The Journal of Open Source Software

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

D. J. Passey [1*] **and Peter J. Mucha** [2*]

1 University of North Carolina at Chapel Hill, United States **2** Dartmouth College, United States
***** These authors contributed equally.

DOI: 10.xxxxxx/draft

Software

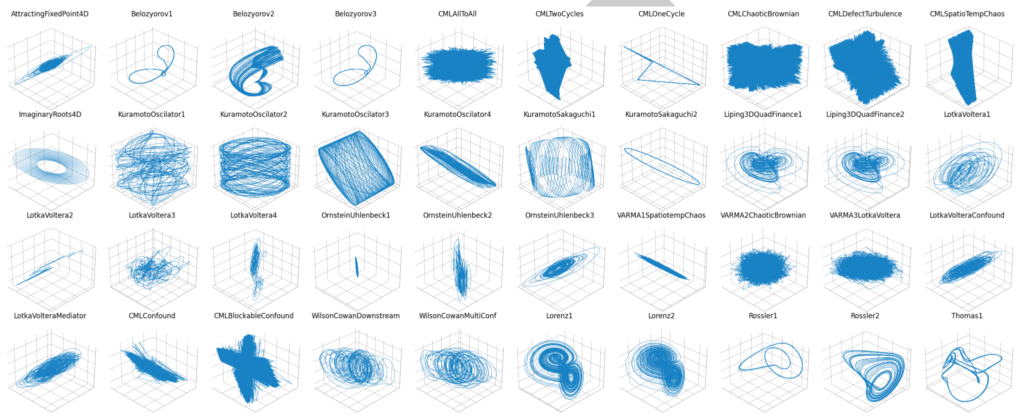
- Review
- Repository
- Archive

Editor: Open Journals

Reviewers:

- @openjournals

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Published: unpublished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? When attempting to infer causal relationships from data, randomized experimental data and counterfactuals are key, but obtaining such datasets is expensive and difficult. Across many fields, like 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 containing 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.

Statement of need

Over the past twenty years we've seen an emergence of multiple frameworks for identifying causal relationships (Imbens & Rubin, 2015), (Pearl, 2009), (Wieczorek & Roth, 2019). The most influential frameworks are probabilistic and while is not a requirement of the frameworks, typically in practice, a linear relationship is 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.

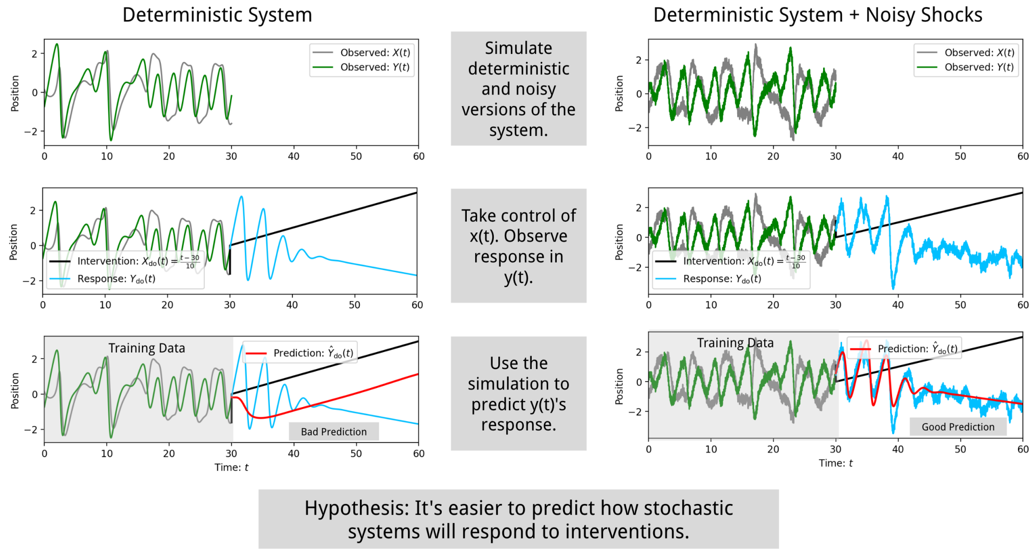


Figure 1: Comparing deterministic and stochastic systems.

Usage

The Interfere package is designed around three tasks: Counterfactual simulation, predictive method optimization and prediction. An example of counterfactual simulation can be summarized in the following code:

```
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)

# Treatment
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)
```

Using the data above, we can fit a method to the observation period and attempt to predict both the intervention response and the counterfactual.

```
cv_objv = interfere.CrossValObjective(
        method_type=interfere.SINDY,
        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
sindy = interfere.SINDY(**params)
sindy.fit(t_train, interv.split_exog(Y))
```

Primary Contributions

The Interfere package provide 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 manipulate the state of a complex system and observe the response. This is no simple feat for complex scientific models that are implemented with a variety of simulation packages. 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.

