairs of images \( \{d_1, ..., d_{10}\} \). Each pair of images is accompanied by a single fixed prompt, and participants indicate their responses \( \{y_i\} \) using a continuous slider. The images are from a fixed set of images generated by a finite number of image features. See Fig. 5 in the supplementary materials for an example design. An experiment consists of a batch of 8 participants, and the experiment design problem is to choose informative designs \( \{d_i\} \) for each participant, given all previously collected data—so that, e.g., designs for the second participant are informed by data collected from the first participant—for a total of 80 design steps.

To estimate the EIG for different designs, we use \( \hat{\mu}_{m+\ell} \), since it yields the best performance on our mixed effects model benchmark (see Table 2). Before running experiments with human participants, we use our data analysis model as a simulated source of data, choosing model parameters such that fixed effects dominate over random effects. We find that—in almost all eventualities—using BOED leads to a more certain (i.e. lower entropy) posterior after about 40 responses, see Fig. 4a.

We then integrate our experiment design loop into a system that enables real-time design choices for data collection with human participants. We allowed 30s between each response for variational posterior updating, EIG estimation, and design optimization. Here, since the design space is discrete and relatively small, we compute EIG estimates for all permissible designs in parallel. The results obtained with human participants (Fig. 4b) exhibit more variability than the simulated results but still substantiate that BOED results in faster learning about the fixed effects. Importantly, the results of our experiment demonstrate that our variational estimators are sufficiently robust and fast to be used for adaptive experiments with a class of models (i.e. mixed effects models) that are of practical importance in many scientific disciplines.

7 DISCUSSION

We have developed efficient EIG estimators that are applicable to a wide range of experimental design problems. Our estimators can be applied to situations where speed is of primary importance and there is tolerance for biased estimates as well as to situations where statistically consistent estimates are required. Moreover, our estimators can be successfully used in adaptive experiments that require a quick turnaround, and we hope that our work will enable practitioners to carry out adaptive experiments previously thought to be impractical.

There is an intimate connection between mutual information estimation and experimental design. Developments in MI estimation are therefore directly beneficial in Bayesian experimental design, where they can be used to estimate EIG. Conversely, our EIG estimators are mutual information estimators and, as such, they have a large number of potential applications outside experiment design, such as estimating objectives for training deep generative models (Alemi et al., 2016; Chen et al., 2018, 2016;
Emphasize that $\hat{\mu}_{VNMC}$ and $\hat{\mu}_{m+\ell}$ are novel estimators in their own right; future work might therefore look at applying them in other MI estimation settings.

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A DETAILS FOR CONVERGENCE RATE

We now provide the details for Theorem 1. Key to proving the aspect of the Theorem relating to the convergence of the variational parameter $\phi_K$ to $\phi^*$ is Assumption 1. Points 1-5 correspond to assumptions H2, H3, H4, H6, and H7 of Moulines and Bach (2011); our proof will rely heavily on theirs. We note that also that our measurability assumption made in the Theorem itself means that their assumption H1 is automatically satisfied.

Assumption 1. Assume:

1. The function $\phi \mapsto f(X, \phi)$ is almost surely convex in its second argument and differentiable with Lipschitz continuous gradient, i.e. $\forall \phi_1, \phi_2 \in \Phi: E[|\nabla f(X, \phi_1) - \nabla f(X, \phi_2)|^2] \leq C |\phi_1 - \phi_2|^2$ with probability 1 for some $C$.

2. The function $f$ is $\mu$-strongly convex; that is, for all $\phi_1, \phi_2 \in \Phi$:
   $$f(X, \phi_1) \geq f(X, \phi_2) + \nabla f(X, \phi_2)^T(\phi_1 - \phi_2) + \frac{\mu}{2} |\phi_1 - \phi_2|^2$$

3. There exists $\sigma > 0$ such that $E[|\nabla f(X, \phi^*)|^2] \leq \sigma^2$

4. The function $\phi \mapsto f(X, \phi)$ is almost surely twice differentiable with Lipschitz continuous Hessian $Hf$, i.e. $\forall \phi_1, \phi_2 \in \Phi$:
   $$E[|Hf(X, \phi_1) - Hf(X, \phi_2)|] \leq C' |\phi_1 - \phi_2|$$

