SAND2023-05920C

Characterizing climate pathways using feature importance on echo state networks

Katherine Goode, Daniel Ries, Kellie McClernon, and Lyndsay Shand

MLDL Workshop

July 18, 2023

SAND2023-05920C

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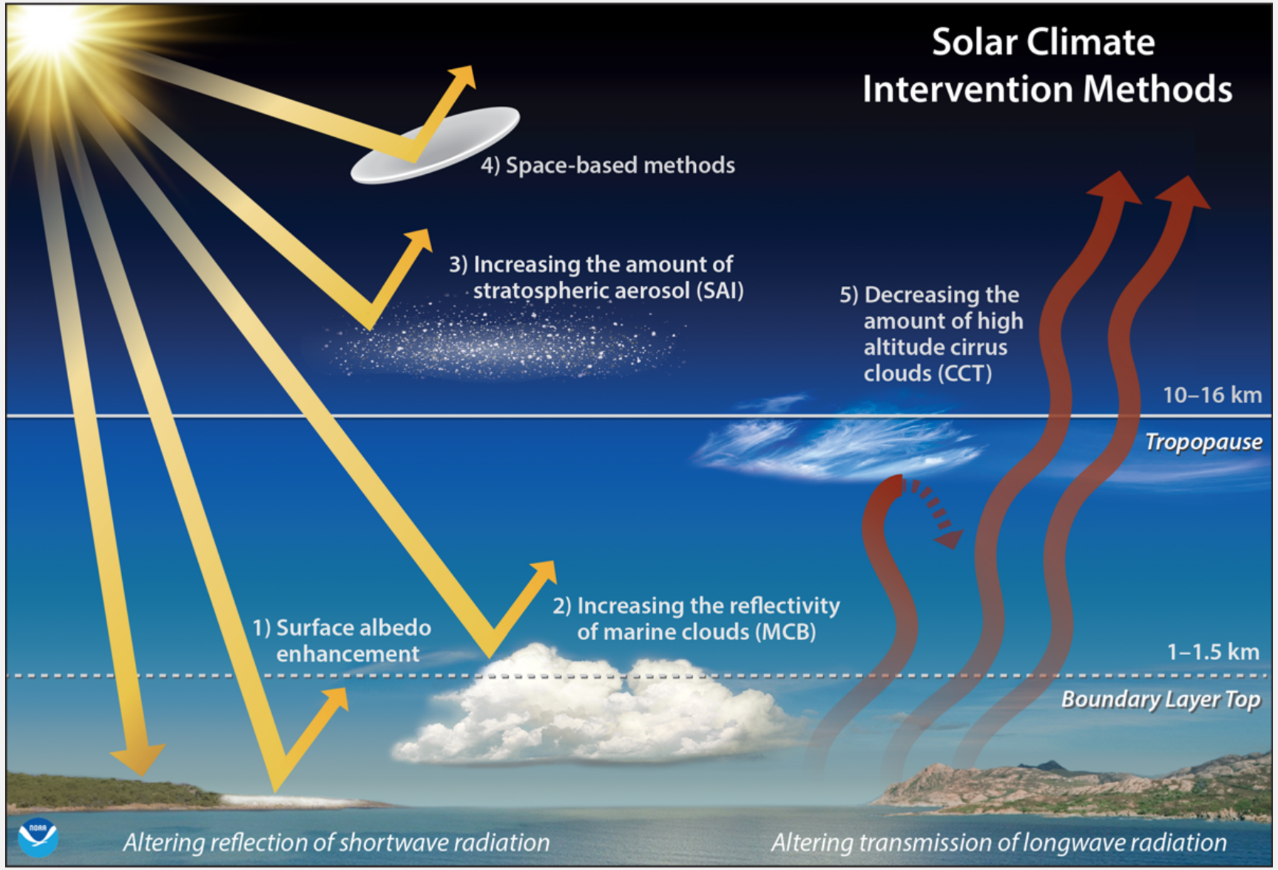
Outline

- Motivation: Climate Interventions
- Approach: Echo State Networks and Feature Importance
- Climate Application: Mount Pinatubo
- Conclusions and Future Work

Motivation

Climate Interventions

Climate Interventions



Threat of climate change has led to proposed interventions…

- Stratospheric aerosol injections
- Marine cloud brightening
- Cirrus cloud thinning
- etc.

What are the downstream effects of such mitigation strategies?

Image source: https://eos.org/science-updates/improving-models-for-solar-climate-intervention-research

Our Objective

Develop algorithms to characterize (i.e., quantify) relationships between climate variables related to a climate event (in observed data)

Example

- Mount Pinatubo eruption in 1991
- Released 18-19 Tg of sulfur dioxide
- Proxy for anthropogenic stratospheric aerosol injection

Mount Pintabuo Pathway

Sulfur dioxide

- Injection of sulfur dioxide (18-19 Tg) into atmosphere [1]

⬇

Aerosol optical depth (AOD)

- Vertically integrated measure of aerosols in air from surface to stratosphere [2]
- AOD increased as a result of injection of sulfur dioxide [1; 2]

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Stratospheric temperature

- Temperatures at pressure levels of 30-50 mb rose 2.5-3.5 degrees centigrade compared to 20-year mean [3]

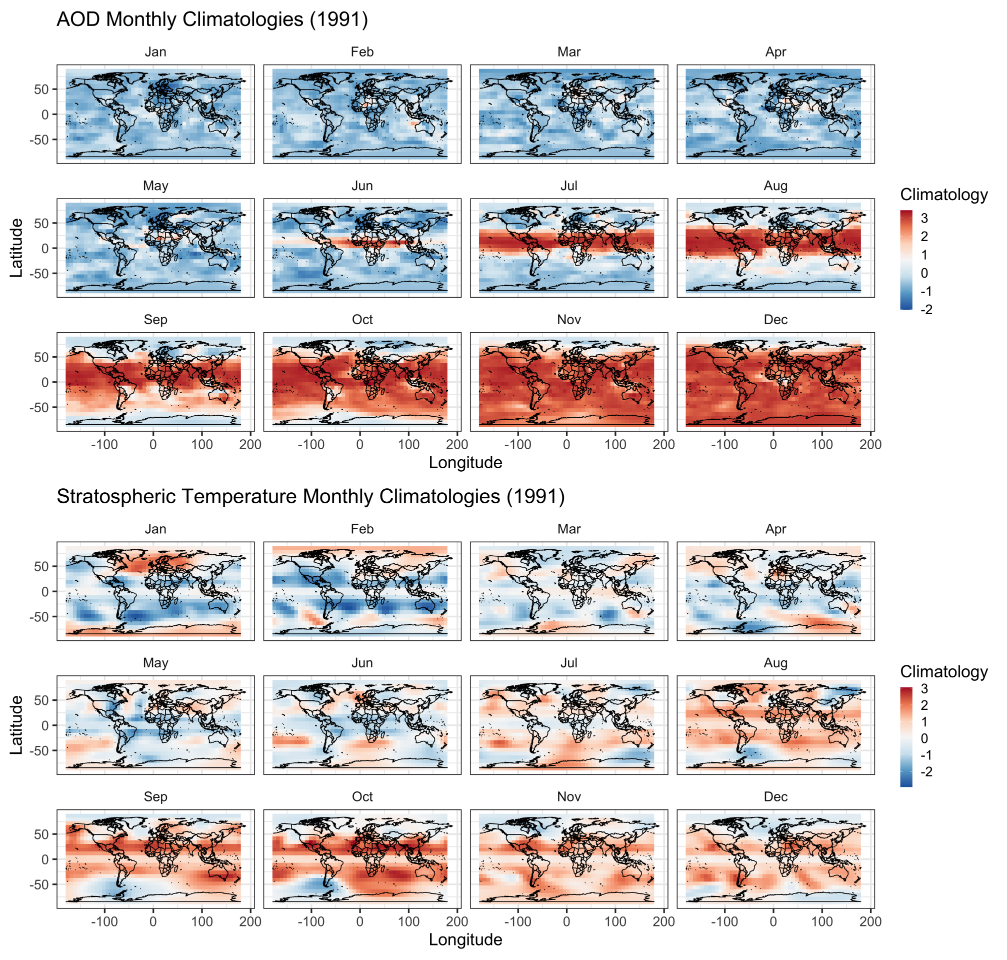


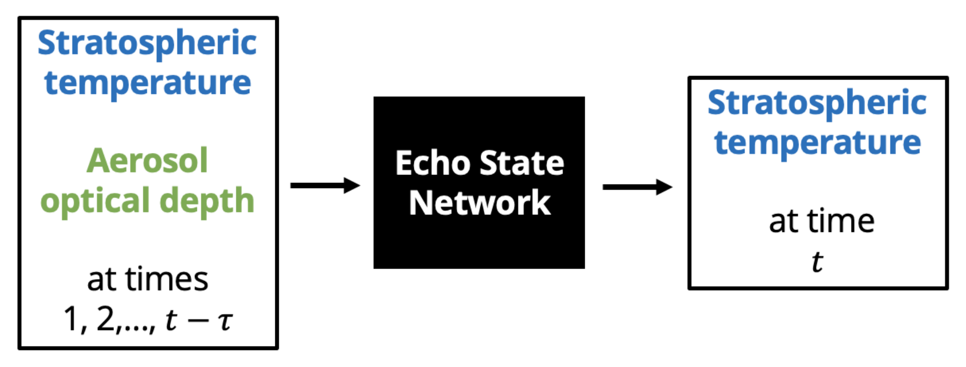
Figure generated using Modern-Era Retrospective Analysis for Research and Applications, Version 2 (MERRA- 2) data [4]

