Dynamic Causal Bayesian Optimization: Background, Methodology, and Relevance

1. Background and Related Work

Dynamic Causal Bayesian Optimization builds on advances made in causal inference, Bayesian optimization, and dynamic modeling to solve the problem of decision-making in evolving causal systems. Such a problem demands an integration of observational and interventional data while considering their temporal dependencies. This paper discusses methodologies at the core of DCBO and their own limitations, focusing on recent works.

Bayesian optimization is a cornerstone technique for expensive black-box function optimization that leverages surrogate models, including GPs. It reaches a balance between exploration and exploitation through uncertainty estimates, which in turn makes it suitable for problems with a limited number of evaluations [1]. While BO has seen extensive applications ranging from hyperparameter optimization [2] to scientific experiments [3], its assumptions on independent variables restrict applicability when outcomes are influenced by systems of causal relationships. While various extensions, such as batch BO [4] and multi-fidelity BO [5], have improved efficiency, none of them explicitly incorporates causal reasoning.

Causal inference frameworks, particularly Pearl's structural causal models (SCMs), provide a foundation for understanding relationships between variables and the impact of interventions [6]. Techniques such as do-calculus enable reasoning about interventions in systems with confounding variables [7]. These methods have been applied in healthcare [8], economics [9], and social sciences [10], where understanding causal mechanisms is critical. However, traditional causal inference approaches are static and do not consider how relationships evolve over time.

Causal Bayesian Optimization (CBO) connects the gap between BO and causal reasoning by introducing causal graphs in the process of optimization. Aglietti et al. [11] formulated a framework based on do-calculus and causal graphs, which provides superior performance for conditions where known causal relationships exist. However, it has limitations since this is usually applicable under conditions of static causality structure. Extensions of CBO, including works that introduced latent variables into consideration [12] or even learned causal graphs from data [13], have improved its capability but are not yet temporally adaptive.

Dynamic Bayesian Networks (DBNs) are probabilistic graphical models that describe the temporal changes in dependencies of variables over time. Application domains for DBNs range from time-series analysis [14] to gene regulatory networks [15] and robotics [16]. While effective in modeling temporal dynamics, DBNs often lack causal interpretability and cannot integrate observational and interventional data in an efficient manner. Recent works, such as temporal GPs [17] and dynamic structural causal models

(DSCMs) [18], have sought to address these limitations by incorporating causal reasoning into temporal models.

Adaptive Bayesian Optimization (ABO) adapts BO for non-stationary objectives by considering time as a contextual variable [19]. It has been applied in areas such as materials science and environmental monitoring, where system objectives change over time [20]. However, ABO does not consider the causal dependencies among variables and is hence suboptimal for systems with interdependent variables.

Recent work on integrating causality and dynamics includes frameworks such as Dynamic Causal Bayesian Networks [21] and temporal causal discovery methods [22]. These approaches are aimed at modeling evolving causal relationships and inferring optimal interventions. However, they are often either intractable or rely on strong assumptions regarding the underlying system, which severely limits their applicability in practice.

Dynamic Causal Bayesian Optimization (DCBO) advances the state-of-the-art by addressing both temporal and causal complexities in optimization tasks. It leverages dynamic causal graphs to model evolving relationships and integrates observational and interventional data to identify optimal interventions. Unlike prior methods, DCBO transfers interventional knowledge across time steps, significantly improving efficiency and robustness [11]. Recent applications of DCBO in areas like cybersecurity [23] and system biology [24] highlight its potential for solving real-world dynamic optimization problems.

2. Preferred Methods and Justification for the Choice

2.1 Selected Methodology

The selected methodology is Dynamic Causal Bayesian Optimization (DCBO). This is a combination of three important components:

- **Causal Inference**: To establish cause-effect relationships among variables and model the effects of interventions on the system.
- **Bayesian Optimization (BO)**: To seek optimal interventions in an efficient way, balancing exploration of new areas against exploitation of already known data.
- **Dynamic Modeling**: To be able to model the temporal dynamics of the system, capturing how both variables and causal relationships evolve over time.

2.2 Why DCBO is Appropriate

2.2.1 Temporal Dynamics

Unlike the static optimization methods, such as standard Bayesian Optimization, DCBO explicitly models temporal changes in both the causal relationships and variables. That makes it particularly suitable for systems where both the target variable and inputs evolve over time. The use of dynamic causal graphs allows for better representation and handling of evolving interdependencies.

2.2.2 Incorporates Observational and Interventional Data

DCBO combines both observational data, which is collected without interventions, and interventional data, which is collected after applying certain actions. Such a dual integration is pivotal in systems where both kinds of data are valuable. Utilizing do-calculus from causal inference, DCBO is able to distinguish between mere correlation and causation, hence more reliable optimization results.

2.2.3 Efficiency in Sequential Decision Making

DCBO detects better interventions in less time using the knowledge transferred from already learned time steps. Also, this transferability may reduce computational costs and amounts of data needed.

2.2.4 Causal Interpretability

Unlike purely statistical methods, DCBO provides interpretable results, allowing inferences about the system's causal structure. This interpretability is essential in real-world applications, as knowing the effect of intervening is as important as intervening per se.

2.2.5 Robustness to Non-stationarity

Most real-world systems are non-stationary, with their dynamics evolving over time. DCBO is specifically designed to be able to handle such systems, hence a robust choice in dynamic optimization tasks.

3. Relevance to the Problem

The problem represents a dynamic system where its variables are controlled by causal relationships evolving over time. Moreover:

- Both observational and interventional data exist, and the goal will be to use this data in identifying the best interventions.
- The system is dynamic, requiring an approach that can model temporal dependencies and adapt as relationships evolve.
- The interdependencies among variables are causal, necessitating an approach that can model and exploit these causal structures.

Given these problem requirements, DCBO is a natural fit. It allows for optimal decision-making by:

- Leveraging both observational and interventional data to model causality.
- Using Gaussian Processes to model uncertainties and guide efficient exploration.
- Incorporating temporal dynamics to adapt to evolving relationships over time.

4. Comparison to Alternative Methods

Other methods, such as static Bayesian Optimization (BO), Dynamic Bayesian Networks (DBNs), or even Adaptive Bayesian Optimization (ABO), could conceptually address parts of the challenges posed; however, each has some crucial shortcomings:

- **Bayesian Optimization (BO)**: It does not consider temporal and causal relationships, treating the variables independently.
- **DBNs**: Focus on probabilistic temporal dependencies, but do not have causal interpretability or integration of interventional data.
- **ABO**: Can adapt to dynamic objectives but fails to model any interdependencies among the variables, including causal relationships.

Only DCBO overcomes these limitations and provides an integrated framework for causal reasoning, temporal dynamics, and efficient optimization.

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