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Interfere: Studying Intervention Response Prediction in Complex Dynamic Models

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Summary

The Interfere package is designed to research *intervention response prediction*, or, more specifically, predicting how a complex, dynamic system will respond to a never-before-seen intervention. When developing predictive methods capable of solving this problem, ideal benchmarking data comes exclusively from carefully controlled, longitudinal experiments. Unfortunately, unavoidable confounding, prohibitive costs and ethical boundaries often stymie attempts to run controlled experiments for many important problems. Synthetic data can be used as an alternative to experimental data and has been employed to benchmark predictive algorithms [cite causal graph etc]. However, in practice, the synthetic data used for benchmarking is often simplistic, and the simulation models used to generate it show a range of familiar shortcomings: static, linear relationships, overly independent noise profiles, and a lack of the complex mechanistic relationships and feedback loops that we find in the real world. As a solution, we propose a middle ground: Scientists in many disciplines, such as economics, ecology, systems biology and others, employ mechanistic dynamic models as an integral part of their research and application toolkit (Baker et al., 2018; Banks et al., 2017; Brayton et al., 2014; Izhikevich & Edelman, 2008). Many of these models are accompanied by a body of evidence demonstrating that they do indeed capture important characteristics of the real world problems they emulate. Instead of using simple synthetic data for benchmarking, we propose using datasets generated by scientific models of complex systems as a ground truth against which we can benchmark and test methods that predict intervention response. The logic is this: if a scientific model captures important characteristics of the world and a method can accurately predict intervention response *for that model* then the method ought to be able to predict intervention response for similar systems in the real world.

Interfere offers the first steps towards this vision by combining (1) a general interface for simulating the effect of interventions on dynamic models, (2) a suite of predictive methods and cross validated hyper parameter optimization tools, and (3) the first known extensible benchmark data set of dynamic intervention response scenarios see Figure 1.

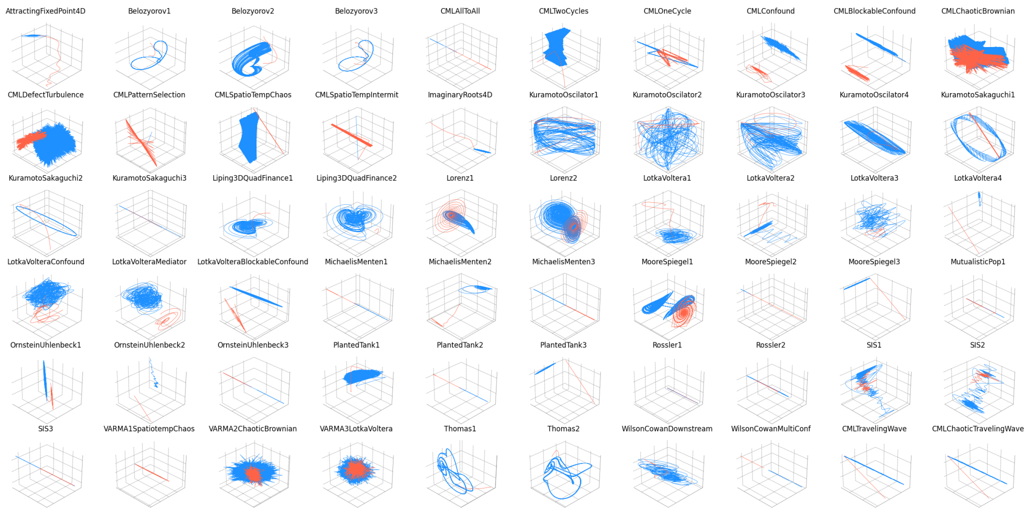

Figure 1: Three-dimensional trajectories of sixty scenarios simulated with the Interfere package. Simulated models are either differential equations or discrete time difference equations. Trajectories in blue represent the natural behavior of the system, while red depicts response to a specified intervention. For models with more than three dimensions, only the three dimensions with highest variance are shown. These sixty scenarios, making up the Interfere Benchmark 1.1.1 for intervention response prediction, are available for download.