Our Approach

Use machine learning…

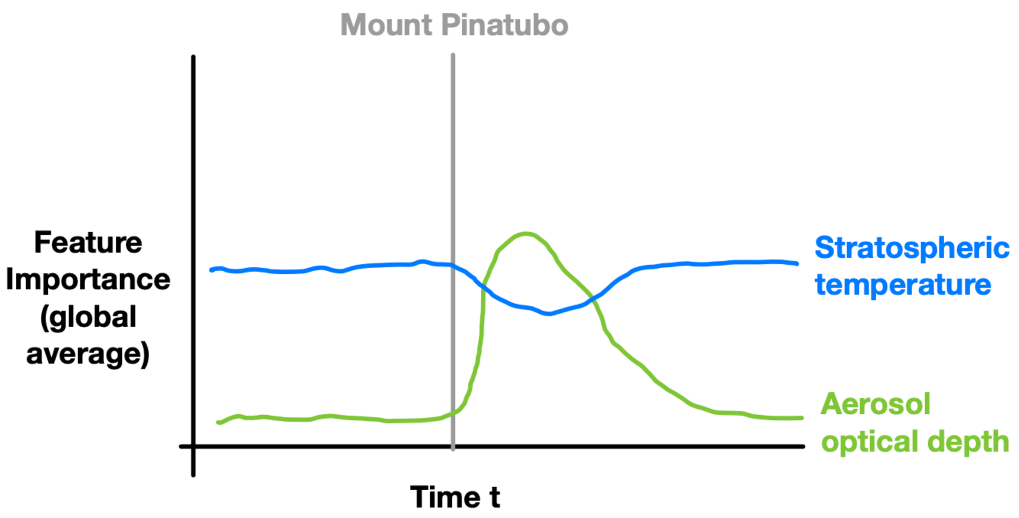
Step 1: Model climate event variables with echo state network

Allow complex machine learning model to capture complex variable relationships



Step 2: Quantify relationships via explainability

Apply feature importance to understand relationships captured by model



Approach

Echo State Networks and Feature Importance

Echo-State Networks

Overview

- Machine learning model for temporal data
  - Sibling to recurrent neural network (RNN)
- Computationally efficient model
  - Compared to RNNs and spatio-temporal statistical models
  - ESN reservoir parameters randomly sampled instead of estimated
- Previous work using ESN for long-term spatio-temporal forecasting
  - McDermott and Wikle [5]

Single-Layer Echo State Network

Output stage: ridge regression

$$\mathbf{y}_t = \mathbf{V}\mathbf{h}_t + \boldsymbol{\epsilon}_t \qquad \boldsymbol{\epsilon}_\mathbf{t} \sim N(\mathbf{0}, \sigma_\epsilon^2 \mathbf{I})$$

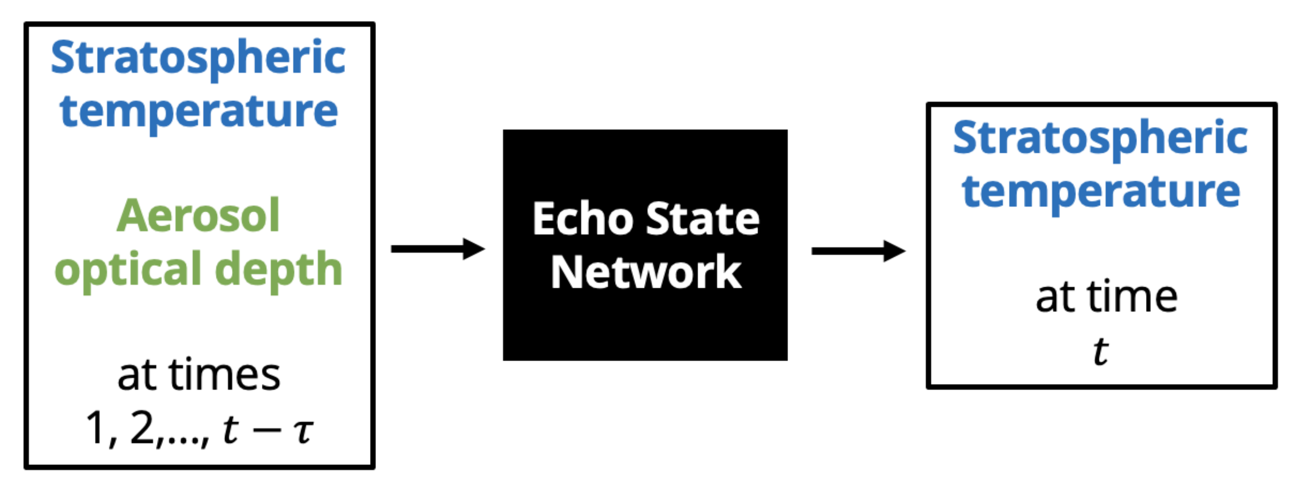
Hidden stage: nonlinear stochastic transformation

$$\mathbf{h}_t = g_h\left(\frac{\nu}{|\lambda_w|}\mathbf{W}\mathbf{h}_{t-1} + \mathbf{U}\tilde{\mathbf{x}}_{t-\tau}\right)$$

$$\tilde{\mathbf{x}}_{t-\tau} = \left[\mathbf{x}'_{t-\tau}, \mathbf{x}'_{t-\tau-\tau^*}, \ldots, \mathbf{x}'_{t-\tau-m\tau^*}\right]'$$

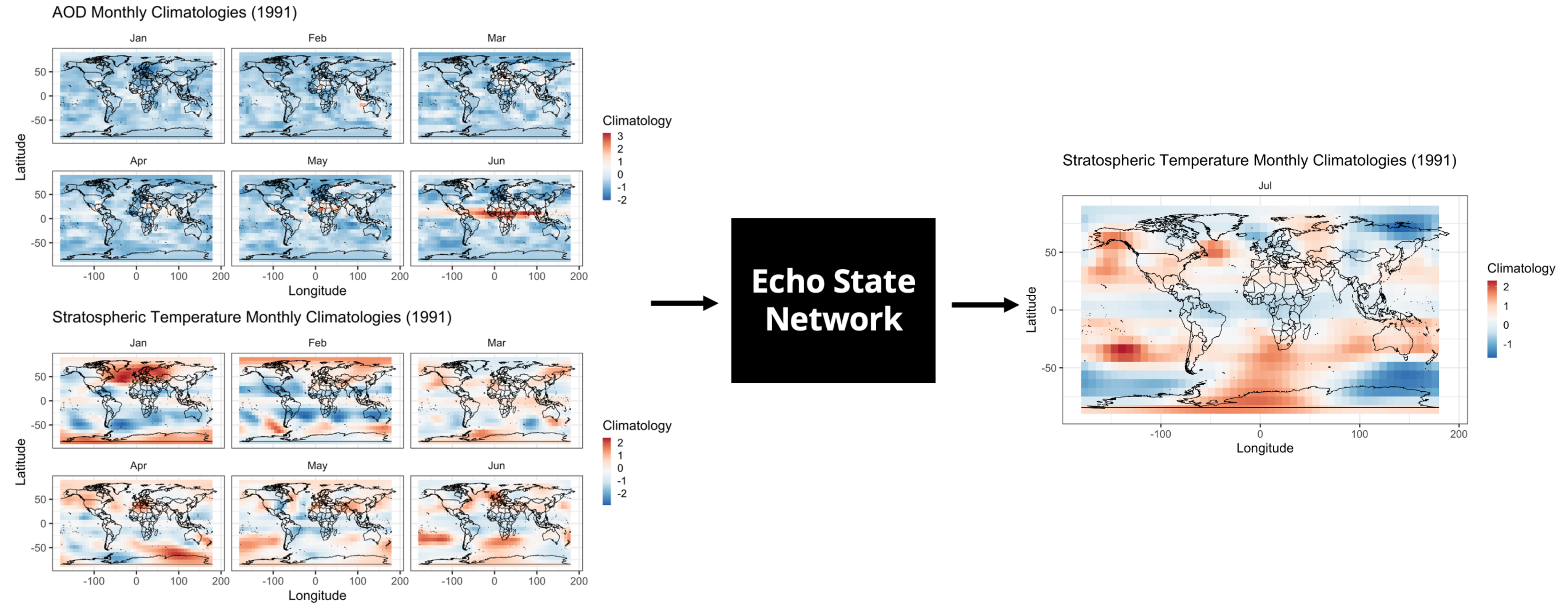
Note: Only parameters estimated are in $\mathbf{V}$.

