An Interpretable and Sparse Neural Network Model for Nonlinear Granger Causality Discovery

Alex Tank, Ian C. Covert, Nicholas J. Foti, Ali Shojaie, Emily B. Fox
University of Washington
alextank@uw.edu, icovert@cs.washington.edu, nfoti@uw.edu
ashojaie@uw.edu, ebfox@uw.edu

Abstract

While most classical approaches to Granger causality detection repose upon linear time series assumptions, many interactions in neuroscience and economics applications are nonlinear. We develop an approach to nonlinear Granger causality detection using multilayer perceptrons where the input to the network is the past time lags of all series and the output is the future value of a single series. A sufficient condition for Granger non-causality in this setting is that all of the outgoing weights of the input data, the past lags of a series, to the first hidden layer are zero. For estimation, we utilize a group lasso penalty to shrink groups of input weights to zero. We also propose a hierarchical penalty for simultaneous Granger causality and lag estimation. We validate our approach on simulated data from both a sparse linear autoregressive model and the sparse and nonlinear Lorenz-96 model.

1 Introduction

Granger causality quantifies the extent to which the past activity of one time series is predictive of another time series. When an entire system of time series is studied, networks of interactions may be uncovered [2]. Classically, most methods for estimating Granger causality assume linear time series dynamics and utilize the popular vector autoregressive (VAR) model [9, 8]. However, in many real world time series the dependence between series is *nonlinear* and using linear models may lead to inconsistent estimation of Granger causal interactions [12, 13]. Common nonlinear approaches to estimating interactions in time series use additive models [12, 4, 11], where the past of each series may have an additive nonlinear effect that decouples across series. However, additive models may miss important nonlinear interactions between predictors so they may also fail to detect important Granger causal connections.

To tackle these challenges we present a framework for interpretable nonlinear Granger causality discovery using regularized neural networks. Neural network models for time series analysis are traditionally used only for prediction and forecasting — *not* for interpretation. This is due to the fact that the effects of inputs are difficult to quantify exactly due to the tangled web of interacting nodes in the hidden layers. We sidestep this difficulty and instead construct a simple architecture that allows us to precisely select for time series that have no linear or nonlinear effects on the output.

We adapt recent work on sparsity inducing penalties for architecture selection in neural networks [1, 7] to our case. In particular, we select for Granger causality by adding a group lasso penalty [14] on the outgoing weights of the inputs, which we refer to as *encoding selection*. We also explore a hierarchical group lasso penalty for automatic lag selection [10]. When the true network of nonlinear interactions is sparse, this approach will select a few time series that Granger cause the output series and the lag of these interactions.

All code for reproducing experiments may be found at `bitbucket.com/atank/nngranger`.

2 Background and problem formulation

Let $x_t \in \mathbb{R}^p$ denote a p-dimensional stationary time series. Granger causality in time series analysis is typically studied using the vector autoregressive model (VAR). In this model, the time series x_t is assumed to be a linear combination of the past K lags of the series

$$x_t = \sum_{k=1}^{K} A^{(k)} x_{t-k} + e_t, \tag{1}$$

where $A^{(k)}$ is a $p \times p$ matrix that specifies how lag k effects the future evolution of the series and e_t is mean zero noise. In this model time series j does not Granger cause time series i iff $\forall k, A_{ij}^{(k)} = 0$. A Granger causal analysis in a VAR model thus reduces to determining which values in $A^{(k)}$ are zero over all lags. In higher dimensional settings, this may be determined by solving a group lasso regression problem

$$\min_{A^{(1)}, \ldots, A^{(K)}} \sum_{t=1}^{T} \left(x_t - \sum_{k=1}^{K} A^{(k)} x_{t-k} \right)^2 + \lambda \sum_{ij} ||(A_{ij}^{(1)}, \ldots, A_{ij}^{(K)})||_2, \tag{2}$$

where $||.||_2$ denotes the the L_2 norm which acts as a group penalty shrinking all values of $(A_{ij}^{(1)}, \ldots, A_{ij}^{(K)})$ to zero together [14] and $\lambda > 0$ is a tuning parameter that controls the level of group sparsity.

A *nonlinear* autoregressive model allows x_t to evolve according to more general nonlinear dynamics

$$x_t = g(x_{(t-1)}, \ldots, x_{(t-K)}) + e_t = \left(g_1(x_{(t-1)}, \ldots, x_{(t-K)}), \ldots, g_p(x_{(t-1)}, \ldots, x_{(t-K)}) \right)^T + \epsilon_t,$$

where g_i is a continuous function that specifies how the past K lags influences series i. In this context, Granger non-causality between two series j and i means that the function g_i does not depend on the $x_{(t-1):(t-K)j}$ variables, the past K lags of series j. Our goal is to estimate nonlinear Granger causal and non-causal relationships using a penalized optimization approach similar to Problem (2) for linear models.