5. There exists $\tau > 0$ such that $E[|\nabla f(X, \phi^*)|^4] \leq \tau^4$ and there exists a positive definite operator $\Sigma$ such that $E[\nabla f(X, \phi^*) \otimes \nabla f(X, \phi^*)] \preceq \Sigma$

6. The function $\mu$ is Lipschitz continuous

It should be noted that, though relatively standard, these assumptions are also quite strong, particularly the assumption of strong convexity of $f$, and may well not hold in practice. In short, the stochastic gradient scheme used in optimizing the bounds may only converge toward a local optimum of the bound $\phi^*$, rather than the global optimum $\phi^*$. When this happens the behavior and rates of convergence will generally be the same, but the error breakdown will become

$$\|\hat{\mu}(d, \phi_K) - \text{EIG}(d)\|_{L^2} \leq \|\hat{\mu}(d, \phi_K) - B(d, \phi_K)\|_{L^2} + \|B(d, \phi_K) - B(d, \phi^*)\|_{L^2} + \|B(d, \phi^*) - \text{EIG}(d)\|. \quad (35a)$$

$$\text{and (see Moulines and Bach (2011) page 4)} \quad E\mu(\phi_K) - \mu(\phi^*) = O(K^{-1/2}). \quad (42)$$

where

$$|B(d, \phi^*) - \text{EIG}(d)| \geq |B(d, \phi^*) - \text{EIG}(d)|.$$

We now present our proof for the result, repeating it from the main paper for convenience.

Theorem 1. Let $\mathcal{X}$ be a measurable space, $\Phi$ a convex subset of a finite dimensional inner product space; let $X_1, X_2, \ldots$ be i.i.d. random variables taking values in $\mathcal{X}$ and $f : \mathcal{X} \times \Phi \rightarrow \mathbb{R}$ a measurable function. Let

$$\mu(\phi) \triangleq E[f(X_1, \phi)] \approx \hat{\mu}_N(\phi) \triangleq \frac{1}{N} \sum_{i=1}^N f(X_i, \phi)$$

and suppose that $\sup_{\phi \in \Phi} \|f(X_1, \phi)\|_{L^2} < \infty$. Then

$$\sup_{\phi \in \Phi} \|\hat{\mu}_N(\phi) - \mu(\phi)\|_{L^2} = O(N^{-1/2}). \quad (27)$$

Now suppose Assumption 1 in Appendix A holds and that $\phi^*$ is the unique minimizer of $\mu$. Using $K$ iterations of the Polyak-Ruppert averaged stochastic gradient descent algorithm of Moulines and Bach (2011) with gradient estimator $\nabla \phi f(X_t, \phi)$ then

$$\|\mu(\phi_K) - \mu(\phi^*)\|_{L^2} = O(K^{-1/2}) \quad (28)$$

and, combining with the first result,

$$\|\hat{\mu}_N(\phi_K) - \mu(\phi^*)\|_{L^2} = O(N^{-1/2} + K^{-1/2}) \quad (29)$$

$$= O(T^{-1/2}) \text{ if } N \asymp K. \quad (30)$$

Proof. We begin by establishing the uniform convergence of $\hat{\mu}_N(\phi)$ to $\mu(\phi)$, for which we simply use the $L^2$ weak law of large numbers. Specifically, we let $Y_n = f(X_n, \phi)$ and $\varepsilon_N(\phi) = \|\hat{\mu}_N(\phi) - \mu(\phi)\|_{L^2}$, then

$$\varepsilon_N^2(\phi) = E\left(\frac{1}{N} \sum_{n=1}^N (Y_n - EY_n)\right)^2 \quad (36)$$

$$= E\left(\frac{1}{N^2} \sum_{n=1}^N (Y_n - EY_n)^2\right) \quad (37)$$

$$= \frac{1}{N^2} N \text{Var}(Y_n) \quad (38)$$

$$\leq \frac{1}{N} \sup_{\phi \in \Phi} \|f(X_1, \phi)\|_{L^2}^2 \quad (39)$$

which is bounded by assumption. Thus

$$\sup_{\phi \in \Phi} \varepsilon_N(\phi) = O(N^{-1/2}) \quad (40)$$

as required.
To establish $L^2$ convergence of the function values, it remains to control the variance of $\mu(\phi_K)$. We now invoke point 6 of Assumption 1 to see that, for some constant $B$ (namely the Lipschitz constant for $\mu$),