Echo-State Networks



Echo-State Networks: Spatio-Temporal Context

Recall that we are working with spatio-temporal data…



Echo-State Networks: Spatio-Temporal Context

Spatio-temporal processes at spatial locations $\{\mathbf{s}_i \in \mathcal{D} \subset \mathbb{R}^2; i = 1, \ldots, N\}$ over times $t = 1, \ldots, T$...

Output variable (stratospheric temperature):

$$\mathbf{Z}_{Y,t} = (Z_{Y,t}(\mathbf{s}_1), Z_{Y,t}(\mathbf{s}_2), \ldots, Z_{Y,t}(\mathbf{s}_N))'$$

Input variables (e.g., lagged aerosol optical depth and stratospheric temperature):

$$\mathbf{Z}_{k,t} = (Z_{k,t}(\mathbf{s}_1), Z_{k,t}(\mathbf{s}_2), \ldots, Z_{k,t}(\mathbf{s}_N))'$$

$$\text{for } k = 1, \ldots, K$$

Stage	Formula	Description
Output data stage	$\mathbf{Z}_{Y,t} \approx \mathbf{\Phi}_Y \mathbf{y}_t$	Basis function decomposition (e.g., PCA)
Output stage	$\mathbf{y}_t = \mathbf{V}\mathbf{h}_t + \boldsymbol{\epsilon}_t$	Ridge regression
Hidden stage	$\mathbf{h}_t = g_h\left(\frac{\nu}{\lvert\lambda_w\rvert}\mathbf{W}\mathbf{h}_{t-1} + \mathbf{U}\tilde{\mathbf{x}}_{t-\tau}\right)$	Nonlinear stochastic transformation
Input data stage	$\mathbf{Z}_{k,t} \approx \mathbf{\Phi}_k \mathbf{x}_{k,t} \quad \text{where } \mathbf{x}_t = [\mathbf{x}'_{1,t}, \ldots, \mathbf{x}'_{K,t}]'$	Basis function decomposition (e.g., PCA)

Feature Importance for ESNs

Goal

- Feature importance aims to quantify effect of input variable on a model's predictions

Background

- Permutation feature importance [6]
- Pixel absence affect with ESNs [7]
- Temporal permutation feature importance [8]

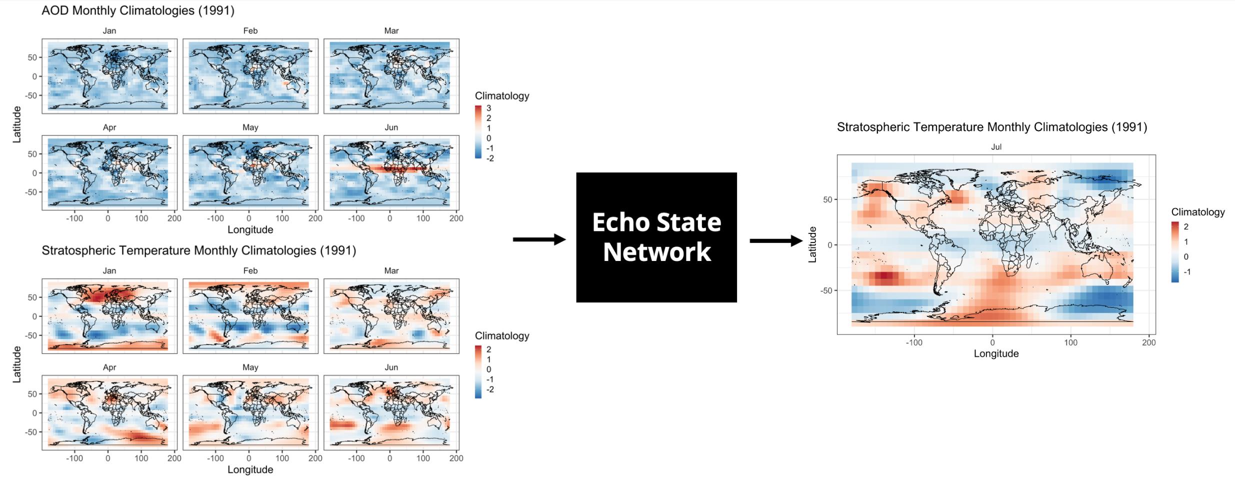
Our Work

- Adapt for ESNs in context of spatio-temporal data

In particular...

Compute feature importance on trained ESN model for:

- input variable over block of times
- on forecasts of response variable at a time



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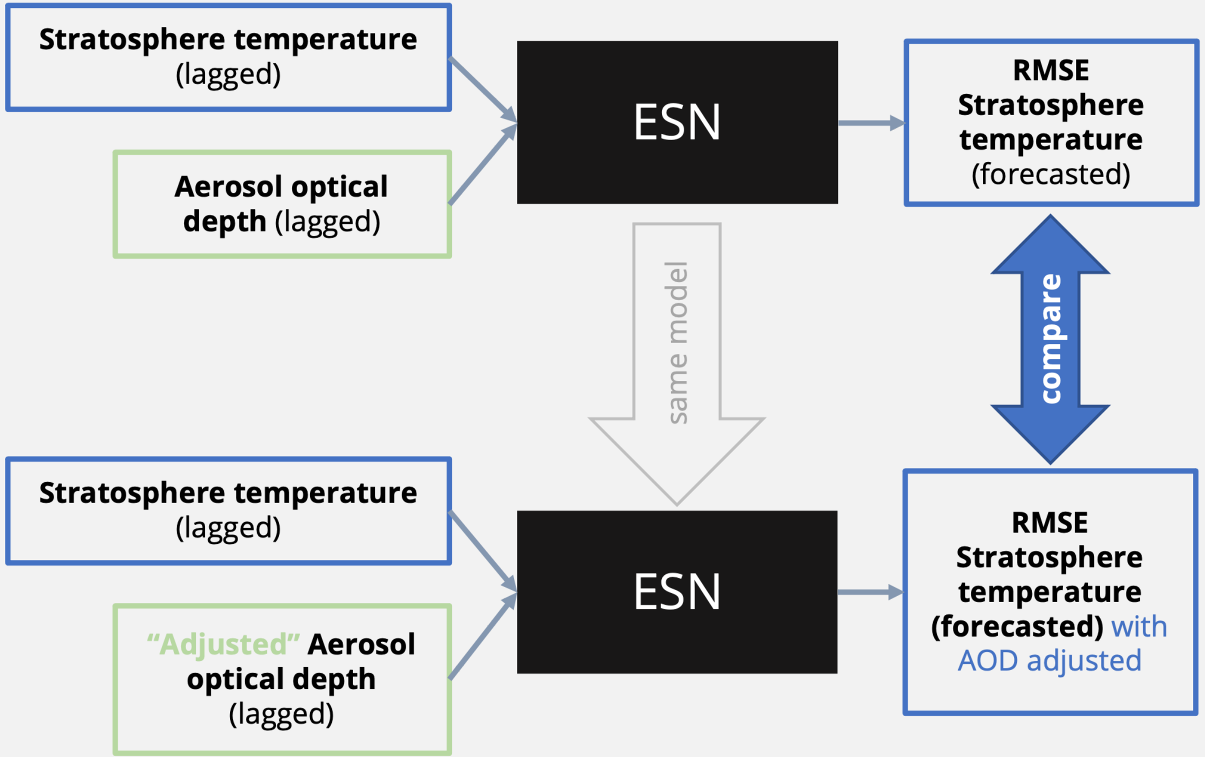


Concept: "Adjust" inputs at times(s) of interest and quantify effect on model performance

- **Permute values**: spatio-temporal permutation feature importance (stPFI)
- **Set values to zero**: spatio-temporal zeroed feature importance (stZFI)

Feature Importance: Difference in RMSEs from "adjusted" and observed spatial predictions:

$$RMSE_{adj,t} - RMSE_{obs,t}$$

Interpretation: Large feature importance indicates "adjusted" inputs lead to a decrease in model performance indicating the model uses those inputs for prediction (i.e., inputs 'important' to model)

Climate Application

Mount Pinatubo

Mount Pinatubo Example: Data

Source

- Modern-Era Retrospective Analysis for Research and Applications, Version 2 (MERRA- 2)

