Interfere: Intervention Response Simulation and Prediction for Stochastic Non-Linear Dynamics

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DOI: 10.xxxxxx/draft

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Submitted: 01 January 1970
Published: unpublished

Summary

The vision of Interfere is simple: What if we used high quality scientific models to benchmark our causal prediction tools? For methods attempting to infer causal relationships from data, randomized experimental data and counterfactuals are key, but obtaining such datasets is expensive and difficult. Across economics, neuroscience, ecology, systems biology and others, mechanistic models are developed to simulate scenarios and predict the response of systems to interventions (Brayton et al., 2014), (Izhikevich & Edelman, 2008), (Banks et al., 2017), (Baker et al., 2018). Because these models are painstaking calibrated with the real world, they have the ability to generate synthetic counterfactual data with complexity characteristics of the real processes they emulate. With this vision in mind, Interfere offers the first steps towards such a vision: (1) A general interface for simulating the effect of interventions on dynamic simulation models, (2) a suite of predictive methods and cross validation tools, and (3) an initial benchmark set of dynamic counterfactual scenarios.

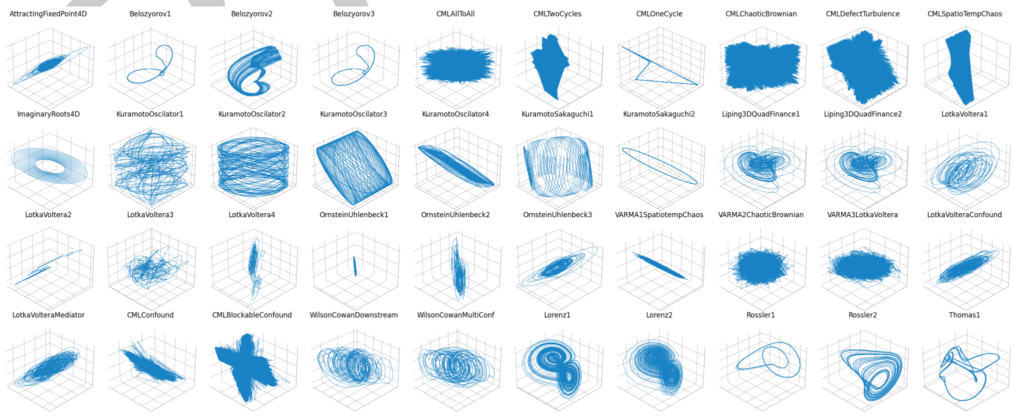

Figure 1: Three dimensional trajectories of forty scenarios simulated with the Interfere package. Many of the models pictured have more than three dimensions and in that case, only the three components of the trajectory with the highest variance are shown. (I'm going to add intervention response trajectories to this)

Statement of need

Over the past twenty years there has been an emergence of multiple frameworks for identifying causal relationships in observational data (Imbens & Rubin, 2015), (Pearl, 2009), (Wieczorek & Roth, 2019). The most influential frameworks are probabilistic and while is not a requirement of the frameworks, in practice, a linear relationship is usually assumed (Runge, 2022). However, when attempting to anticipate the response of complex systems in the medium and long term, linear models are insufficient. (For example, static linear models cannot predict scenarios where things get worse before they get better.) Thus, there is a need for causal models with more complexity. Currently, there are very few techniques that are able to fit causal dynamic non-linear models to data. Because of this, we see an opportunity to bring together both the insights from recent breakthroughs in causal inference and the descriptive power of mechanistic modeling. In order to facilitate this cross pollination, we identified a key causal problem: predicting how a complex system responds to a previously unobserved intervention, and designed the Interfere package as a focal point for building and benchmarking tools aimed at intervention response prediction. The dynamic models contained in Interfere present challenges for causal inference that can likely only be addressed with the incorporation of mechanistic assumptions. As such, the Interfere package creates a much-needed link between the causal inference community and mechanistic modeling community.