3 Neural networks for Granger causality estimation

We model the nonlinear dynamics with a multilayer perceptron (MLP). In a forecasting setting, it is common to model the full set of outputs x_t using an MLP where the inputs are $x_{(t-1):(t-K)}$. There are two problems with applying this approach to our case. First, due to sharing of hidden layers, it is difficult to specify necessary conditions on the weights that simultaneously allows series j to influence series i but not influence series i' for $i \neq i'$. Necessary conditions for Granger causality are needed because we wish to add selection penalties during estimation time. Second, a joint MLP requires all g_i functions to depend on the same lags, however in practice each g_i may have different lag orders.

3.1 Granger causality selection on encoding

To tackle these challenges we model each g_i with a separate MLP, so that effects from inputs to outputs are easier to disentangle. Assume that for each i, g_i takes the form of an MLP with L layers and let the vector h_t^l denote the values of the lth hidden layer at time t. Let $\mathbf{W} = \{W^1, \ldots, W^L\}$ denote the weights at each layer and let the first layer weights be written as $W^1 = \{W^{11}, \ldots, W^{1K}\}$. The first hidden values at time t are given by:

$$h_t^l = \sigma \left(\sum_{k=1}^{K} W^{1k} x_{t-k} + b^l \right) \tag{3}$$

where σ is an activation function and b^l is the bias at layer l. The output, x_{ti}, is given by

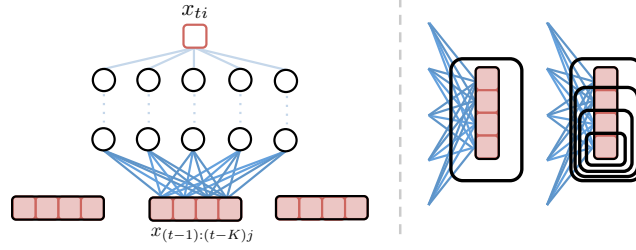$$x_{ti} = w_O^T h_t^L + \epsilon_t. \tag{4}$$

Figure 1: Schematic for modeling Granger causality using MLPs. (left) If the outgoing weights for series j, shown in dark blue, are penalized to zero, then series j does not influence series i. (right) The group lasso penalty jointly penalizes the full set of outgoing weights while the hierarchical version penalizes the nested set of outgoing weights, penalizing higher lags more.

where w_O^T is the linear output decoder. In Equation (3), if the jth column of the weight matrix, $W_{:j}^{1k}$, is zero for all k, then time series j does not Granger cause series i. Thus, analogous to the VAR case, one may select for Granger causality by adding a group lasso penalty on the columns of the W^{k1} matrices to the least squares MLP optimization problem for each g_i,

$$\min_{\mathbf{W}} \sum_{t=1}^{T} \left(x_{it} - g_i(x_{(t-1):(t-K)}, \mathbf{W}) \right)^2 + \lambda \sum_{j=1}^{p} ||(W_{:j}^{11}, \ldots, W_{:j}^{1K})||_F. \tag{5}$$

For large enough λ, the solutions to Eq. (5) will lead to many zero columns in each W^{1k} matrix, implying only a small number of estimated Granger causal connections.

The zero outgoing weights are sufficient but not necessary to represent Granger non-causality. Indeed, series i could be Granger non-causal of series j through a complex configuration of the weights that exactly cancel each other. However, since we wish to *interpret* the outgoing weights of the inputs as a measure of dependence, it is important that these weights reflect the true relationship between inputs and outputs. Our penalization scheme acts as a prior that biases the network to represent Granger non-causal relationships with zeros in the outgoing weights of the inputs, rather than through other configurations. Our simulation results in Section 4 validate this intuition.

3.2 Simultaneous Granger causality and lag selection

We may simultaneously select for Granger causality and select for the lag order of the interaction by adding a *hierarchical* group lasso penalty [10] to the MLP optimization problem,

$$\min_{\mathbf{W}} \sum_{i=1}^{T} \left(x_{it} - g_i(x_{(t-1):(t-K)}, \mathbf{W}) \right)^2 + \lambda \sum_{j=1}^{p} \sum_{k=1}^{K} ||(W_{:j}^{1k}, \ldots, W_{:j}^{1K})||_F. \tag{6}$$

The hierarchical penalty leads to solutions such that for each j there exists a lag k such that all $W_{:j}^{1k'} = 0$ for $k' > k$ and all $W_{:j}^{1k'} \neq 0$ for $k' \leq k$. Thus, this penalty effectively selects the lag of each interaction. The hierarchical penalty also sets many columns of W^{1k} to be zero across all k, effectively selecting for Granger causality. In practice, the hierarchical penalty allows us to fix K to a large value, ensuring that no Granger causal connections at higher lags are missed.