Training Years

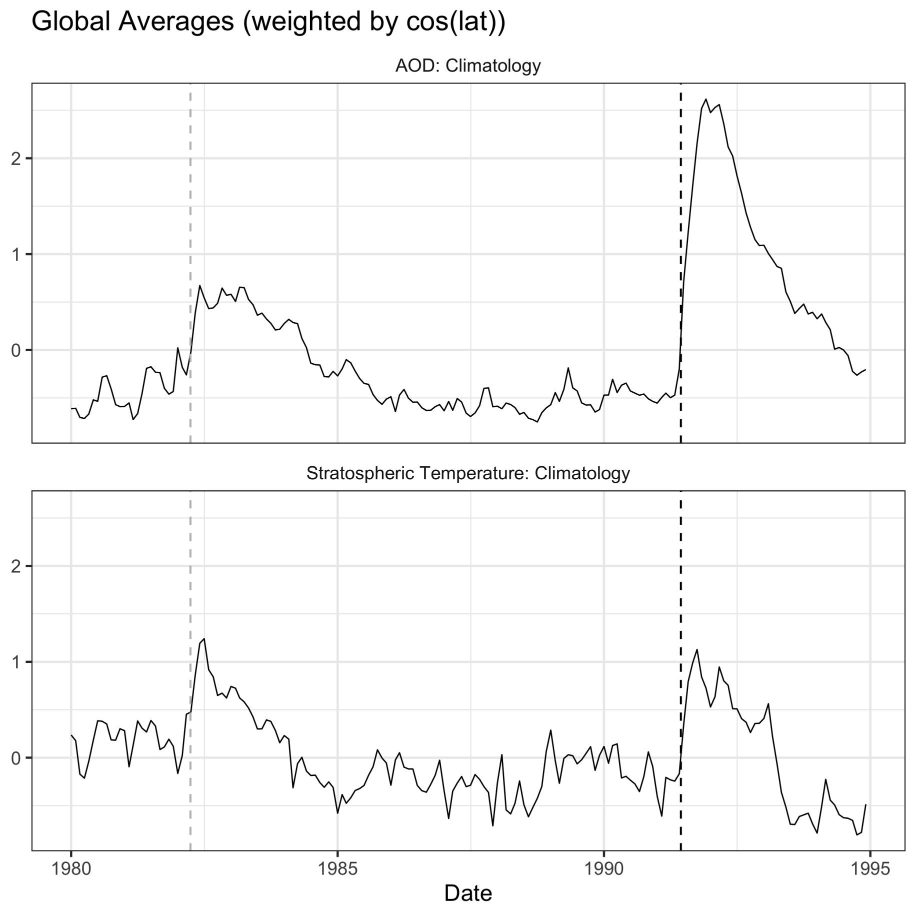
- 1980 to 1995
- Includes eruptions of Mount Pinatubo (1991) and El Chichón (1982)

Time Interval

- Monthly

Latitudes

- -86 to 86 degrees



Mount Pinatubo Example: Model

ESN Output

- Stratospheric Temperature (50mb)

ESN Inputs

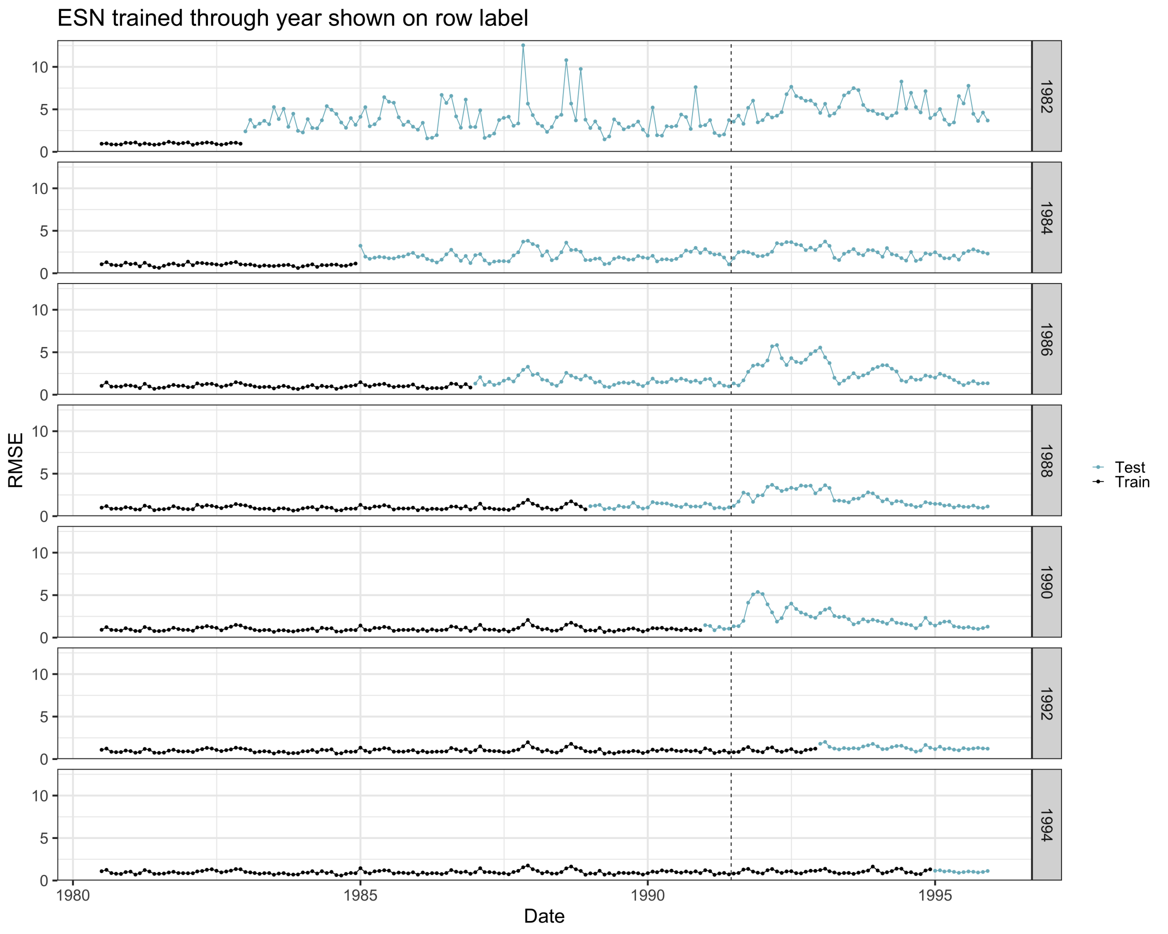
- Lagged Stratospheric Temperature (50mb)
- Lagged AOD

Forecast Lag

- One month

Preprocessing (all variables)

- Climatologies
- Principal components (first 5)



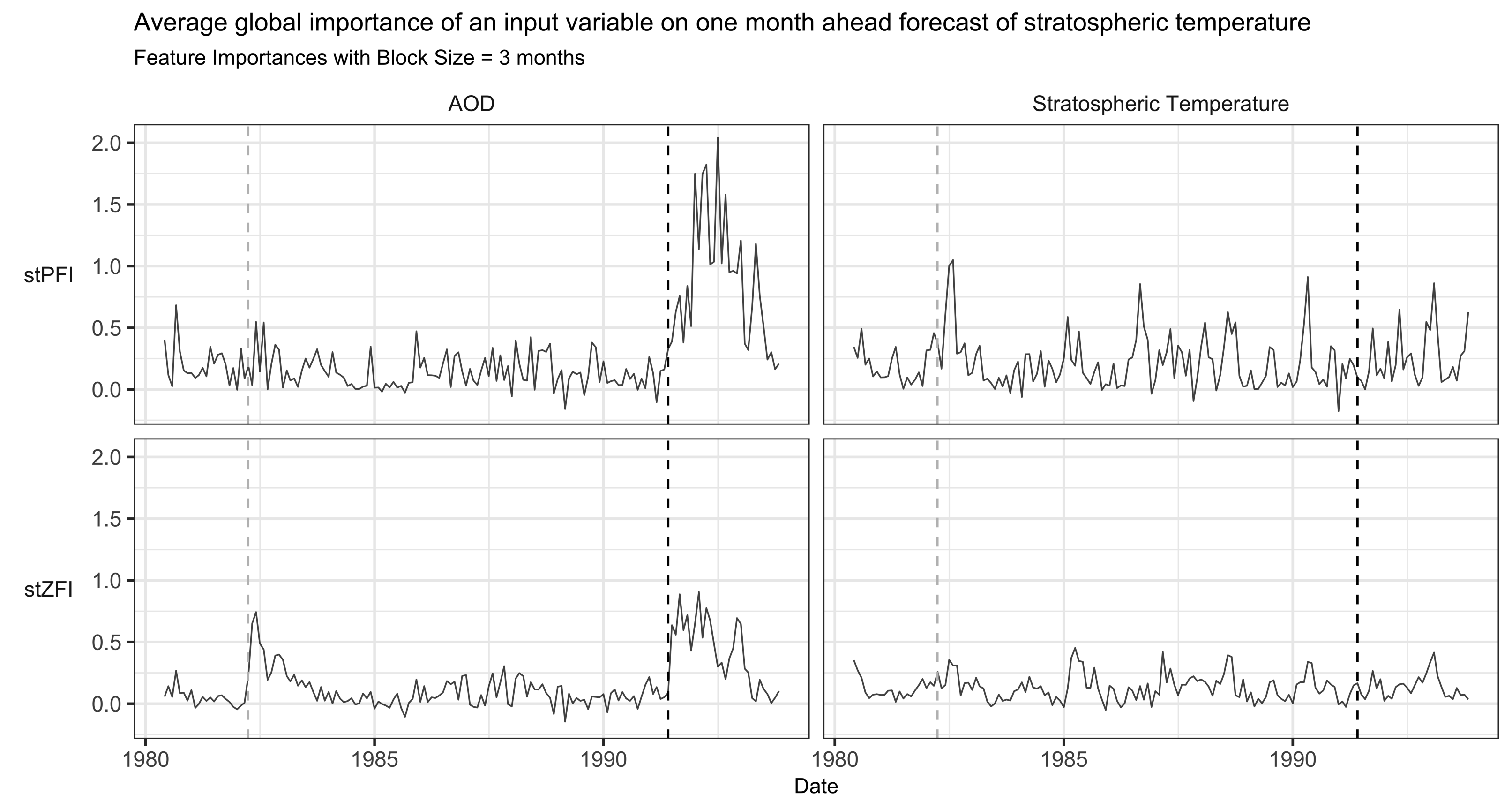
Mount Pinatubo Example: Feature Importance