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).

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
HodgkinHuxleyPyclustering	Neuron action-potential dynamics based on Hodgkin-Huxley equations	(Hodgkin & Huxley, 1952)	Non-linear

Dynamic Model Class	Short Description	Source	Properties
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
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

Dynamic Model Class	Short Description	Source	Properties
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.

References

Akiba, T., Sano, S., Yanase, T., Ohta, T., & Koyama, M. (2019). Optuna: A next-generation hyperparameter optimization framework. *The 25th ACM SIGKDD International Conference on Knowledge Discovery & Data Mining*, 2623–2631.

Azul Garza, C. C., Max Mergenthaler Canseco. (2022). *StatsForecast: Lightning fast forecasting with statistical and econometric models*. PyCon Salt Lake City, Utah, US 2022. https://github.com/Nixtla/statsforecast

Baker, R. E., Peña, J.-M., Jayamohan, J., & Jérusalem, A. (2018). Mechanistic models versus machine learning, a fight worth fighting for the biological community? *Biology Letters*, *14*(5), 20170660. https://doi.org/10.1098/rsbl.2017.0660

Banks, H. T., Banks, J. E., Bommarco, R., Curtsdotter, A., Jonsson, T., & Laubmeier, A. N. (2017). Parameter estimation for an allometric food web model. *International Journal of Pure and Apllied Mathematics*, *114*(1). https://doi.org/10.12732/ijpam.v114i1.12

Belozyorov, V. Y. (2015). Exponential-algebraic maps and chaos in 3D autonomous quadratic systems. *International Journal of Bifurcation and Chaos*, *25*(04), 1550048.

Black, F., & Scholes, M. (1973). The pricing of options and corporate liabilities. *Journal of Political Economy*, *81*(3), 637–654.

Brayton, F., Laubach, T., & Reifschneider, D. (2014). The FRB/US model: A tool for macroeconomic policy analysis. *FEDS Notes*, *2014-04*, 03.

Brunton, S. L., Proctor, J. L., & Kutz, J. N. (2016). Discovering governing equations from data by sparse identification of nonlinear dynamical systems. *Proceedings of the National Academy of Sciences*, *113*(15), 3932–3937. https://doi.org/10.1073/pnas.1517384113

Challu, C., Olivares, K. G., Oreshkin, B. N., Ramirez, F. G., Canseco, M. M., & Dubrawski, A. (2023). NHITS: Neural Hierarchical Interpolation for Time Series Forecasting. *Proceedings of the AAAI Conference on Artificial Intelligence*, *37*(6), 6989–6997. https://doi.org/10.1609/aaai.v37i6.25854

Cliff, O. M., Bryant, A. G., Lizier, J. T., Tsuchiya, N., & Fulcher, B. D. (2023). Unifying pairwise interactions in complex dynamics. *Nature Computational Science*, *3*(10), 883–893. https://doi.org/10.1038/s43588-023-00519-x

Fazio, R., & Jannelli, A. (2006). Mathematical and numerical modeling for a bio-chemical aquarium. *Applied Mathematics and Computation*, *174*(2), 1370–1383.

Gardiner, C. (2009). *Stochastic methods* (Vol. 4). Springer Berlin Heidelberg.

Hamilton, J. D. (2020). *Time series analysis*. Princeton university press.

Harding, S., Leishman, Q., Lunceford, W., Passey, D. J., Pool, T., & Webb, B. (2024). Global forecasts in reservoir computers. *Chaos: An Interdisciplinary Journal of Nonlinear Science*, *34*(2), 023136. https://doi.org/10.1063/5.0181694

Hening, A., & Nguyen, D. H. (2018). Stochastic lotka–volterra food chains. *Journal of Mathematical Biology*, *77*, 135–163.

Hodgkin, A. L., & Huxley, A. F. (1952). A quantitative description of membrane current and its application to conduction and excitation in nerve. *The Journal of Physiology*, *117*(4), 500.

Imbens, G. W., & Rubin, D. B. (2015). *Causal Inference for Statistics, Social, and Biomedical Sciences: An Introduction* (1st ed.). Cambridge University Press. https://doi.org/10.1017/CBO9781139025751

Izhikevich, E. M., & Edelman, G. M. (2008). Large-scale model of mammalian thalamocortical systems. *Proceedings of the National Academy of Sciences*, *105*(9), 3593–3598. https://doi.org/10.1073/pnas.0712231105

Kaneko, K. (1991). Coupled map lattice. In *Chaos, Order, and Patterns* (pp. 237–247). Springer.