4 Simulation Experiments

4.1 Linear Vector Autoregressive Model

First, we study how our approach performs on data simulated from a VAR model in order to show that it can capture the same structure as existing Granger causality methods. We randomly generate sparse A matrices and apply our group lasso regularization scheme to estimate the Granger causality graph. In Figure 3 (left) we show the estimated graphs for multiple T and λ settings and in Figure 4 we show the distribution of AUC values obtained from ROC curves for graph estimation using 10 random seeds. The ROC curves are computed by sweeping over a grid of λ values. The AUC values quickly approach the value one as T increases, suggesting that our method is consistent for VAR data.

Figure 2: Estimates of Granger causal interactions for a single series, x_{ti}, of a VAR process using the hierarchical penalty. Plots are shown for various λ settings.
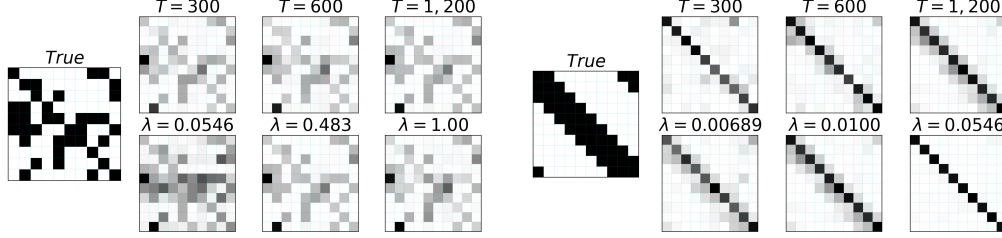

Figure 3: A comparison of the true graphs to the estimated graphs for multiple λ settings and multiple T for data generated from (left) VAR and (right) Lorenz models. Top row in both plots vary λ for a fixed T and bottom row vary T with λ fixed. The weight of each edge is the L_2 norm of the outgoing weights of the respective input series.

To visualize the performance of the hierarchical penalty we show the estimated graph, including lags, for a single g_i on a $p = 10$, $T = 1000$ example in Figure 2. At lower λ values both more series are estimated to have Granger causal interactions and higher order lags are included.

4.2 Nonlinear Lorenz-96 Model

Second, we apply our approach to simulated data from the Lorenz-96 model [6], a nonlinear model of climate dynamics. The dynamics in a p-dimensional Lorenz model are

$$\frac{dx_{ti}}{dt} = (x_{i+1} - x_{i-2}) x_{i-1} - x_i + F, \tag{7}$$

where $x_{-1} = x_p$, $x_0 = x_p$, and $x_{N+1} = x_1$ and F is a forcing constant (we take $F = 5$). We numerically simulate the Lorenz-96 model using Euler's method, which results in a multivariate, nonlinear autoregressive time series with sparse Granger causal connections. When generating the series with Euler's method, the self connections are much stronger than the off diagonal interactions since the derivative in Eq. (7) is multiplied by the Euler step size (we use .01). We show estimated graphs for multiple λ and T values in Figure 3 (right) from data generated from a $p = 10$ model. In Figure 4 we show box plots of AUC values for multiple T values over 10 random seeds. Overall, the AUC values approach the value one, suggesting consistency of our approach in this nonlinear model.

5 Concurrent and future work

We are currently extending the work in two directions. First, the method herein performs selection on the encoding stage. Alternatively, we could use separate networks to learn features of each series then perform selection on the decoding layer. Second, we are actively working on extensions using recurrent networks based on both long-short term memory networks [3] and echo state networks [5].
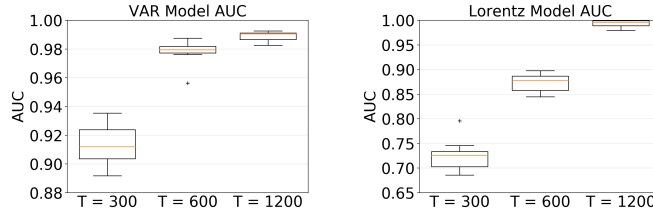

Figure 4: Box plots of AUC values for data simulated from (left) VAR and (right) Lorenz models.

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