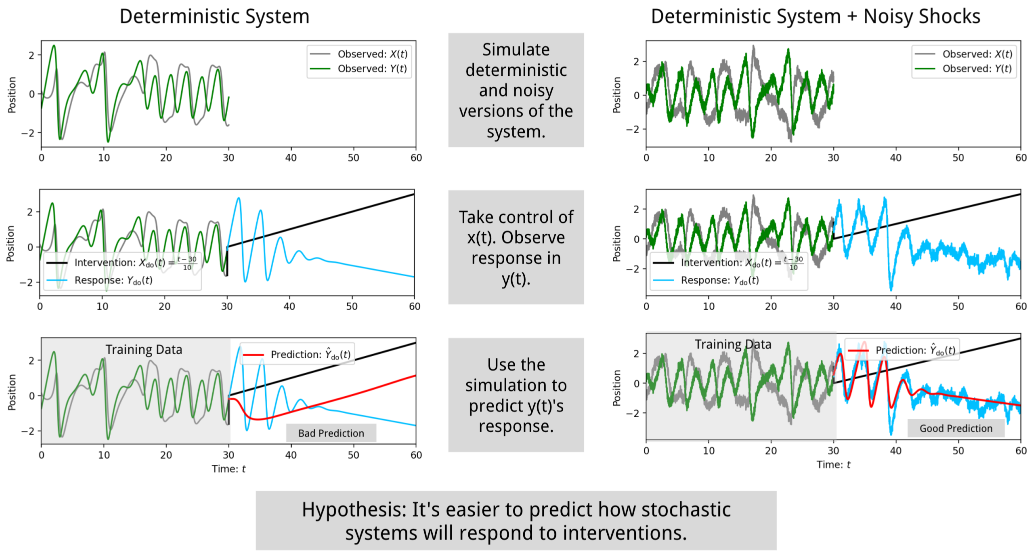

Figure 2: Example experimental setup possible with Interfere: Comparing intervention response prediction for deterministic and stochastic systems.

Primary Contributions

The Interfere package provides three primary contributions to the scientific community.

1. Dynamically Diverse Counterfactuals at Scale

The "dynamics" submodule in the interfere package contains over fifty dynamic models. It contains a mix of linear, nonlinear, chaotic, continuous time, discrete time, stochastic, and deterministic models. The models come from a variety of diciplines including economics, finance, ecology, biology, neuroscience and public health. Each model inherits the from the Interfere BaseDynamics type and gains the ability to take exogenous control of any observed state and to add measurement noise. Most models also gain the ability to make any observed state stochastic where magnitude of stochasticity can be controlled by a simple scalar parameter or fine tuned with a covariance matrix.

Because of the difficulty of building models of complex systems, predictive methods for complex dynamics are typically benchmarked on less than ten dynamical systems (Challu et al., 2023), (Brunton et al., 2016), (Vlachas et al., 2020), (Pathak et al., 2018), (Prasse & Van Mieghem, 2022). As such, Interfere offers a clear improvement over current benchmarking methods for prediction in complex dynamics.

Most importantly, Interfere is built around interventions: the ability to take exogenous control of the state of a complex system and observe the response. Imbuing scientific models with general exogenous control is no small feat because models can be complex and are implemented in a variety of ways. Thus Interfere offers the ability to produce multiple complex dynamic *counterfactual scenarios* at scale. This unqiue feature enables large scale evaluation of dynamic causal prediction methods—tested against systems with properties of interest to scientists.

2. Cross Disciplinary Forecast Methods

A second contribution of interfere is the integration of dynamic *forecasting* methodologies from deep learning, applied mathematics and social science. The Interere "ForecastingMethod" class is expressive enough to describe, fit and predict with multivariate dynamic models and intervene on the states of the models during prediction. This cross diciplinary mix of techniques affords new insights into the problem of intervention response prediction.

3. Opening Up Intervention Response to the Scientific Community

The third major contribution of Interfere is that it poses the intervention response problem—a highly applicable question, to the broader community. The Interfere Benchmark 1.0.0 has the potential provide simple comprehensive evaluation of computational methods on the intervention response problem and therefore streamline future progress towards correctly anticipating how complex systems will respond to new scenarios.

Usage

The Interfere package is designed around three tasks: Counterfactual simulation, predictive method optimization and prediction.

1. Counterfactual Simulation of Intervention Response

The following code contains and example of counterfactual intervention response simulation.

```python
import numpy as np
import interfere
import optuna

initial_cond = np.random.rand(3)
t_train = np.arange(0, 10, 0.05)
dynamic_model = interfere.dynamics.Belozyorov3DQuad()
# Observation Period.
Y = dynamic_model.simulate(t_train, initial_cond)
# Forecasting period.
t_test = np.arange(t_train[-1], 12, 0.05)
# Dynamic treatment do(x1(t) = sin(t))
interv = interfere.SignalIntervention(np.sin, 1)
Y_treat = dynamic_model.simulate(t_test, Y, intervention=interv)
# Counterfactual
Y_cntr = dynamic_model.simulate(t_test, initial_cond)
```

2. Cross Validation and Hyperparameter Optimization

We can fit a method to the observation period generated in the previous section using Interfere's cross validation objective function along with a hyperparameter optimizer (Optuna). Every

Interfere method comes with preset hyperparameter ranges to explore.

```
method_type = interfere.VAR
cv_objv = interfere.CrossValObjective(
        method_type=method_type,
        data=Y,
        times=t_train,
        train_window_percent=0.3,
        num_folds=5,
        exog_idxs=interv.intervened_idxs,
)
study = optuna.create_study(name="Interfere Demo Study")
study.optimize(cv_objv, ntrials=10)

params = study.best_params
```

3. Intervention Response Prediction

Using the best parameters from the hyperparameter optimization run, we can fit a method to the observation data, treating the states we plan to manipulate as exogenous. We then supply an exogenous signal to the method and forecast a response.

```
method = method_type(**params)
Y_endog, Y_exog = interv.split_exog(Y)
method.fit(t_train, Y_endog, Y_exog)

# Simulate intervention response.
pred_Y_treat = method.simulate(
    t_test,
    prior_states=Y,
    intervention=interv
)
```

Related Software and Mathematical Foundations

Predictive Methods

The Interfere package draws extensively on the Nixtla open source ecosystem for time series forecasting. Nixtla's NeuralForecast proves three of the methods that are integrated with Interfere's interface and StatsForecast provides one of the methods (Olivares et al., 2022), (Azul Garza, 2022). Nixtla also provided the inspiration for the cross validation and hyperparameter optimization workflow. Interfere also integrates with predictive methods from the PySINDy and StatsModels packages (Kaptanoglu et al., 2022), (Seabold & Perktold, 2010). An additional reservoir computing method for global forecasts comes from (Harding et al., 2024). Hyperparameter optimization is designed around the Optuna framework (Akiba et al., 2019).