$$\text{Var}[\mu(\phi_K)] = \mathbb{E} \left[ (\mu(\phi_K) - \mathbb{E} [\mu(\phi_K)])^2 \right]$$

\begin{align}
&\leq \mathbb{E} \left[ (\mu(\phi_K) - \mu(\mathbb{E} \phi_K))^2 \right] \\
&\leq B^2 \mathbb{E} \left[ (\phi_t - \mathbb{E} \phi_t)^2 \right] \\
&\leq B^2 \|\phi_K - \phi^*\|^2_{L^2}
\end{align}

By (41) we conclude $\sqrt{\text{Var}[\mu(\phi_K)]} = \mathcal{O}(K^{-1/2})$. Thus $I(\phi_K)$ converges in $L^2$ at the required rate.

Finally, if $\epsilon_K = \|\hat{\mu}_K(\phi_K) - \mu(\phi^*)\|_{L^2}$ then

$$\epsilon_K \leq \|\hat{\mu}_K(\phi_K) - \mu(\phi^*)\|_{L^2} + \|\mu(\phi^*) - \mu(\phi^*\land\hat{\mu}_K(\phi_K))\|_{L^2}$$

$$\leq \|\hat{\mu}_K(\phi_K) - \mu(\phi^*)\|_{L^2} + \sup_{\phi \in \Theta} \|\hat{\mu}_K(\phi) - \mu(\phi)\|_{L^2}$$

$$= \mathcal{O}(N^{-1/2} + K^{-1/2})$$

$$= \mathcal{O}(T^{-1/2})$$

as required. \qed

\section*{B \hspace{1em} EXPERIMENT DETAILS}

We note that all experiments had a finite design space $D$ and we learned separate variational parameters for each $d$. This is not a requirement of our methods; this simple choice allows the fairest comparison with other methods, which also do not pool information between designs.

\subsection*{B.1 \hspace{1em} A/B TEST}

Recall the model

$$\theta \sim N(0, \Sigma_\theta)$$

$$y|\theta, d \sim N(X_d \theta, I).$$

In this example we set the number of participants to be $n = 10$ with 11 designs ($n_A = 0, \ldots, 11$) and the prior covariance matrix to be

$$\Sigma_\theta = \begin{pmatrix} 10^2 & 0 \\ 0 & 1.82^2 \end{pmatrix}$$

We chose families of variational distributions that include the true posterior (or true marginal). For the amortised posterior, we set $\phi = (A, \Sigma_p)$ with $\phi$ trained separately for each $d$ and let

$$q_p(\theta|y, d, \phi) \sim N(Ay, \Sigma_p)$$

where $A$ is a $10 \times 2$ matrix and $\Sigma_p$ is positive definite. For the marginal, we simply take $\phi = (\mu_m, \Sigma_m)$ and

$$q_m(y|d, \phi) \sim N(\mu_m, \Sigma_m).$$

For NMC and Laplace, no variational families need to be specified.

For LFIRE, we used a parametrization $\phi = (b, \delta, \Lambda)$ and used the ratio estimate

$$\log \hat{r}(y|\theta, d, \phi) = b - (\theta - \delta)^T \Lambda (\theta - \delta)$$

where $\Lambda$ is positive definite. This form was chosen to mimic the approximation made by the posterior method, and so reduce the effect of architecture on performance.

For DV, we used a similar critic, namely we set $\phi = (A, \Lambda)$ and

$$T(y, \theta|d, \phi) = -(\theta - Ay)^T \Lambda (\theta - Ay)$$

where $\Lambda$ is positive definite.

The ground truth EIG($d$) was computed analytically.

