Model-based Causal Bayesian Optimization

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March 16, 2023

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Bayesian Optimization

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- If the function is not expensive to evaluate, just sample at many points via grid search, numeric gradient estimation, and more.
- Idea: find the global optimum in a minimum number of steps.
- Incorporate prior belief and update the prior with (some) samples to get a posterior that is better at approximating.

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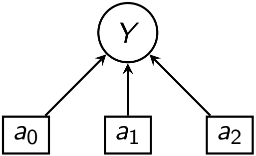
- Black Box Setup



Causal Bayesian Optimization

- Exploit structural knowledge in the form of a causal graph specified by a DAG, assuming that actions can be modeled as interventions on a structural causal model

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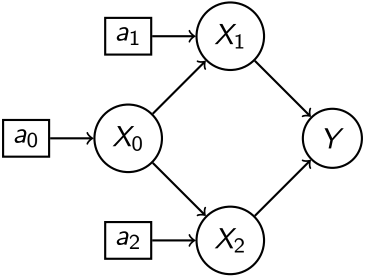

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$$\sigma_{i,t}^2(z_i, a_i, l) = \boxed{k_i}((z_i, a_i, l); (z_i, a_i, l)) - \boxed{k_{i,t}}(z_i, a_i, l)^\top (K_t + b_i^2 I)^{-1} \boxed{k_{i,t}}(z_i, a_i, l)$$

Statistical Model

$$[K_t]_{(t_1,l),(t_2,l')} = k_i((z_{i,t_1,l}, a_{i,t_1,l}, l); (z_{i,t_2,l'}, a_{i,t_2,l'}, l'))$$

$$\begin{aligned} k_{i,t}(z_i, a_i, l)^\top =& [k_i((z_{i,1,1}, a_{i,1,1}, 1); (z_i, a_i, l)), \ldots, \\ & k_i((z_{i,t,d}, a_{i,t,d}, d); (z_i, a_i, l))]^\top \end{aligned}$$

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- Single scalar-output $\mathcal{GP}$ with kernel k for modeling all output components, but introduce the component index as part of the input space

Assumptions

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Comes with the assumption that $f_i(\cdot)$ belongs to an RKHS space of smooth functions, $\mathcal{S} = \mathcal{Z}_i \times \mathcal{A}_i$.

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Assumptions on the Norm

Comes with the assumption that the RKHS norm of $f_i(\cdot)$ is bounded $||f_i||_{k_i} \leq \mathcal{B}_i > 0$. Also $\implies$ L_f-Lipschitz continous.

Acquisition function

Optimistically pick interventions that yield the highest expected return among all system models that are still plausible given past observations.

$$a_{:,t} = \arg\max_{a \in \mathcal{A}} \max_{\tilde{F} \in \mathcal{M}_t} \mathbb{E}_w \left[y \mid \tilde{F}, a \right]$$

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set of functions with bounded RKHS norm

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$$a_{:,t} = \arg\max_{a \in \mathcal{A}} \max_{\eta(\cdot)} \mathbb{E}_w \left[y \mid \tilde{F}, a \right]$$

choosing optimistic but plausible models given the confidence bounds

Implementing Soft Interventions

Require: Parameters $\{\beta_t\}_{t\geq 1}, \Omega$, prior means $\mu_{i,0} = 0$, kernel functions $k_{i,0}\ \forall i \in [0, \ldots, m]$

1: **for** $t = 1, 2, \ldots$ **do**

2: Construct confidence bounds

3: Select $a_t \in \arg\max_{a \in \mathcal{A}} \max_{\eta(\cdot)} \mathbb{E}[y \mid \{\tilde{f}\}, a]$

4: Observe samples $\{z_{i,t}, x_{i,t}\}_{i=0}^{m}$

5: Use $\mathcal{D}_t$ to update posterior $\{\mu_{i,t}(\cdot), \sigma_{i,t}^2(\cdot)\}_{i=0}^{m}$

6: **end for**

Hard Interventions?

- Naturally generalizes to hard interventions, perform the combinatorial optimization over the set of nodes $\mathcal{I}$

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For practical use-cases with large $|\mathcal{I}|$

Minimal intervention set (Lee et al., 2019) to prune sets of intervention targets that contain redundant interventions.

Implementing Hard Interventions

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1: **for** $t = 1, 2, \dots$ **do**

2: Construct confidence bounds

3: Select $I, a_I \in \arg\max_{I,a_I} \max_{\eta} \mathbb{E}[y \mid \{\tilde{f}\}, do(X_I = a_I)]$

4: Observe samples $\{z_{i,t}, x_{i,t}\}_{i=0}^{m}$

5: Use $\mathcal{D}_t$ to update posterior $\{\mu_{i,t}(\cdot), \sigma^2_{i,t}(\cdot)\}_{i=0}^{m}$

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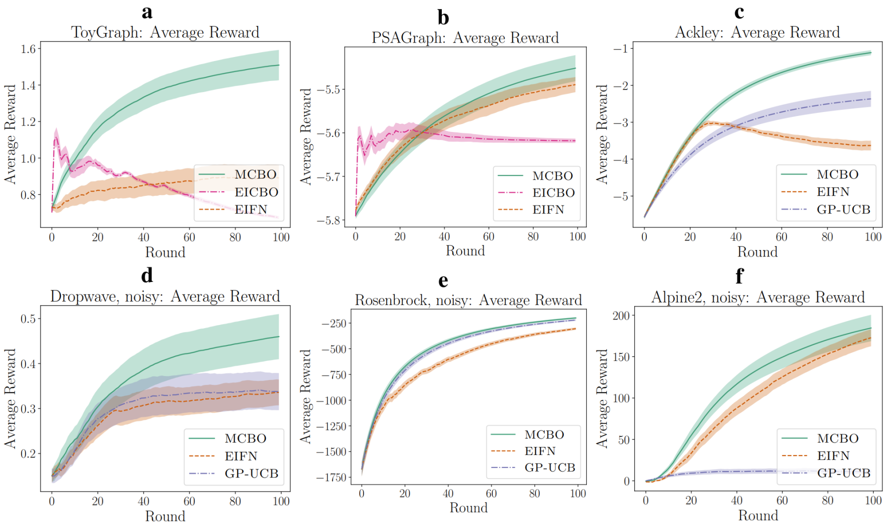
Main Results



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- Combines models in two lines of literature, causal BayesOpt that considered "hard interventions", BO for function networks that considered "soft interventions
- Can be efficiently implemented with popular gradient-based optimizers
- Potentially exponential improvement in cumulative regret, with respect to the number of actions, compared to standard BO, first sublinear cumulative regret bound for CBO

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Next Steps

- Assumes no unobserved confounding
- More real-world applications
- Heuristics or choices for how modeling η changes performance

Thank You