Key Point

Peak of importance for AOD (and lack of peak of importance for lagged stratospheric temperatures), provides evidence that volcanic eruption impact on temperature can be traced through AOD

FI Metric

Weighted RMSE (weighted by cosine of the latitude)



Conclusions and Future Work

Summary and Conclusions

Summary

- Interested in quantifying relationships between climate variables associated with pathway of climate event
- Motivated by increasing possibility of climate interventions
- Our machine learning approach:
  - Use ESN to model variable relationships
  - Understand variable relationships using proposed spatio-temporal feature importance

Conclusion

- Approach provided evidence of AOD being an intermediate variable in Mount Pinatubo climate pathway affecting stratospheric temperature

Future (Current) Work

ESN extensions

- Addition of multiple layers
- ESN ensembles
- Bayesian ESNs

Spatio-temporal feature importance

- Implement proposed retraining technique [9] to lessen detection of spurious relationships due to correlation
- Adapt to visualize on spatial scale
- Comparison to other newly proposed explainability techniques for ESNs (layer-wise relevance propagation) [10]

Mount Pinatubo application

- Inclusion of additional pathway variables (e.g., SO2, radiative flux, surface temperature)
- Importance of grouped variables

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[10] M. Landt-Hayen, P. Kröger, M. Claus, et al. "Layer-Wise Relevance Propagation for Echo State Networks Applied to Earth System Variability". In: *Signal, Image Processing and Embedded Systems Trends*. Ed. by D. C. Wyld. Computer Science & Information Technology (CS & IT): Conference Proceedings 20. ARRAY(0x55588c8d8680), 2022, pp. 115-130. ISBN: 978-1-925953-80-0. DOI: doi:10.5121/csit.2022.122008. URL: https://doi.org/10.5121/csit.2022.122008.

Thank you

Katherine Goode

kjgoode@sandia.gov

goodekat.github.io

Back-Up Slides

ESN Details

Quadratic Echo State Network

Output Stage: Ridge regression

$$\mathbf{Y}_t = \mathbf{V}_1\mathbf{h}_t + \mathbf{V}_2\mathbf{h}_t^2 + \boldsymbol{\epsilon}_t \quad \boldsymbol{\epsilon}_t \sim Gau\left(\mathbf{0}, \sigma_\epsilon^2\mathbf{I}\right)$$

- **Response matrix**: Principal component scores (time series) that capture spatial trends
- **Ridge regression coefficients** (linear)
- **Ridge regression coefficients** (quadratic)
- **Ridge regression error variance**

Embedding Vector: Inputs

$$\tilde{\mathbf{x}}_t = \left[\mathbf{x}_t', \mathbf{x}_{t-\tau^*}', \mathbf{x}_{t-2\tau}', \ldots, \mathbf{x}_{t-m\tau^*}'\right]'$$

- Number of previous times to include in embedding vector
- Lag between embedding vector times

Hidden Stage: Nonlinear stochastic transformation of input vectors)

$$\mathbf{h}_t = g_h\left(\frac{\nu}{|\lambda_w|}\mathbf{W}\mathbf{h}_{t-1} + \mathbf{U}\tilde{\mathbf{x}}_t\right)$$

- **Scaling parameter**: Helps control the amount of memory in the system (between 0 and 1 for stability)
- **Previous time's hidden units**
- **Embedding vector** (covariates): Principal component scores
- **Nonlinear activation function** (e.g., sigmoidal function such as a hyperbolic tangent function)
- **Spectral radius**: Largest eigenvalue of **W**
- **Reservoir weight matrices**: Determine which and to what degree, past embeddings and current embeddings will be used to construct features $\boldsymbol{h}_t$ for the quadratic regression

Reservoir Weight Matrices: Details

$$\mathbf{W} = [w_{i,l}]_{i,l} \qquad \mathbf{U} = [u_{i,j}]_{i,j}$$

$$w_{i,l} = \gamma_{i,l}^w Unif(-a_w, a_w) + (1 - \gamma_{i,l}^w)\delta_0$$

$$u_{i,j} = \gamma_{i,j}^u Unif(-a_u, a_u) + (1 - \gamma_{i,j}^u)\delta_0$$

$$\gamma_{i,l}^w \sim Bern(\pi_w) \qquad \gamma_{i,j}^u \sim Bern(\pi_u)$$

- **Previous time hidden unit weight matrix**: Can be thought of analogously to a transition matrix in a vector autoregressive model in that it can capture transition dynamic interactions between various inputs
- **Indicator variables**
- **Uniform distribution parameters**: Set to small values to help prevent overfitting
- **Dirac function**
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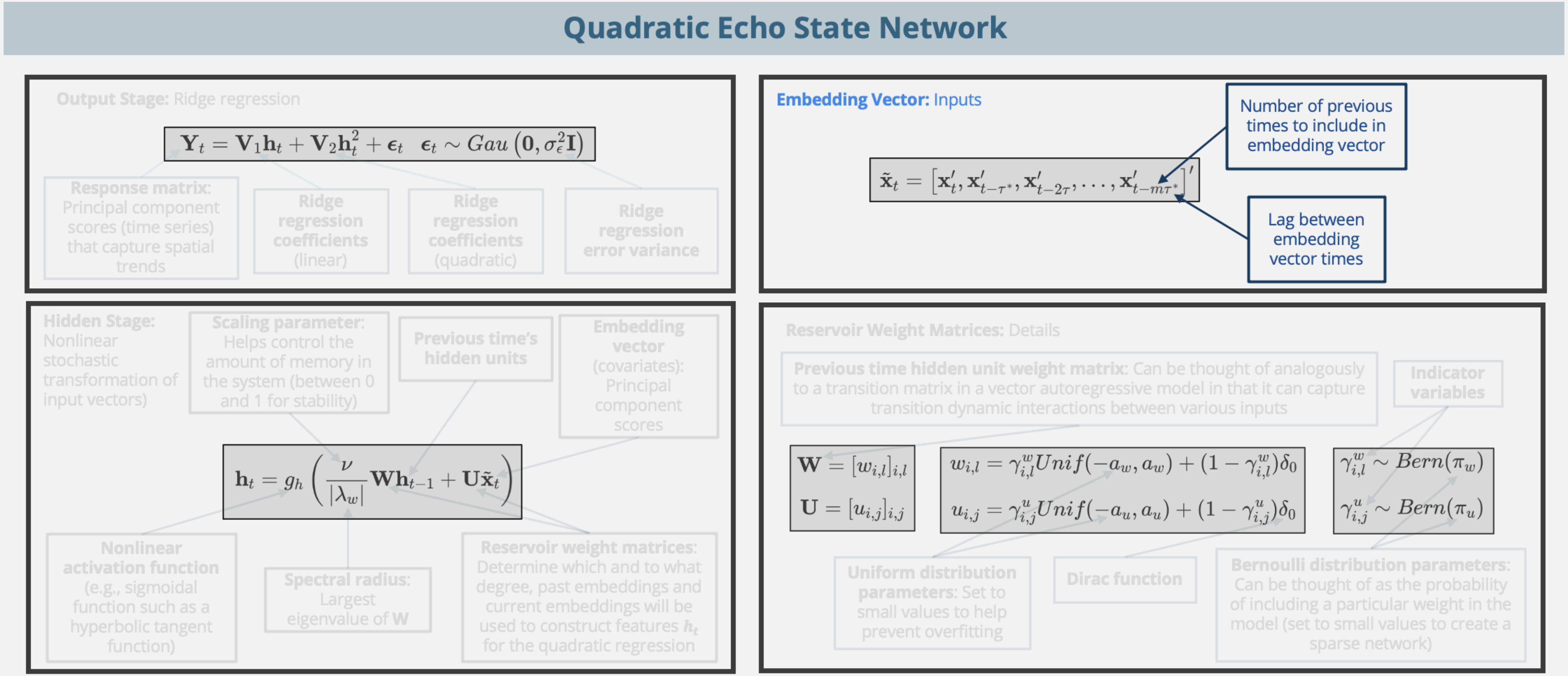
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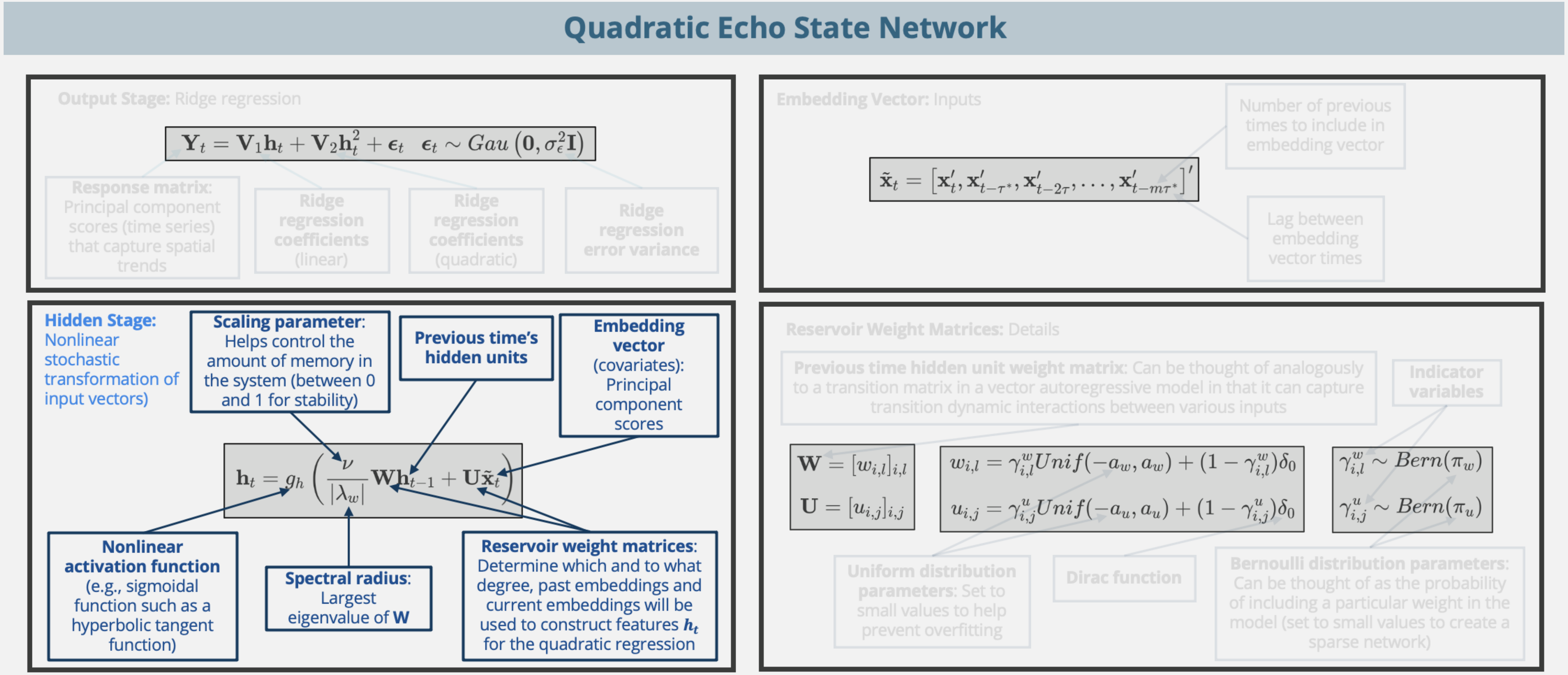