\subsection*{B.2 \hspace{1em} LOCATION FINDING}

Recall the model

$$\theta \sim N(\mu, \sigma^2_\theta)$$

$$\eta|\theta, d \sim N(d - \theta, \sigma^2_\eta(1 + |d|)^2)$$

$$y = f(\eta)$$

where

$$f : \mathbb{R} \to [\epsilon, 1 - \epsilon]$$

$$x \mapsto \begin{cases} 
\epsilon & \text{if } x \leq \text{logit}(\epsilon) \\
1 - \epsilon & \text{if } x \geq \text{logit}(1 - \epsilon) \\
\frac{1}{1 - e^{-x}} & \text{otherwise}
\end{cases}$$

and $\text{logit}(p) = \log p - \log (1 - p)$. For this example we set $\mu = -20, \sigma = 20$ and $\sigma = 1$. We took designs on a linearly spaced grid in $[-80, 80]$. For the variational family for the posterior, we took $\phi = (w, \sigma, \mu_0, \mu_1, \sigma_1)$ and then

$$q_p(\theta|y, d, \phi) \sim N(\mu_p, \sigma^2_p)$$

where $\hat{\eta} = d - \text{logit}(y)$

$$\mu_p = w \hat{\eta} + (1 - w) \mu_0 + \mu_1 1_{\{y = \epsilon\}}$$

$$\sigma^2_p = \sigma^2 + \sigma^2_\mu 1_{\{y = \epsilon\}} + \sigma^2_\sigma 1_{\{y = 1 - \epsilon\}}$$

For the marginal, we simply took $\phi = (\mu_m, \sigma_m)$ and

$$q_m(y|d, \phi) \sim f#N(\mu_m, \sigma^2_m).$$

where $\#$ denotes the push-forward measure.

For LFIRE, we used the parametrization $\phi = (b, b_0, b_1, \delta, \lambda)$ with ratio estimate

$$\hat{\eta} = d - \text{logit}(y)$$

$$\log \hat{r}(y|\theta, d, \phi) = b - \lambda(\hat{\eta} - \delta)^2$$

$$+ b_0 1_{\{y = \epsilon\}} + b_1 1_{\{y = 1 - \epsilon\}}$$
For DV, the critic had parametrization \( \phi = (b_0, b_1, \delta, \delta_0, \delta_1, \lambda_0, \lambda_1) \) and we set
\[
\hat{\eta} = d - \logit(y) \tag{64}
\]
\[
\lambda = \lambda_i + \lambda_0 \mathbf{1}_{y_0} + \lambda_1 \mathbf{1}_{y_1} \tag{65}
\]
\[
\delta = \delta_i + \delta_0 \mathbf{1}_{y_0} + \delta_1 \mathbf{1}_{y_1} \tag{66}
\]
\[
T(y, \theta | d, \phi) = -\lambda(\hat{\eta} - \delta)^2 + b_0 \mathbf{1}_{y_0} + b_1 \mathbf{1}_{y_1} \tag{67}
\]
Both these forms were chosen to minimize the differences between the functional forms used for different methods.

The ground truth EIG\( (d) \) was computed by running the marginal method, which is statistically consistent for this example because the true marginal is contained in the variational family, to convergence.

### B.3 Mixed Effects Regression for Mechanical Turk Experiment

We begin by describing the experiment itself. Participants were presented with a question of the form seen in Figure 5 with the possible images shown in Figure 6. There were two image feature dimensions with 3 levels each. A single image \( i \) could therefore be represented as a \( 1 \times 6 \) matrix \( X_i \) with two entries 1 and the rest 0. With the left image \( i_1 \) and right image \( i_2 \), the question was represented as \( X_d = X_{i_1} - X_{i_2} \) encoding the assumed left-right symmetry. We then considered a model for the \( it \) participant

\[
\theta \sim N(0, \Sigma_\theta) \tag{68}
\]
\[
\sigma^2_\psi \sim \Gamma(\alpha_\psi, \beta_\psi) \tag{69}
\]
\[
\psi | \sigma^2_\psi \sim N(0, \sigma^2_\psi I_6) \tag{70}
\]
\[
\sigma^2_k \sim \Gamma(\alpha_k, \beta_k) \tag{71}
\]
\[
\log k_i \sim N(0, \sigma_k^2) \tag{72}
\]
\[
\mathbf{y} | \psi, k, d \sim N(k_i (X_d \theta + X_d \psi_i), \sigma^2_\psi) \tag{73}
\]
\[
y = f(\mathbf{y}) \tag{74}
\]

where \( f \) is the censored sigmoid defined in (56) and \( i \in \{1, \ldots, 8\} \) as there were 8 different participants.

