



Flexibility, interpretability, and scalability in time series modeling

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Modern sources of time series





Theory not applicable because typically assume no time dependencies

Now time series are "in"



Lots of replicated series

- Lots of correspondence data
- Lots of trials of a robot navigating every part of the maze
- Lots of transcribed audio



Inferring brain networks: Costly data collection, significant subject-to-subject variability

Lots of replicated series

- Lots of correspondence data
- Lots of trials of a robot navigating every part of the maze
- Lots of transcribed audio



Demand forecasting of new item: Tons of data, but not for question of interest

Lots of replicated series

- Lots of correspondence data
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Rare disease (or event) modeling: Need to focus on tails of distribution

Lots of	
replicated	
series	

- Lots of correspondence data
- Lots of trials of a robot navigating every part of the maze
- Lots of transcribed audio

Manageable contextual memory

- Seen this structure in a maze before
- Seen these words in this context before
- Seen patient with these symptoms and test results before



Changing context (non-stationarity): Patient recovering or deteriorating, event-driven changes, etc.

Lots of replicated series	 Lots of correspondence data Lots of trials of a robot navigating every part of the maze Lots of transcribed audio
Manageable contextual memory	 Seen this structure in a maze before Seen these words in this context before Seen patient with these symptoms and test results before
Clear prediction objective	 Word error rate for speech recognition BLEU score for machine translation Reward function in reinforcement learning

Few, low-trustworthy labels

No clear prediction metric

Structure learning, interpretability



- my www. man May man white
- what when by the property of the hold of the second
- when the manufacture of the second of the se

Interpretable interactions

Modeling sparsely sampled, nonstationary time series Handling bias in stochastic gradients of sequential data

Granger causality: Directed, lagged interactions in time series



Why are interactions important?



Functional networks in the brain



Gene regulatory networks

Granger causality selection – Linear model



Series i does not Granger cause series j iff $A_{ji,k} = 0$ $\forall k$

Lag k interaction

Granger causality selection – Linear model



$$\min_{A_1,\ldots,A_K} \underbrace{\sum_{t=K}^T \left(x_t - \sum_{k=1}^K A_k x_{t-k} \right)^2}_{\text{reconstruction error}} + \lambda \underbrace{\sum_{ij} ||(A_{ji,1},\ldots,A_{ji,K})||_2}_{\text{group lasso penalty}},$$

The issue with a linear approach



Functional networks in the brain

Gene regulatory networks

Modeling nonlinear dynamics



Tank, Covert, Foti, Shojaie, Fox, NIPS Time Series Workshop 2017, under review 2019

Identifying Granger causality



Tank, Covert, Foti, Shojaie, Fox, NIPS Time Series Workshop 2017, under review 2019

Using penalized neural networks



Tank, Covert, Foti, Shojaie, Fox, NIPS Time Series Workshop 2017, under review 2019

Penalized multilayer perceptron (MLP)



Penalized multilayer perceptron (MLP)

series j does not Granger cause series i if group j weights are 0

place group-wise penalty on layer 1 weights

group inputs by: (Klags of series j)



Penalized multilayer perceptron (MLP)



Lag selection via hierarchical group lasso





$$\begin{array}{ll} \text{forget gate} & f_t = \sigma \left(W^f x_t + U^f h_{(t-1)} \right) \\ \text{input gate} & i_t = \sigma \left(W^{in} x_t + U^{in} h_{(t-1)} \right) \\ \text{output gate} & o_t = \sigma \left(W^o x_t + U^o h_{(t-1)i} \right) \\ \text{cell state} & c_t = f_t \odot c_{t-1} + i_t \odot \sigma \left(W^c x_t + U^c h_{(t-1)} \right) \\ \text{hidden state} & h_t = o_t \odot \sigma(c_t) \\ \text{evolution} \end{array}$$



series j does not Granger cause series i if jth column of weights W is 0



DREAM3 challenge

Difficult **non-linear dataset** used to benchmark Granger causality detection

Simulated gene expression and regulation dynamics for:

- 2 E.Coli and 3 Yeast
- 100 series (network size)
- 46 replicates
- 21 time points

Very different structures

Structure extracted from currently established gene regulatory networks



DREAM3 results

% AUROC



Capturing contemporaneous interactions via structured deep generative models



Ainsworth, Foti, Lee, Fox, ICML 2018

Interpretable interactions

Modeling sparsely sampled, nonstationary time series Handling bias in stochastic gradients of sequential data



3467 Maple Street

For Rent \$2,500 Rent Zestimate' \$2,430 1265 Cedar Way Pre-Foreclosure Zestimate' \$250,000

> 3451 Alder Street For Sale \$266,000 Zestimate' \$260,000

1265 Oak Way Sold on 3/31/13 Sold for \$237,000

modeling a local housing index



Census tracts in Seattle, WA

What is the value of housing in each region over time?