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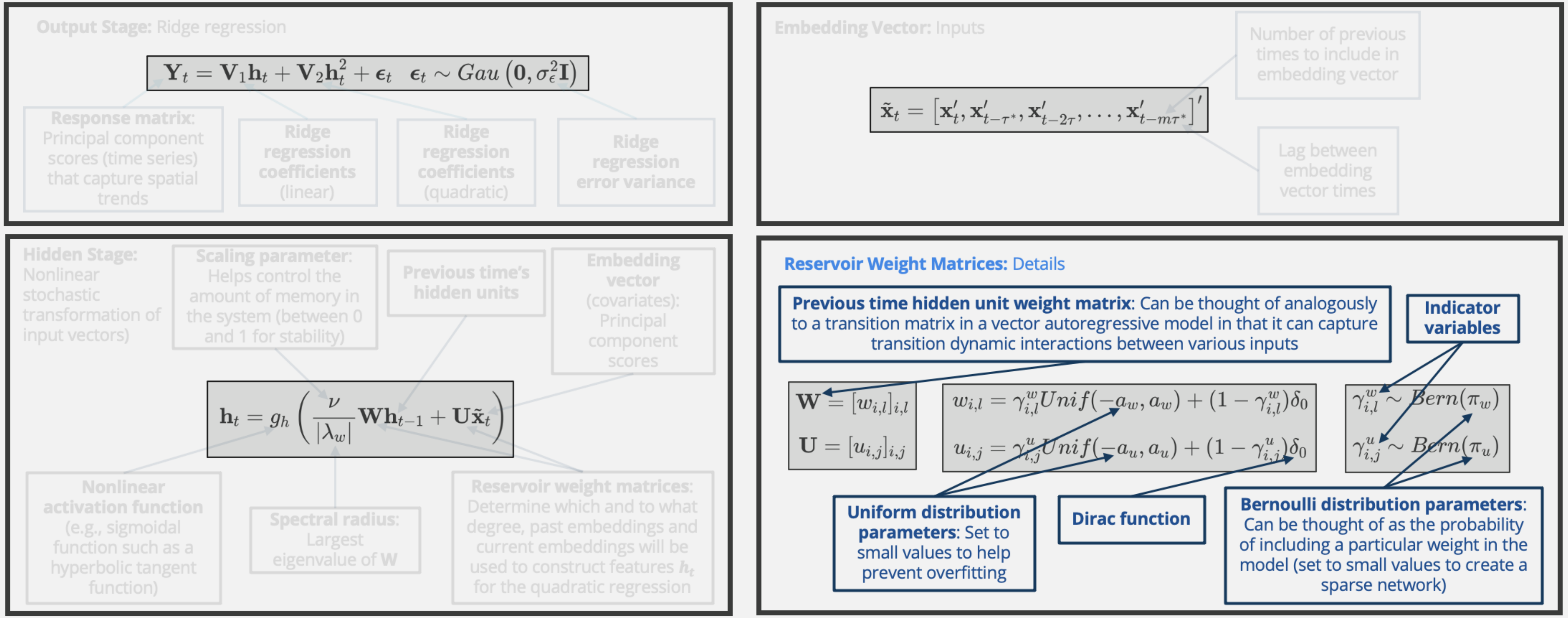
ESN Details

Quadratic Echo State Network



Feature Importance: Spatio-Temporal Context

Compute FI on the trained ESN model for...

- spatio-temporal input variable k
- over the block of times $\{t, t-1, \ldots, t-b+1\}$
- on the forecasts of the spatio-temporal response variable at time $t+\tau$.

	$x_{1,t,1}$	…	x_{1,t,P_1}	$x_{2,t,1}$	…	x_{2,t,P_2}	…	$x_{K,t,1}$	…	x_{K,t,P_K}
$t=1$										
$t=2$										
$t=3$										
$t=4$										
$t=5$										
…										
$t=T$										

	$y_{1,t}$	…	$y_{Q,t}$
$t=1$			
$t=2$			
$t=3$			
$t=4$			
$t=5$			
…			
$t=T$			

Feature Importance: Spatio-Temporal Context

	$x_{1,t,1}$	…	x_{1,t,P_1}	$x_{2,t,1}$	…	x_{2,t,P_2}	…	$x_{K,t,1}$	…	x_{K,t,P_K}
$t = 1$										
$t = 2$										
$t = 3$										
$t = 4$										
$t = 5$										
…										
t = T										

	$y_{1,t}$	…	$y_{Q,t}$
$t = 1$			
$t = 2$			
$t = 3$			
$t = 4$			
$t = 5$			
…			
t = T			

Two Approaches: "Adjust" inputs by either

- Permutation: spatio-temporal permutation feature importance (stPFI)
- Set values to zero: spatio-temporal zeroed feature importance (stZFI)

Feature Importance: Difference in RMSEs from observed and "adjusted" spatial predictions

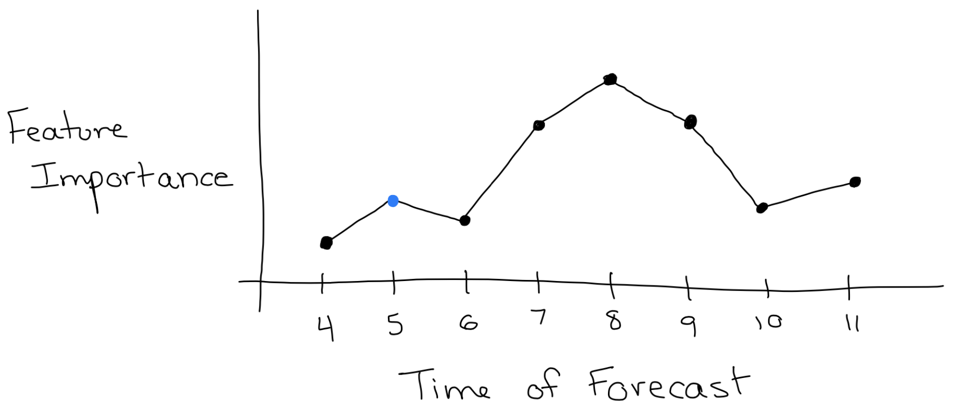
$$\mathcal{I}_{t,t+\tau}^{(k,b)} = \mathcal{M}\left(\mathbf{y}_{t+\tau}, \hat{\mathbf{y}}_{t+\tau}^{(k,b)}\right) - \mathcal{M}\left(\mathbf{y}_{t+\tau}, \hat{\mathbf{y}}_{t+\tau}\right)$$