Finding forecasting methods to integrate with Interfere was difficult due to the (1) lack of multivariate dynamic forecasting methods (2) lack of dynamic methods that allow exogenous variables (3) the fact that many methods only offer a fixed forecast window do not implement recursive prediction.

Dynamic Models

See the table below for a full list of dynamic models with attributions that are currently implemented in the interfere package. The dynamic models in were implemented directly from mathematical descriptions except for two which adapt existing simulations from the PyClustering package (Novikov, 2019).

Dynamic Model Class	Short Description	Source	Properties
ArithmeticBrownianMotion	Brownian motion with linear drift and constant diffusion	(Øksendal, 2005)	Stochastic, Linear
Coupled Logistic Map	Discrete-time logistic map with spatial coupling	(Lloyd, 1995)	Non-linear, Chaotic
StochasticCoupledMapLattice	Coupled map lattice with stochastic noise	(Kaneko, 1991)	Non-linear, Stochastic, Chaotic
Michaelis-Menten	Model for enzyme kinetics and biochemical reaction networks	(Srinivasan, 2022)	Non-linear, Stochastic
Lotka-VolteraSDE	Stochastic Lotka-Volterra predator-prey model	(Hening & Nguyen, 2018)	Non-linear, Stochastic
Kuramoto	Coupled oscillator model to study synchronization	(Rodrigues et al., 2016)	Non-linear, Stochastic
Kuramoto-Sakaguchi	Kuramoto model variant with phase frustration	(Sakaguchi & Kuramoto, 1986)	Non-linear, Stochastic
Hodgkin-HuxleyPyclustering	Neuron action-potential dynamics based on Hodgkin-Huxley equations	(Hodgkin & Huxley, 1952)	Non-linear
Stuart-LandauKuramoto	Coupled oscillators with amplitude-phase dynamics	(Cliff et al., 2023)	Non-linear, Stochastic
MutualisticPopulation	Dynamics of interacting mutualistic species	(Prasse & Van Mieghem, 2022)	Non-linear
OrnsteinUhlenbeck	Mean-reverting stochastic differential equation	(Gardiner, 2009)	Stochastic, Linear
Belozyorov3DQuad	3-dimensional quadratic chaotic system	(Belozyorov, 2015)	Non-linear, Chaotic
Liping3DQuadFinance	Chaotic dynamics applied in financial modeling	(Liping et al., 2021)	Non-linear, Chaotic
Lorenz	Classic chaotic system describing atmospheric convection	(Lorenz, 2017)	Non-linear, Chaotic
Rossler	Simplified 3D chaotic attractor system	(Rössler, 1976)	Non-linear, Chaotic
Thomas	Chaotic attractor with simple structure and rich dynamics	(Thomas, 1999)	Non-linear, Chaotic
DampedOscillator	Harmonic oscillator with damping and noise	(Classical linear model)	Linear, Stochastic

Dynamic Model Class	Short Description	Source	Properties
SIS	Epidemiological model (Susceptible-Infected-Susceptible)	(Prasse & Van Mieghem, 2022)	Non-linear, Stochastic
VARMADynamics	Vector AutoRegressive Moving Average for time series modeling	(Hamilton, 2020)	Linear, Stochastic
Wilson-Cowan	Neural mass model for neuronal population dynamics	(Wilson & Cowan, 1972)	Non-linear
GeometricBrownianMotion	Stochastic model widely used in financial mathematics	(Black & Scholes, 1973)	Non-linear, Stochastic
PlantedTankNitrogenCycle	Biochemical cycle modeling nitrogen transformation in aquatic systems	(Fazio & Jannelli, 2006)	Non-linear
GenerativeForecaster	Predictive forecasting models trained on simulation, then used to generate data	(Written for Interfere)	Stochastic
StandardNormalNoise	IID noise from standard normal distribution	(Cliff et al., 2023)	Stochastic
StandardCauchyNoise	IID noise from standard Cauchy distribution	(Cliff et al., 2023)	Stochastic
StandardExponentialNoise	IID noise from standard exponential distribution	(Cliff et al., 2023)	Stochastic
StandardGammaNoise	IID noise from standard gamma distribution	(Cliff et al., 2023)	Stochastic
StandardTNoise	IID noise from Student's t-distribution	(Cliff et al., 2023)	Stochastic

Acknowledgements

This work was supported by NSF GRFP.

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