Variational Bayesian Optimal Experimental Design

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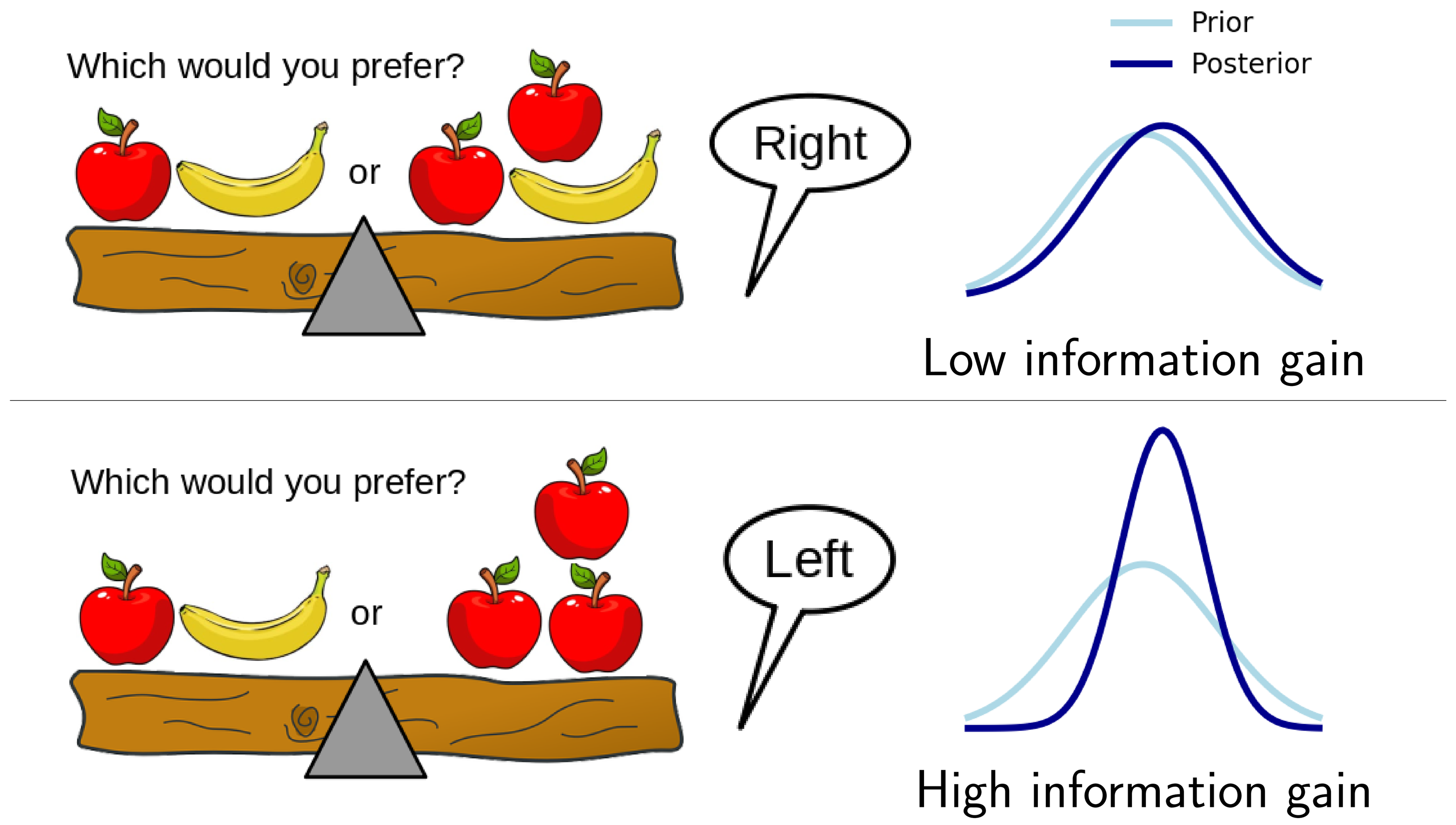
Overview

- In Bayesian experimental design, we want to find experiment designs that have maximal expected information gain (EIG)
- Computing EIG is challenging because it is the expectation of an intractable integrand
- We use an **amortized variational** approximations to the integrand to avoid recomputing similar integrals again and again
- We establish EIG bounds to train the variational approximations

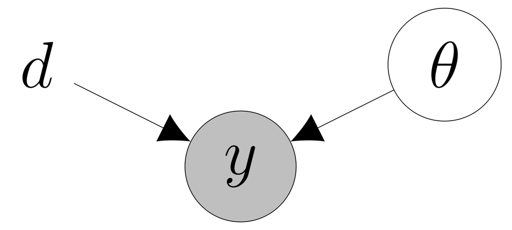
Bayesian optimal experimental design (BOED)

Motivation How do we design an experiment, e.g. pose a question to a participant, that will lead to high quality inference?