The actual prior values of the parameters used were

\[
\Sigma_\theta = 100 I_6 \tag{75}
\]
\[
\alpha_\psi = \beta_\psi = 2 \tag{76}
\]
\[
\alpha_k = \beta_k = 2 \tag{77}
\]
\[
\sigma_k = 10 \tag{78}
\]

We begin by discussing the variational families used to estimate the EIG. Because we used this model to run an adaptive experiment, we also required a variational family to learn the full posterior (over random effects and hyperparameters as well as \( \theta \)). This is detailed at the end.

For the posterior estimator of EIG, we took \( \phi = (A, \Sigma_p) \) and
\[
\hat{\eta} = \logit(y) \tag{79}
\]
\[
q_p(\theta | y, d, \phi) \sim N(A \hat{\eta}, \Sigma_p) \tag{80}
\]
For the marginal + likelihood estimator, we set \( \phi = (\mu_m, \sigma_m, \mu_t, \sigma_t, \xi) \) and took
\[
q_m(y | d, \phi) \sim f \# N(\mu_m, \sigma^2_m) \tag{81}
\]
\[
q_k(\theta | d, \phi) \sim f \# N(\epsilon^2 X_d \theta + \mu_t, \sigma_k^2) \tag{82}
\]
For LFIRE, we used \( \phi = (b, \delta, \lambda) \) and then took
\[
\hat{\eta} = \logit(y) \tag{83}
\]
\[
\log \hat{r}(y | \theta, d, \phi) = b - \lambda(\hat{\eta} - \delta)^2 \tag{84}
\]
For DV, we used \( \phi = (\lambda, \xi) \) and
\[
\hat{\eta} = \logit(y) \tag{85}
\]
\[
T(y, \theta | d, \phi) = -\lambda(\hat{\eta} - \epsilon^2 X_d \theta)^2 \tag{86}
\]
For benchmarking, we computed the ground truth using a variant of NMC. Specifically, we note that
\[
p(y | d) = \mathbb{E}_{y \sim \psi; k} [p(y | \theta, \psi, k, d)] \tag{87}
\]
\[
p(y | \theta, d) = \mathbb{E}_{y \sim \psi; k} [p(y | \theta, \psi, k, d)] \tag{88}
\]
and for this model, we can sample directly from \( p(\psi, k) \). These identities allow us to estimate the marginal and likelihood by Monte Carlo, and then combine in a NMC estimator for \( EIG(d) \). Whilst inefficient, this estimator is statistically consistent.

When optimizing the EIG to select designs \( d \), we estimated \( EIG \) across all candidate designs—this simple approach isolates the effect of our new \( EIG \) estimators.

For the full variational inference of the posterior used when we receive actual data, we used a partial mean-field approximation. Specifically, we set \( q(\theta, \psi, \{\psi_i\}_{i=1}^8, \sigma_k, \{k_i\}_{i=1}^8) \) to be
\[
\theta \sim N(\mu_\theta, \Sigma_\theta) \tag{89}
\]
\[
\sigma^2_\psi \sim \Gamma(\alpha_\psi, \beta_\psi) \tag{90}
\]
\[
\psi_i | \theta \sim N(A \theta - \mu_\psi, \Sigma_\psi) \tag{91}
\]
\[
\sigma^2_k \sim \Gamma(\alpha_k, \beta_k) \tag{92}
\]
\[
\log k_i \sim N(\mu_k, \sigma_k^2) \tag{93}
\]
and we learned the variational parameters \( \mu_\theta, \Sigma_\theta, \alpha_\psi, \beta_\psi, A, \mu_\psi, \Sigma_\psi, \alpha_k, \beta_k, \mu_k, \sigma_k \) by conventional (not amortized) variational inference. Note that, under this approximate posterior, \( \theta \) is multivariate Gaussian so we can compute its entropy analytically.
Figure 5: A screenshot of the question answering interface used by human participants in the adaptive experiment in Sec. 6.3.

Figure 6: The nine characters we used in the adaptive experiment in Sec. 6.3. They vary along two feature dimensions: the mouth (smile, frown, showing teeth) and eyebrows.
Finally, for the simulated results, we took 
\[ \theta = \left( -30 \ 30 \ 0 \ -12 \ -6 \ 18 \right). \] (94)
We simulated the random effects \( \psi, k \) from the prior and used the prior value \( \sigma_\eta = 10 \).