Feature Importance: Spatio-Temporal Context

	$x_{1,t,1}$	…	x_{1,t,P_1}	$x_{2,t,1}$	…	x_{2,t,P_2}	…	$x_{K,t,1}$	…	x_{K,t,P_K}
$t = 1$										
$t = 2$										
$t = 3$										
$t = 4$										
$t = 5$										
…										
t = T										

	$y_{1,t}$	…	$y_{Q,t}$
$t = 1$			
$t = 2$			
$t = 3$			
$t = 4$			
$t = 5$			
…			
t = T			

Visualization: Feature importance of $\mathbf{x}_1$ during times $\{t, t-1, t-2\}$ on forecast of $\mathbf{y}_t$ at time $t+1$:



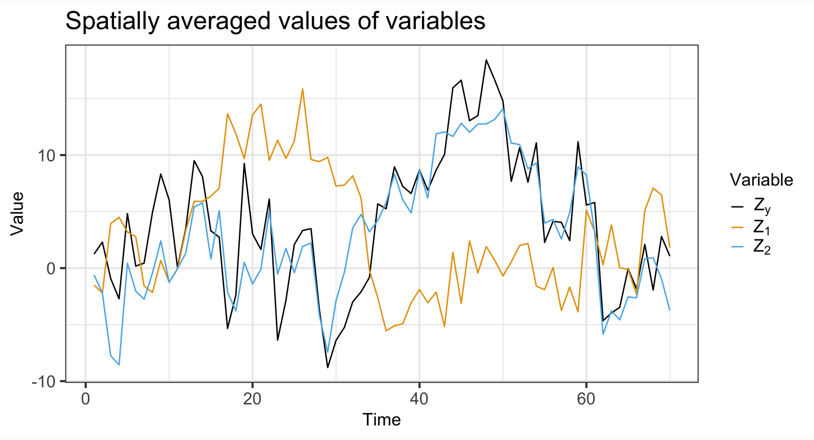
Simulated Data Demonstration

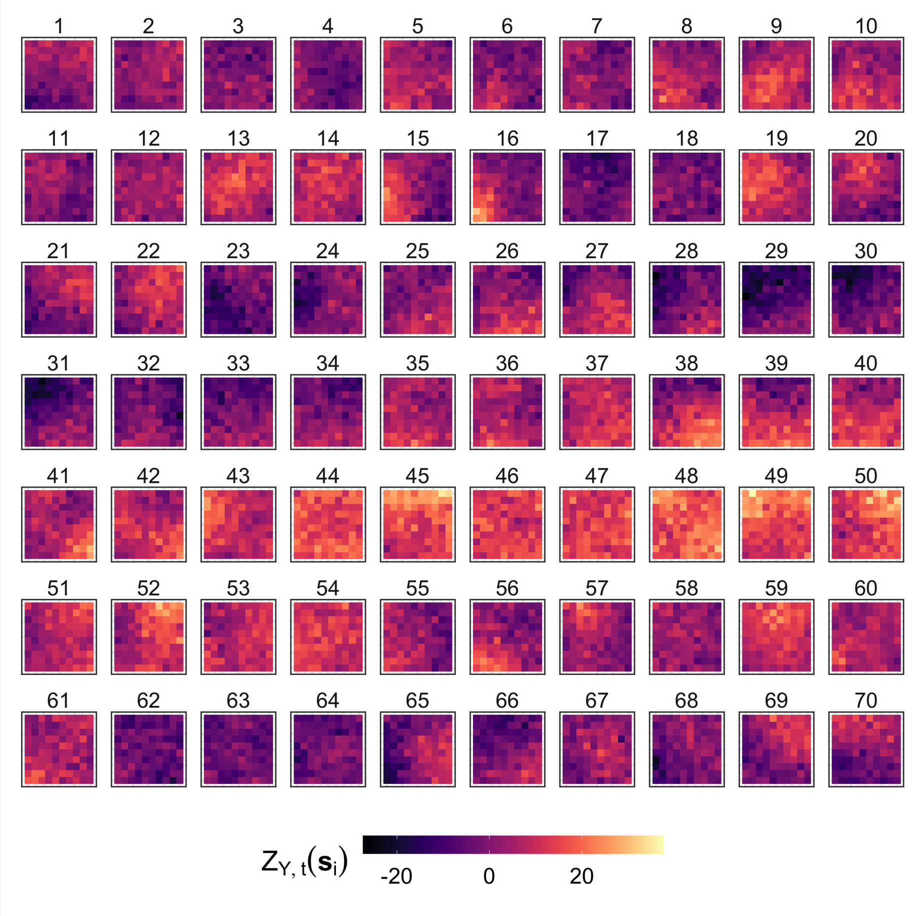
Simulated response

$$Z_{Y,t}(\mathbf{s}_i) = Z_{2,t}(\mathbf{s}_i)\beta + \delta_t(\mathbf{s}_i) + \epsilon_t(\mathbf{s}_i)$$

where

- $Z_{2,t}$ spatio-temporal covariate
- $\delta_t(\mathbf{s}_i)$ spatio-temporal random effect
- $\epsilon_t(\mathbf{s}_i) \overset{iid}{\sim} N(0, \sigma_\epsilon^2)$