Design choose d	Experiment obtain y	Inference on θ



Bayesian model for experimental design: **design** d, **outcome** y and **latent variable** of interest θ



with prior $p(\theta)$ and likelihood $p(y|\theta,d)$.
The **information gain** of the experiment is the reduction in entropy from the prior to the posterior

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

The **expected information gain (EIG)** [1] is

$$\mathrm{EIG}(d) = \mathbb{E}_{y\sim p(y|d)}\left[H[p(\theta)] - H[p(\theta|y,d)]\right].$$

The optimal design d^* is the one which maximizes EIG over the space of feasible designs

Estimating EIG

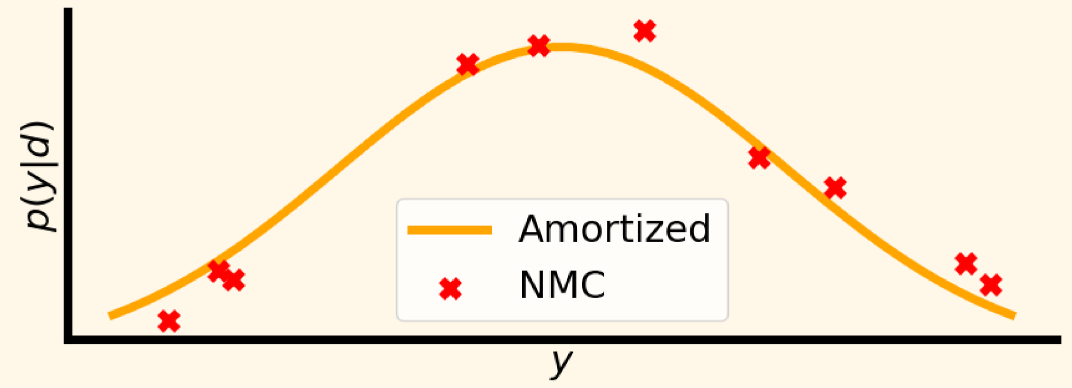
$$\mathrm{EIG}(d) = \mathbb{E}_{\theta,y\sim p(\theta)p(y|\theta,d)}\left[\log\frac{\boxed{p(\theta|y,d)}}{p(\theta)}\right] = \mathbb{E}_{\theta,y\sim p(\theta)p(y|\theta,d)}\left[\log\frac{p(y|\theta,d)}{\boxed{p(y|d)}}\right].$$

We do not know $p(y|d)$ or $p(\theta|y,d) \implies$ no standard Monte Carlo
Traditional solution is Nested Monte Carlo (NMC) [2]

$$\mathrm{EIG}(d) \approx \frac{1}{N}\sum_{n=1}^{N}\log\frac{p(y_n|\theta_n,d)}{\frac{1}{M}\sum_{m=1}^{M}p(y_n|\theta_m,d)}$$

where $\theta_n, y_n \overset{\text{i.i.d.}}{\sim} p(\theta)p(y|\theta,d)$ and $\theta_m \overset{\text{i.i.d.}}{\sim} p(\theta)$.

Use amortization: learn the functional form of the integrand instead of repeatedly re-estimating $p(y|d)$



To learn this functional form, we use variational bounds on EIG

Marginal upper bound: $\mathrm{EIG}(d) \le \mathbb{E}_{p(\theta)p(y|\theta,d)}\left[\log\frac{p(y|\theta,d)}{q_m(y|d,\phi)}\right]$, or

Posterior lower bound: $\mathrm{EIG}(d) \ge \mathbb{E}_{p(\theta)p(y|\theta,d)}\left[\log\frac{q_p(\theta|y,d,\phi)}{p(\theta)}\right]$.