Statement of Need

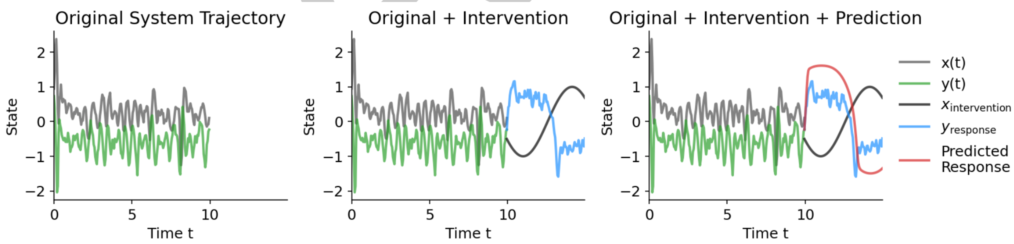

Figure 2: Original System Trajectory (Left): The natural, uninterupted evolution of the quadratic Belozyorov system (Belozyorov, 2015) simulated using the Interfere package with a small amount of stochastic noise. **System Trajectory After Intervention (Center):** The effect that taking exogenous control of $x(t)$ by via do$(x(t) = \sin(t))$ beginning at time $t = 10$ has on y. The intervention (black) and response (blue), depict a clear departure from the natural behavior of the system (green and gray). **Intervention Response Prediction (Right):** Example of forecasting the response of the Belozyorov system to the sinusoidal intervention. The ground truth response, $y(t)$ for $t > 10$ is plotted in blue. Here, an equation discovery algorithm, SINDy, (Brunton et al., 2016) is fit to the data that occurs prior to the intervention and makes an attempt to predict the intervention response (red curve).

Over the past twenty years, multiple frameworks have emerged for identifying causal relationships in observational data (Imbens & Rubin, 2015; Pearl, 2009; Wieczorek & Roth, 2019). The most influential frameworks are probabilistic and, while it is not a necessary condition for identifying causality, a static, linear relationship has often been assumed. However, when attempting to anticipate the response of complex dynamic systems in the medium and long term, a linear approximation of the dynamics can be insufficient. Therefore, non-linear, dynamic techniques have been employed for causal discovery and forecasting (e.g. Runge, 2022). Nevertheless, there are relatively few techniques that are able to fit causal dynamic nonlinear models to data.

Leveraging recent advancements in causal inference and historical work in dynamic modeling and simulation, we focus on a key problem — predicting how a complex system responds to a previously unobserved intervention — and designed the Interfere package for benchmarking tools aimed at this intervention response prediction. The dynamic models contained in Interfere present challenges for this prediction that likely require incorporating mechanistic assumptions alongside probabilistic frameworks for causality. Interfere allows researchers to validate predictive dynamic methods against simulated intervention scenarios, encouraging cross-pollination between probabilistic causal inference and modeling/simulation perspectives.

Primary Contributions

Interfere provides three primary contributions: (1) dynamically diverse counterfactuals, (2) cross-disciplinary forecast methods, and (3) comprehensive and extensible benchmarking.