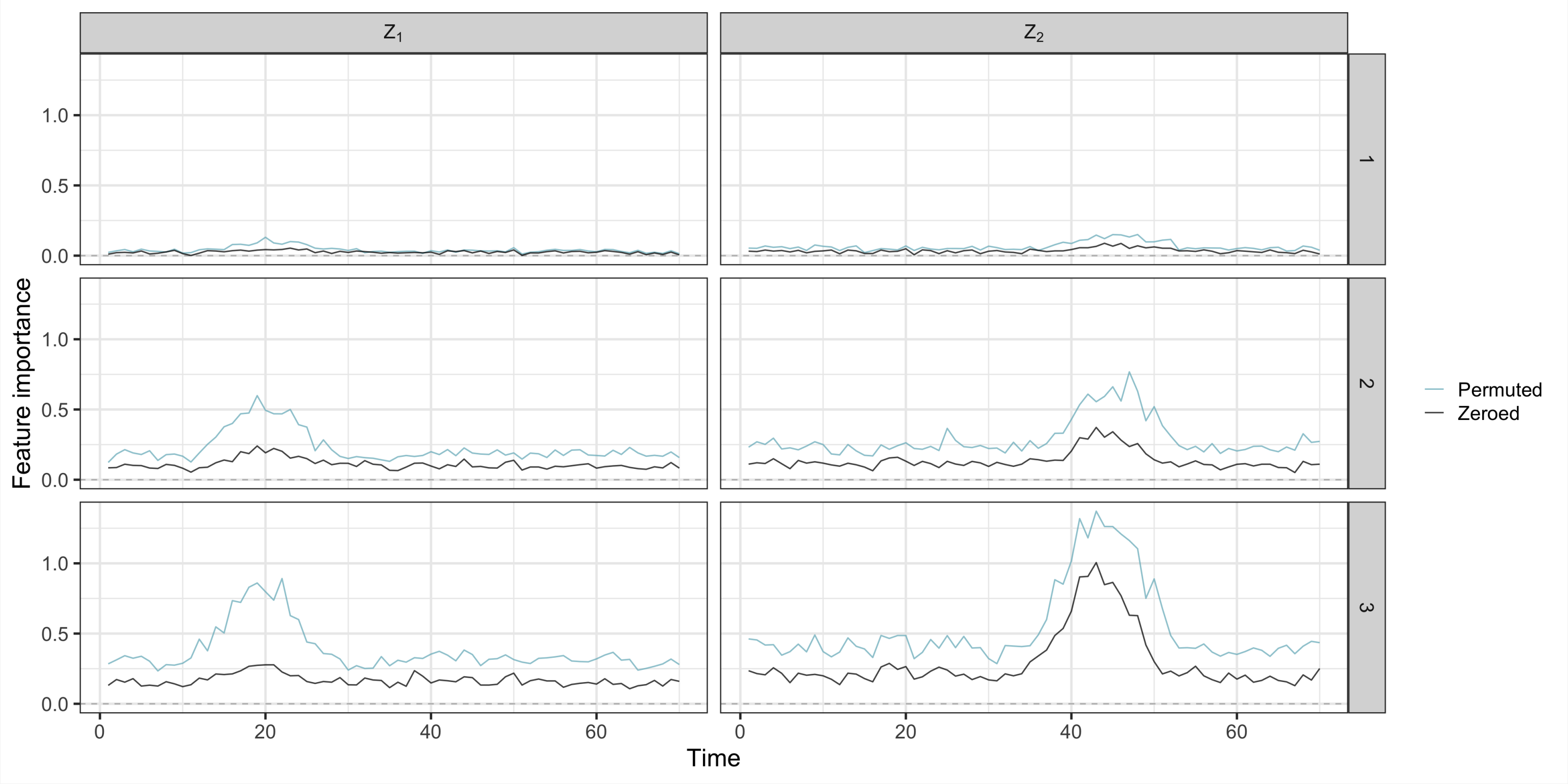
Simulated Data Demonstration

Fit an ESN

- Forecast $Z_{Y,t}$
- Inputs $Z_{1,t-\tau}$ and $Z_{2,t-\tau}$

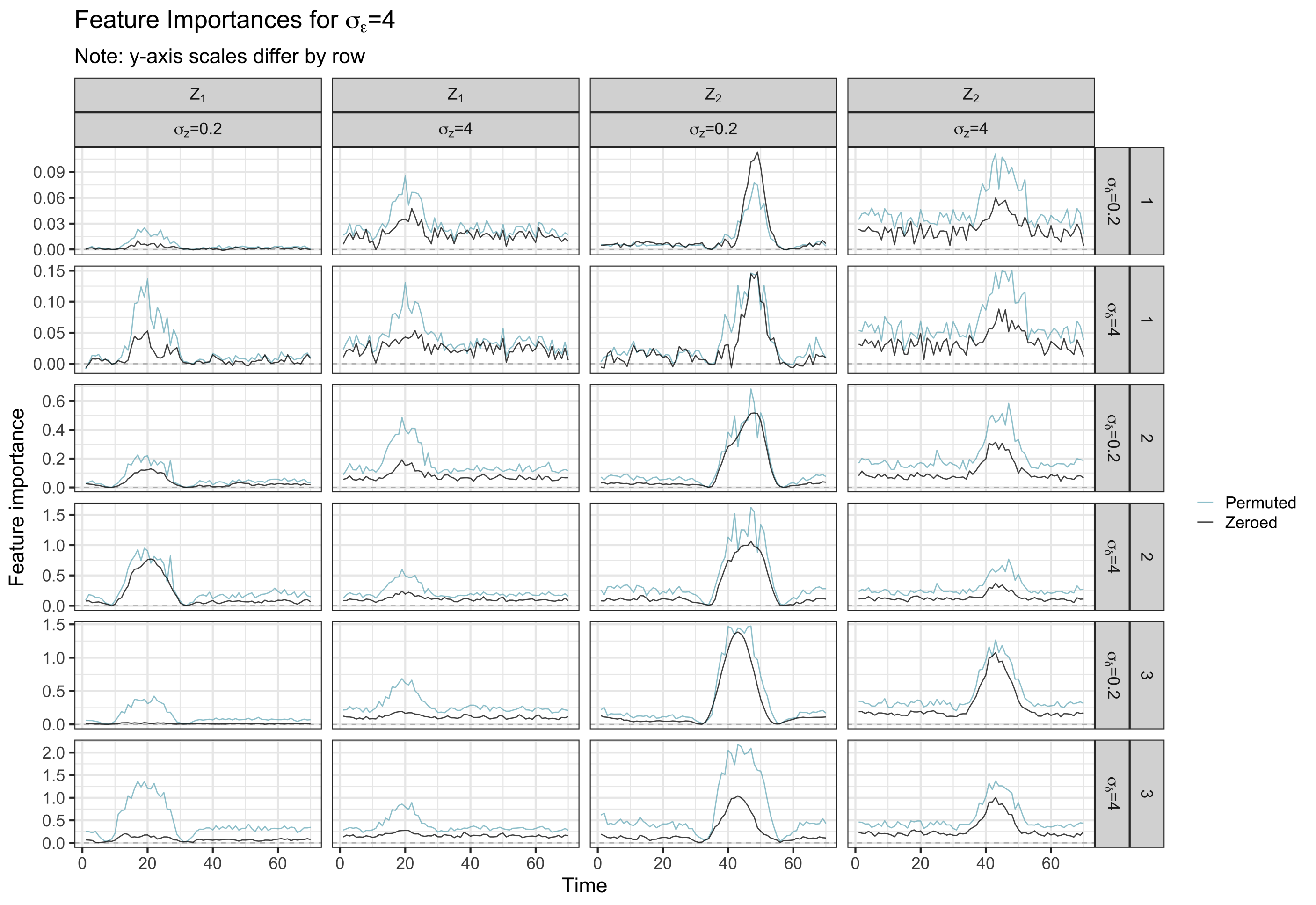
Compute stPFI and stZFI

- Blocks of size 1 to 3

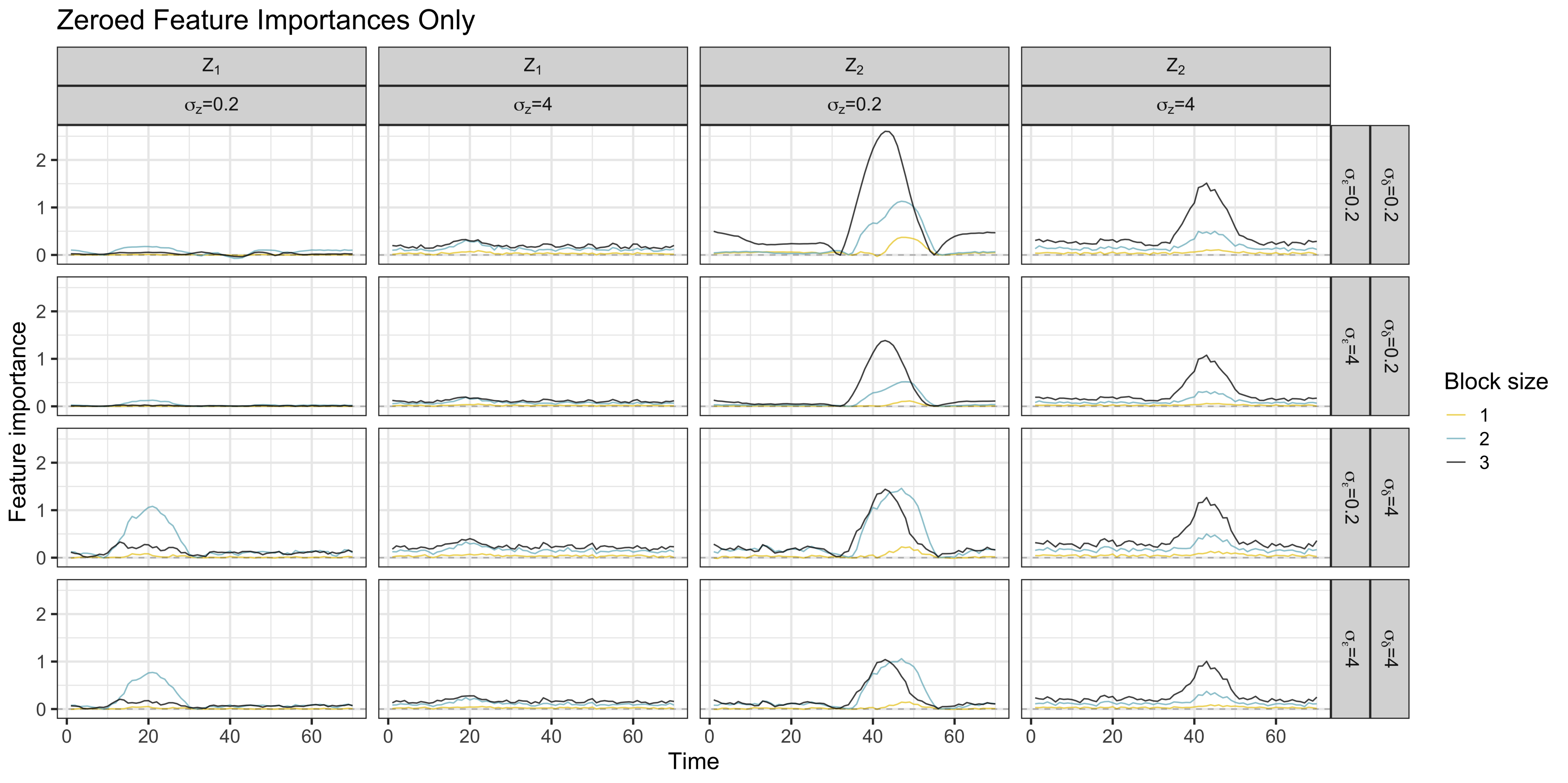


Each line represents the importance of the block of lagged times of an input variable on the forecast at time t

Simulated Data: Effect of Variability on FI



Simulated Data: Effect of Variability on FI



Effect of Correlation on FI

Effect of Correlation on PFI

Correlation between features can lead to biased PFI values dues to the model being forced to extrapolate

- When a correlated variable is permuted, it can lead to observations not in the training data
- Model is forced to extrapolate for that observation
- **Extrapolation can lead to a major effect on prediction making a variable seem more important than it is**

Example

Data is simulated so that X1 affects Y but X2 does not:

(Left) Within training data (stars) random forest correctly determines relationship between X1, X2, and Y (contour lines) but incorrect outside of training data

(Right) When X2 is permuted, observation could land outside training data and lead to change in prediction (i.e., large PFI)

Source: Hooker, Mentch, and Zhou (2021)