### B.4 Extrapolation

Recall the model 
\[ \psi \sim N(\mu_\psi, \Sigma_\psi) \]
\[ \theta|\psi \sim \text{Bernoulli}(\logit^{-1}(X_\theta \psi)) \]
\[ y|\psi, d \sim \text{Bernoulli}(\logit^{-1}(X_d \psi)) \]
where \( X_\theta = (1 \ -\frac{1}{2}) \) and \( X_d = (-1 \ d) \) for \( d \in \mathbb{R} \).

For the posterior method we set \( \phi = (l_0, l_1) \) and 
\[ l_p(y) = l_1 y + l_0 (1 - y) \] (96)
\[ q_p(\theta|y, d, \phi) \sim \text{Bernoulli}(\logit^{-1}(l_p(y))). \] (97)
We computed the prior entropy, which is not analytically tractable here, using a MC estimator, noting that \( \theta \) has a finite sample space.

For the marginal + likelihood method, we let \( \phi = (l_0, l_1) \) and then 
\[ q_m(y|d, \phi) \sim \text{Bernoulli}(\logit^{-1}(l)) \] (98)
\[ l_\phi(\theta) = l_1 \theta + l_0 (1 - \theta) \] (99)
\[ q_\phi(\theta|y, d, \phi) \sim \text{Bernoulli}(\logit^{-1}(l_\phi(\theta))). \] (100)
Finally, for DV, we let \( \phi = (w_y, w_\theta, w_\psi \theta) \) and took 
\[ T(\theta|y, d, \phi) = w_y y + w_\theta \theta + w_\psi \psi \theta. \] (101)

The ground truth EIG was computed using MC, noting that the sample spaces for \( y, \theta \) are finite in this example.

### C Additional Experiments

#### C.1 Death Process

We examine experimental design for the simple continuous time process considered in (Cook et al., 2008) and (Kleinegesse and Gutmann, 2018), arising in epidemiology. Consider a population with fixed size \( N \) that is initially healthy at time \( t = 0 \), with individuals becoming infected at a constant rate \( b \) as time evolves. We consider a design space \( d = (t_1, t_2) \), where \( 0 \leq t_1 \leq t_2 \), corresponding to the times at which we measure the number of infected individuals. We place a log-normal prior on the infection rate \( b \).

For this example, we investigate how the choice of variational family affects the asymptotic bias. In Fig. 7 we compare the EIG surfaces obtained using four estimators: i) an exact method that uses brute force quadrature; ii) \( \hat{\mu}_{\text{post}} \) with a log-normal variational distribution; iii) \( \hat{\mu}_{\text{post}} \) with a truncated normal variational distribution; and iv) the Laplace approximation \( \hat{\mu}_{\text{laplace}} \). The log-normal family matches the true posterior best, giving mean absolute errors \( \sim 10^{-3} \). The second posterior method and the Laplace approximation both make the same distributional assumption, but Laplace results in absolute errors that are about 30% higher than for the posterior method. See Fig. 8 for a closer analysis of the errors of the approximate methods.

#### Experimental Details

The likelihood for observing \( (I_1, I_2) \) infected individuals from a population of size \( N \) at times \( (t_1, t_2) \) is given by (Ehrenfeld, 1962): 
\[ p(I_1, I_2|b, t_1, t_2) = \frac{N!}{I_1!(I_2-I_1)!(N-I_2)!} \left[ 1 - e^{-bt_1} \right]^{I_1} \times \]
\[ \left[ 1 - e^{-b(t_2-t_1)} \right]^{I_2-I_1} \left[ e^{-bt_1} \right]^{I_1} \left[ e^{-bt_2} \right]^{N-I_2} \] (102)
The prior over the infection rate \( b > 0 \) is taken to be 
\[ \log b \sim N(\mu_b, \sigma_b) \] (103)
so that the joint density is given by 
\[ p(I_1, I_2, b|t_1, t_2) = p(I_1, I_2|b, t_1, t_2) p(b) \] (104)
In our experiment we choose \( N = 10, \mu_b = 0, \) and \( \sigma_b = 0.25 \). The figures are scaled such that the maximum EIG over the design space (as computed with the exact method) is 1.0. For all four EIG estimation methods we use quadrature and exact summation over the outcomes \( (I_1, I_2) \) where appropriate to obtain maximally accurate results. That is, the obtained results are only constrained by the methods themselves and not the computational budget used. Note that we do not make use of any kind of amortization.

