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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

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Editor: Open Journals

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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Published: unpublished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? 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.

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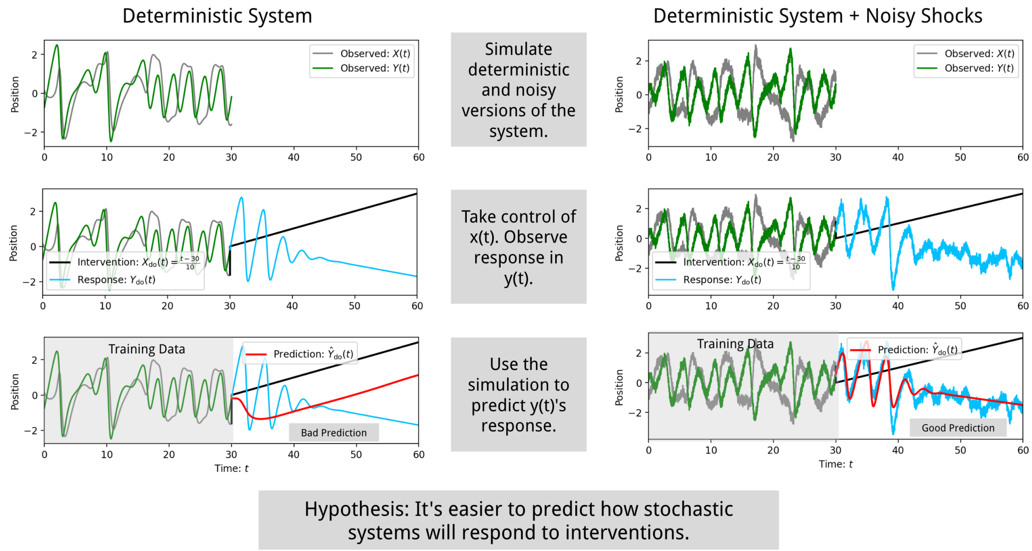

Figure 1: Comparing deterministic and stochastic systems.

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.

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

Dynamic Model Class	Short Description	Source	Properties
HodgkinHuxleyPyclustering	Neuron action-potential dynamics based on Hodgkin-Huxley equations	(Hodgkin & Huxley, 1952)	Non-linear
StuartLandauKuramoto	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

Dynamic Model Class	Short Description	Source	Properties
Standard-CauchyNoise	IID noise from standard Cauchy distribution	(Cliff et al., 2023)	Stochastic
StandardEx-ponential-Noise	IID noise from standard exponential distribution	(Cliff et al., 2023)	Stochastic
Standard-Gam-maNoise	IID noise from standard gamma distribution	(Cliff et al., 2023)	Stochastic
StandardT-Noise	IID noise from Student's t-distribution	(Cliff et al., 2023)	Stochastic

Acknowledgements

This work was supported by NSF GRFP.

References

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.

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.

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.

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.

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

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.

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.

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.