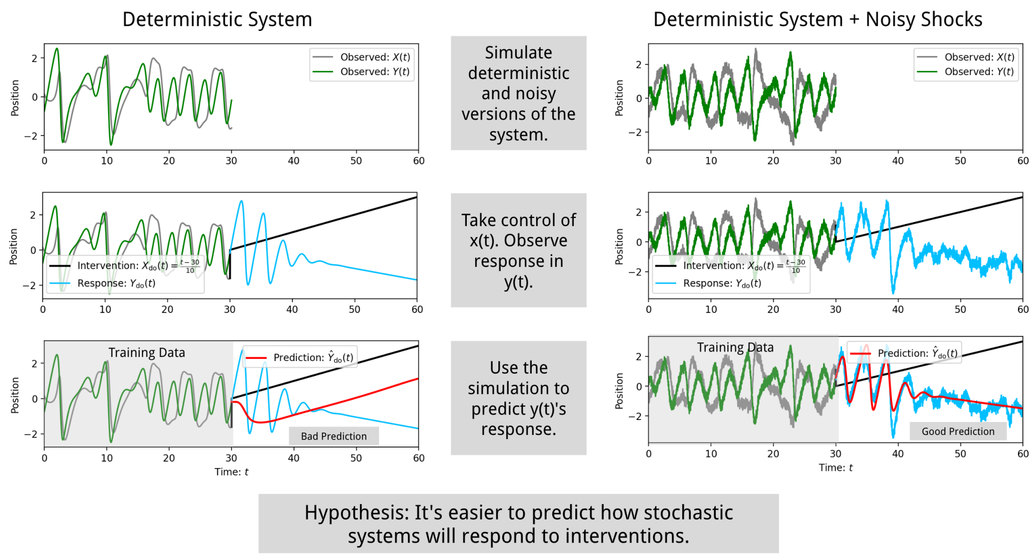

Figure 3: Example experimental setup possible with Interfere: Can stochasticity help reveal associations between variables? Interfere can be used to compare intervention response prediction for deterministic and stochastic versions of the same system.

1. Dynamically Diverse Counterfactuals at Scale

Whereas most predictive methods for complex dynamics are typically benchmarked on fewer than ten systems (Brunton et al., 2016; Challu et al., 2023; Pathak et al., 2018; Prasse & Van Mieghem, 2022; Vlachas et al., 2020), Interfere's "dynamics" submodule contains over fifty dynamic models, with a mix of linear, nonlinear, chaotic, continuous-time, discrete-time, stochastic, and deterministic models, from a variety of disciplines including finance, ecology, biology, neuroscience and public health. Most importantly, Interfere is built for studying interventions: each model inherits the Interfere BaseDynamics type, with possible exogenous control of any observed state, added measurement noise, and, for most models, stochasticity controlled by a scalar parameter or fine tuned with a covariance matrix. Interfere thus offers a user-friendly framework to produce complex dynamic intervention response and standard forecasting scenarios at scale.

2. Cross Disciplinary Forecast Methods

Interfere integrates dynamic *forecasting* methodologies from deep learning (LSTM, NHITS), applied mathematics (SINDy, Reservoir Computers) and social science (VAR). The Interfere

"ForecastingMethod" class is expressive enough to describe, fit and predict with multivariate dynamic models and apply interventions to the states of the models during prediction.

3. Comprehensive and Extensible Benchmarking

Interfere organizes a variety of dynamic scenarios into the Interfere Benchmark, a comprehensive and extensible set containing 60 intervention response scenarios for testing, each simulated with different levels of stochastic noise. Each scenario is housed in a JSON file, with metadata annotation, documentation, versioning and commit hashes marking the commit of Interfere that was used to generate the data. The scenarios were reviewed by hand with some systems exposed to exogenous input to ensure that none of the key variables settle into a steady state. Additionally, all interventions were chosen so that the target variable response significantly departs from its prior behavior. We aim for this benchmark to facilitate future progress towards correctly anticipating how complex systems will respond to never before seen scenarios.

Related Software and Mathematical Foundations

Predictive Methods

Interfere draws from the Nixtla open source ecosystem for time series forecasting. We implemented intervention support for LSTM and NHITS from the NeuralForecast package, and for ARIMA from the StatsForecast package (Azul Garza, 2022; Olivares et al., 2022). We followed Nixtla's example for cross validation and hyperparameter optimization approaches. We integrated predictive methods from the PySINDy (Kaptanoglu et al., 2022) and StatsModels (Seabold & Perktold, 2010) packages. We also include ResComp, a reservoir computing method for global forecasts from (Harding et al., 2024). Hyperparameter optimization is designed around the Optuna framework (Akiba et al., 2019).

While other forecasting methods exist, integrating a method with Interfere requires that the method is capable of (1) multivariate endogenous dynamic forecasting, (2) support for exogenous variables, and (3) support for flexible length forecast windows or recursive predictions. Few forecasting methods meet these criteria, and it is our hope that this package will encourage development of additional methods.

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