#### C.2 Sequential Location Finding

We conduct a simple sequential BOED experiment based on the location finding example introduced in Sec. 6.1. At each iteration \( t \) we use variational inference with a Gaussian variational distribution to update the prior and the marginal OED estimator to choose the design \( d_t \). For comparison we consider a heuristic design strategy in which \( d_t \) is chosen to be the (approximate) posterior mean of \( \theta \) at iteration \( t \). See Fig. 9 for the results, which indicate that selecting designs using BOED results in lower uncertainty about the unknown location than the heuristic strategy. Data was simulated from the data analysis model, with the true location set to \( \theta = 44.6 \).
D CONSISTENT EIG ESTIMATION WITH CONTROL VARIATES

Let \( \hat{p}(y) = \frac{1}{M} \sum_{m=1}^{M} p(y|\theta_m) \) with \( \theta_m \sim p(\theta) \) denote a Monte Carlo estimator of the marginal likelihood \( p(y) \). Then we can write

\[
\text{EIG} = E_{p(y, \theta)} [\log p(y|\theta) - \log \hat{p}(y)]
\]

\[
\approx E_{p(y, \theta)} [\log p(y|\theta) - \log q_m(y)]
\]

Suppose furthermore that: (i) we have a marginal variational distribution \( q_m(y) \) at our disposal; and (ii) \( q_m(y) \) and the likelihood \( p(y|\theta) \) are both exponential family distributions. The distribution \( q_m(y) \) could, for example, be learned using the same procedure used in Sec. 3.2. Then we can write

\[
\text{EIG} \approx E_{p(y, \theta)} [\log p(y|\theta) - \log \hat{p}(y)]
\]

\[
= E_{p(y, \theta)} [\log q_m(y) - \log \hat{p}(y)] + \quad (105)
\]

\[
E_{p(y, \theta)} [\log p(y|\theta) - \log q_m(y)]
\]

Since the integral w.r.t. \( y \) in the final expectation can be computed analytically given our assumptions, we make the substitution

\[
E_{p(\theta)} [E_{p(y|\theta)} [\log p(y|\theta) - \log q_m(y)]] \rightarrow
\]

\[
E_{p(\theta)} [\text{analytic function of } \theta] \quad (106)
\]

This expectation w.r.t. \( \theta \) can be efficiently estimated with Monte Carlo. Importantly, the variance of the NMC term \( E_{p(y, \theta)} [\log \hat{p}(y)] \) can be substantially reduced by the control variate provided by \( \log q_m(y) \), so long as \( q_m(y) \approx p(y) \).\(^3\) Finally, note that just like \( \hat{\mu}_{\text{NMC}} \), this estimator is consistent, i.e. it will converge to the EIG as \( N, M \to \infty \).

E KL\((q|p)\) VERSUS KL\((p|q)\)

A notable feature of our variational bounds is that they feature the forward KL divergence \( \text{KL}(p|q) \) as opposed to the reverse KL divergence \( \text{KL}(q|p) \) that is typically found in variational inference. This difference is worth exploring in some detail. As discussed in the main text, an importance consequence of the KL\((p|q)\) formulation is that we can easily compute gradient estimates of the variational bound whenever we can sample from the model joint distribution \( p(y, \theta) \). In particular we do not encounter any of the difficulties that can occur with discrete latent variables in variational inference.

Here we explore how the reverse KL divergence exhibits discontinuous behavior that could be problematic in the context of EIG estimation. The EIG is defined w.r.t. a nested expectation \( E_{p(y)} E_{p(\theta|y)} \). To clarify what is going on it is sufficient to focus on the inner expectation \( E_{p(\theta|y)} \), i.e. we fix the observation \( y \) — and thus the posterior \( p(\theta|y) \) — and drop\(^4\) the term containing the prior \( p(\theta) \) to consider the ‘partial’ KL divergence

\[
E_{p(\theta|y)} [\log q(\theta)]
\]

(107)

which is an approximation to the (negative) entropy of the posterior, i.e.