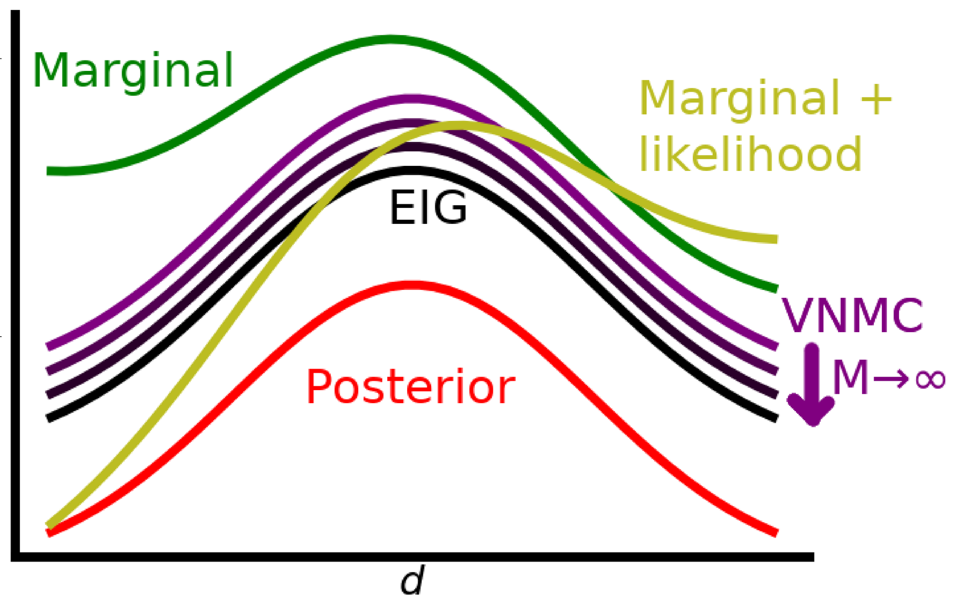
We train ϕ by stochastic gradient minimization or maximization.
Extend posterior to get a bound that becomes arbitrarily tight as $M\to\infty$

Variational NMC: $\mathrm{EIG}(d) \le \mathbb{E}_{p(\theta_0)p(y|\theta_0,d)q_v(\theta_{1:M}|y,\phi)}\left[\log\frac{p(y|\theta_0,d)}{\frac{1}{M}\sum_{m=1}^{M}\frac{p(\theta_m)p(y|\theta_m,d)}{q_v(\theta_m|y,d,\phi)}}\right]$

Extend marginal for the **implicit likelihood** scenario

Marginal + likelihood: $\mathrm{EIG}(d) \approx \mathbb{E}_{p(\theta)p(y|\theta,d)}\left[\log\frac{q_\ell(y|\theta,d,\psi)}{q_m(y|d,\phi)}\right]$

		Implicit	Bound	Consistent
Ours	Posterior	✓	Lower	✗
	Marginal	✗	Upper	✗
	VNMC	✗	Upper	✓
	M. + ℓ.	✓	✗	✗
Baseline	NMC	✗	Upper	✓
	Laplace	✗	✗	✗
	LFIRE	✓	✗	✗
	DV	✓	Lower	✗

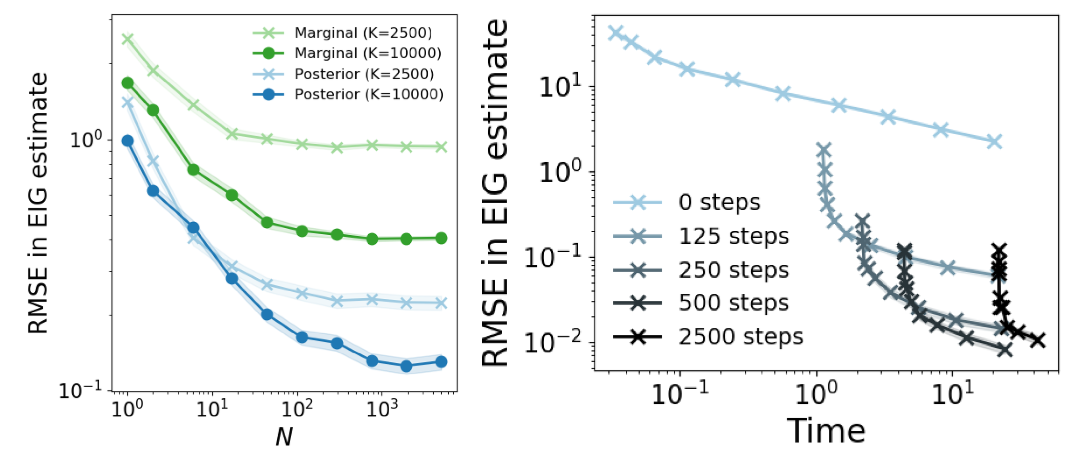


Convergence rates

For any one of our variational bounds $\mathcal{B}$, we train ϕ for K steps and then take an N-sample Monte Carlo estimate $\hat{\mu}$ of the bound. We decompose the EIG estimation error using the triangle inequality

$$\begin{aligned}\|\hat{\mu}(d,\phi_K)-\mathrm{EIG}(d)\|_2 \le &\|\hat{\mu}(d,\phi_K)-\mathcal{B}(d,\phi_K)\|_2 && \text{Monte Carlo error} && \mathcal{O}(N^{-1/2})\\ &+\|\mathcal{B}(d,\phi_K)-\mathcal{B}(d,\phi^*)\|_2 && \text{Optimization error} && \mathcal{O}(K^{-1/2})\\ &+|\mathcal{B}(d,\phi^*)-\mathrm{EIG}(d)| && \text{Asymptotic bias} && \mathcal{O}(M^{-1}) \quad \text{for VNMC [2]}\end{aligned}$$

For VNMC, the total cost of the estimator is $T = MN + K$. If we take $M=\sqrt{N}$ we obtain an overall convergence rate $\mathcal{O}(T^{-1/3})$, but unlike NMC we make use of fast variational training.