Kaptanoglu, A. A., Silva, B. M. de, Fasel, U., Kaheman, K., Goldschmidt, A. J., Callaham, J., Delahunt, C. B., Nicolaou, Z. G., Champion, K., Loiseau, J.-C., Kutz, J. N., & Brunton, S. L. (2022). PySINDy: A comprehensive python package for robust sparse system identification. *Journal of Open Source Software*, *7*(69), 3994. https://doi.org/10.21105/joss.03994

Liping, C., Khan, M. A., Atangana, A., & Kumar, S. (2021). A new financial chaotic model in Atangana-Baleanu stochastic fractional differential equations. *Alexandria Engineering Journal*, *60*(6), 5193–5204.

Lloyd, A. L. (1995). The coupled logistic map: A simple model for the effects of spatial heterogeneity on population dynamics. *Journal of Theoretical Biology*, *173*(3), 217–230.

Lorenz, E. N. (2017). Deterministic Nonperiodic Flow 1. In *Universality in Chaos, 2nd edition* (pp. 367–378). Routledge.

Novikov, A. V. (2019). PyClustering: Data mining library. *Journal of Open Source Software*, *4*(36), 1230. https://doi.org/10.21105/joss.01230

Øksendal, B. K. (2005). *Stochastic differential equations: An introduction with applications* (6th ed., corrected third printing 2005). Springer. ISBN: 978-3-540-04758-2

Olivares, K. G., Challú, C., Garza, A., Canseco, M. M., & Dubrawski, A. (2022). *NeuralForecast: User friendly state-of-the-art neural forecasting models.* PyCon Salt Lake City, Utah, US 2022. https://github.com/Nixtla/neuralforecast

Pathak, J., Hunt, B., Girvan, M., Lu, Z., & Ott, E. (2018). Model-Free Prediction of Large Spatiotemporally Chaotic Systems from Data: A Reservoir Computing Approach. *Physical Review Letters*, *120*(2), 024102. https://doi.org/10.1103/PhysRevLett.120.024102

Pearl, J. (2009). *Causality* (2nd ed.). Cambridge University Press. https://doi.org/10.1017/CBO9780511803161

Prasse, B., & Van Mieghem, P. (2022). Predicting network dynamics without requiring the knowledge of the interaction graph. *Proceedings of the National Academy of Sciences*, *119*(44), e2205517119. https://doi.org/10.1073/pnas.2205517119

Rodrigues, F. A., Peron, T. K. D., Ji, P., & Kurths, J. (2016). The Kuramoto model in complex networks. *Physics Reports*, *610*, 1–98.

Rössler, O. E. (1976). An equation for continuous chaos. *Physics Letters A*, *57*(5), 397–398.

Runge, J. (2022). *Discovering contemporaneous and lagged causal relations in autocorrelated* *nonlinear time series datasets*. arXiv. https://doi.org/10.48550/arXiv.2003.03685

Sakaguchi, H., & Kuramoto, Y. (1986). A soluble active rotater model showing phase transitions via mutual entertainment. *Progress of Theoretical Physics*, *76*(3), 576–581.

Seabold, S., & Perktold, J. (2010). Statsmodels: Econometric and statistical modeling with python. *9th Python in Science Conference*.

Srinivasan, B. (2022). A guide to the Michaelis–Menten equation: Steady state and beyond. *The FEBS Journal*, *289*(20), 6086–6098.

Thomas, R. (1999). Deterministic chaos seen in terms of feedback circuits: Analysis, synthesis," labyrinth chaos". *International Journal of Bifurcation and Chaos*, *9*(10), 1889–1905.

Vlachas, P. R., Pathak, J., Hunt, B. R., Sapsis, T. P., Girvan, M., Ott, E., & Koumoutsakos, P. (2020). Backpropagation algorithms and Reservoir Computing in Recurrent Neural Networks for the forecasting of complex spatiotemporal dynamics. *Neural Networks*, *126*, 191–217. https://doi.org/10.1016/j.neunet.2020.02.016

Wieczorek, A., & Roth, V. (2019). Information Theoretic Causal Effect Quantification. *Entropy*, *21*(10), 975. https://doi.org/10.3390/e21100975

Wilson, H. R., & Cowan, J. D. (1972). Excitatory and inhibitory interactions in localized populations of model neurons. *Biophysical Journal*, *12*(1), 1–24.