\[
E_{p(\theta|y)} [\log p(\theta|y)] \approx E_{p(\theta|y)} [\log q(\theta)]
\]

(108)

Here \( q(\theta) \) is one of the variational distributions \( q_{\text{forward}} \) and \( q_{\text{reverse}} \), which we define to be given by

\[
q_{\text{forward}} \equiv \arg \min_{q \in Q} \text{KL}(p(\theta|y)|q(\theta))
\]

(109)

and

\[
q_{\text{reverse}} \equiv \arg \min_{q \in Q} \text{KL}(q(\theta)|p(\theta|y))
\]

(110)

Here \( Q \) is some family of variational distributions. Crucially, \( q \) appears twice on the RHS of (110) (i.e. once in the measure and once in the logarithm), while it only appears once on the RHS of (109). This can result in the well-known behavior of mode-locking — and thus mode-dropping — which in our context can result in significant misestimates of the posterior entropy. Furthermore, since this mode-locking behavior is discontinuous (so that it can occur for a particular design \( d \) but not for a neighboring design \( d' \)) it can potentially result in large design-dependent bias in EIG estimation. For a quantitative exploration of this phenomenon for two bimodal posteriors and a Normal family of variational distributions \( Q \) see Figures 10 and 11.

\(^3\)Note that there is no opportunity for variance reduction if we do not have an analytic result for the quantity \( E_{p(y|\theta)} [\log q_m(y)] \); however, it is not strictly necessary that we have an analytic result for \( E_{p(y|\theta)} [\log p(y|\theta)] \).

\(^4\)This term is constant w.r.t the variational problem.
Figure 7: EIG surfaces estimated by four methods for the two-dimensional design \((t_1, t_2)\) for the continuous time model described in Sec. C.1. The optimal design \((t_1^*, t_2^*)\) determined by each method is indicated with a cross. The posterior method with a LogNormal variational distribution yields nearly exact results. The posterior method with a Truncated Normal distribution and the Laplace method are not as accurate but still result in designs with large EIG. Note that the EIG has been scaled for interpretability and that all four figures use a common scale. The errors of these estimators are examined more closely in Figure 8.

Figure 8: Absolute EIG errors corresponding to the estimates depicted in Fig. 7. The optimal design \((t_1^*, t_2^*)\) determined by an exact method is indicated with a star. The absolute error of the LogNormal Posterior estimate is \(\sim 10^{-3}\) across the design space. The mean absolute error of the Laplace EIG estimates across the design space is about 30% higher than for the Posterior method with a Truncated Normal variational distribution. In this case the Laplace method results in an upper bound, while (as always) both Posterior methods yield a lower bound. All three figures have the same scale as Fig. 7, except for the LogNormal errors, which have been scaled by an additional factor of 100.

Figure 9: On the left we depict an adaptively learnt posterior distribution for the location finding example in Sec. C.2. Depicted in red are the mean and 90% confidence interval for a variational approximation to the posterior over \(\theta\). Also illustrated are the designs chosen at each iteration, with red and blue crosses corresponding to heuristic and BOED design strategies, respectively. On the right we depict how the posterior entropy evolves for experiments run according to the two design strategies. After 25 iterations, BOED has achieved notably lower posterior uncertainty about the unknown location.
Figure 10: Normal variational distributions found by fitting to a target posterior that is a mixture with two distinct Normal components. In both subfigures the target posterior has $\pi_1 = 0.6$, $\pi_2 = 0.4$, $\sigma_1 = 0.5$, and $\sigma_2 = 1.0$. In the top subfigure the gap between the two components is $\Delta \mu_{\text{post}} = 3.0$, while in the bottom subfigure $\Delta \mu_{\text{post}} = 3.3$. In contrast to the behavior resulting from $\text{KL}(p|q)$, the mode-seeking behavior of $\text{KL}(q|p)$ leads to a large change in the corresponding optimal variational distribution from top to bottom and a correspondingly large change in the ‘partial’ KL.

Figure 11: Posterior entropy estimates as inferred by fitting with the reverse and forwards KL divergences. The (negative) posterior entropy as estimated with $\text{KL}(p|q)$ exhibits a sharp discontinuity as the gap between the two components crosses $\Delta \mu_{\text{post}} \approx 3.18$. 