(Left) Posterior and marginal with K training steps, then N samples

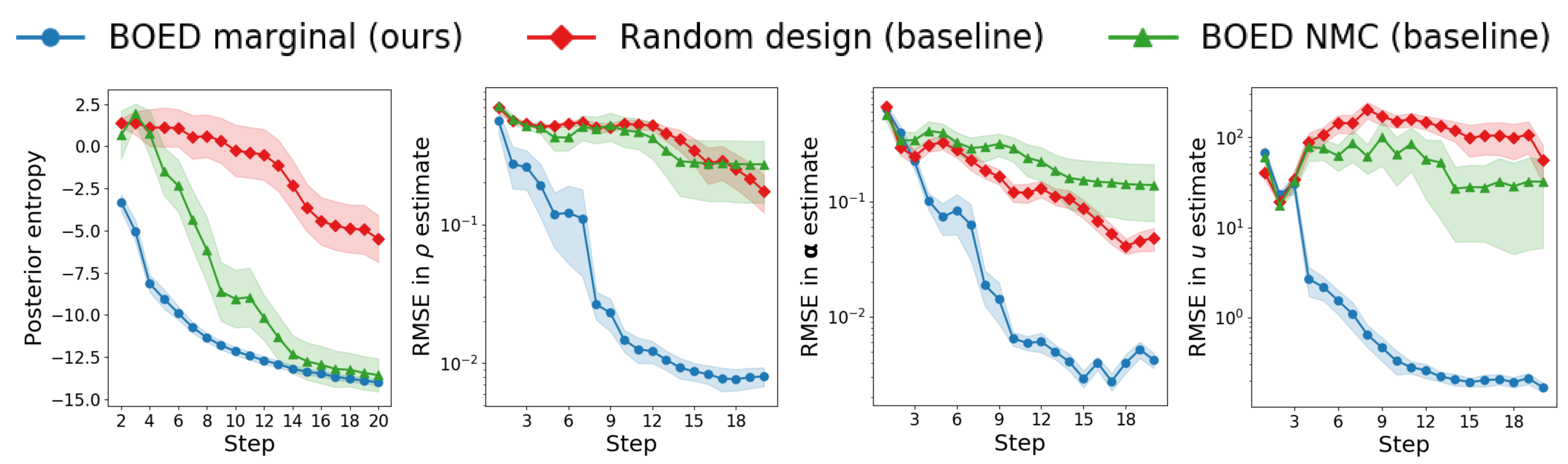
(Right) VNMC with K training steps, then N and $M=\sqrt{N}$ samples

Experiments

Bias-variance of EIG estimators

	A/B test		Econ. preference		Mixed effects	
	Bias^2	Var	Bias^2	Var	Bias^2	Var
Posterior	1.33×10^{-2}	7.15×10^{-3}	4.26×10^{-2}	8.53×10^{-3}	2.21×10^{-3}	2.70×10^{-3}
Marginal	7.45×10^{-2}	6.41×10^{-3}	$\mathbf{1.10\times10^{-3}}$	$\mathbf{1.99\times10^{-3}}$	-	-
VNMC	$\mathbf{3.44\times10^{-3}}$	$\mathbf{3.38\times10^{-3}}$	4.17×10^{-3}	9.04×10^{-3}	-	-
M. + ℓ.	-	-	-	-	$\mathbf{3.05\times10^{-3}}$	$\mathbf{7.72\times10^{-5}}$
NMC	4.70×10^{0}	3.47×10^{-1}	7.60×10^{-2}	8.36×10^{-2}	-	-
Laplace	$\mathbf{1.92\times10^{-4}}$	$\mathbf{1.47\times10^{-3}}$	8.42×10^{-2}	9.70×10^{-2}	-	-
LFIRE	2.29×10^{0}	6.20×10^{-1}	1.30×10^{-1}	1.41×10^{-2}	1.41×10^{-1}	6.67×10^{-2}
DV	4.34×10^{0}	8.85×10^{-1}	9.23×10^{-2}	8.07×10^{-3}	9.10×10^{-3}	5.56×10^{-4}

End-to-end sequential experiment



(a) Entropy (b) RMSE of ρ (c) RMSE of α (d) RMSE of u

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[1] Dennis V Lindley. *Bayesian statistics, a review*, volume 2. SIAM, 1972.

[2] Tom Rainforth, Robert Cornish, Hongseok Yang, Andrew Warrington, and Frank Wood. On nesting Monte Carlo estimators. In *International Conference on Machine Learning*, pages 4264–4273, 2018.