Challenge: Spatiotemporally sparse data



Challenge: Spatiotemporally sparse data

Tract 281980

Tract 340184









Ren, Fox, Bruce, Annals of Applied Statistics 2017



Cluster and correlate multiple time series



Ren, Fox, Bruce, Annals of Applied Statistics 2017
Seattle City analysis



Robustness to even finer scales



Heuristically defined neighborhoods

Smaller than census tracts

5% improvement in predictive performance!

Another data-scarce study: Dynamics of homelessness

Data challenges:

CAGO

Count method varies from metro

Counts occur on single night

to metro and across time

OF HOMELESS PERSO
 % sheltered varies widely

between metros

Observe most in shelters and

IN fraction on the streets

measurement bias!

Goals:

- Studying time-varying homeless populations **locally**
- Infer effect of increases in rent to homelessness rate
- Forecast future homeless population for decision-making
- Robustly quantify **uncertainty**

Per-metro count-based dynamical model



(Nonstationary) population dynamics

Noisy census counts (observed)

Log odds of homelessness regressed on Zillow Rent Index (ZRI)

Total # homeless (unobserved)

Count accuracy

Counted # homeless (observed)



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Log odds of homelessness regressed on Zillow Rent Index (ZRI)

Total # homeless (unobserved)

Count accuracy

Counted # homeless (observed)



(Nonstationary) population dynamics

Noisy census counts (observed)

Log odds of homelessness regressed on Zillow Rent Index (ZRI)

Total # homeless (unobserved)

Count accuracy

Counted # homeless (observed)

Adjusting for dynamics of count accuracy and total population, is homelessness rate increasing?

States of emergency

Status quo

Progress



% increase in unsheltered count accuracy

• 0% • 2%

If rent increases x%, do # homeless increase?



Interpretable interactions

Modeling sparsely sampled, nonstationary time series Handling bias in stochastic gradients of sequential data

Recap: Mechanisms for coping with limited data



clusters and hierarchies



sparse directed interactions





low-dimensional embeddings

switching between simpler dynamics

Interpretable interactions

Modeling sparsely sampled, nonstationary time series Handling bias in stochastic gradients of sequential data



Discrete-time state space models





Examples: HMMs, AR-HMMs, linear Gaussian state space models, switching linear dynamical systems, nonlinear state space models, ...

Learning challenge for SSMs

$$\log \Pr(y, u \mid \theta) = \sum_{t} \log \Pr(y_t \mid u_t, \theta) + \log \Pr(u_t \mid u_{t-1}, \theta)$$

Emissions Transitions y_{t-1}



$$\log \Pr(y \mid \theta) = \sum_{t} \log \Pr(y_t \mid y_{< t}, \theta)$$

Fisher's Identity:

$$\nabla_{\theta} \log \Pr(y \mid \theta) = \mathbb{E}_{u \mid y, \theta} \left[\nabla_{\theta} \log \Pr(y, u \mid \theta) \right]$$

Expectation conditioned on full sequence



Algorithms for SSMs

Complexity O(K²T) (or O(N³T) for continuous latent states)

 $\mathbf{A}^{(t)}$



Stochastic gradients + SSMs



Issue with naïve approach...

A(t

Information outside minibatch not propagated!



Solution: Account for memory decay to still act locally

A naïve stochastic gradient for SSMs

Fisher's Identity: $\nabla_{\theta} \log \Pr(y \mid \theta) = \mathbb{E}_{u \mid y, \theta} \left[\nabla_{\theta} \log \Pr(y, u \mid \theta) \right]$ $= \sum_{t=1}^{I} \mathbb{E}_{u|y,\theta} \left[\nabla_{\theta} \log \Pr(y_t, u_t \mid u_{t-1}, \theta) \right]$ Expectation conditioned on full sequence Naive gradient estimator: $\nabla_{\theta} \operatorname{log} \operatorname{Pr}(y \mid \theta) = \operatorname{Pr}(\mathcal{S})^{-1} \cdot \sum_{t \in \mathcal{S}} \mathbb{E}_{u \mid y_{\mathcal{S}}, \theta} \left[\nabla_{\theta} \operatorname{log} \operatorname{Pr}(y_t, u_t \mid u_{t-1}, \theta) \right]$ Only take expectation conditioning on subsequence

An unbiased, but impractical alternative

Fisher's Identity:

$$\nabla_{\theta} \log \Pr(y \mid \theta) = \mathbb{E}_{u \mid y, \theta} \left[\nabla_{\theta} \log \Pr(y, u \mid \theta) \right]$$
$$= \sum_{t=1}^{T} \mathbb{E}_{u \mid y, \theta} \left[\nabla_{\theta} \log \Pr(y_t, u_t \mid u_{t-1}, \theta) \right]$$

Unbiased gradient estimator:

$$\widehat{\nabla_{\theta} \log \Pr(y \mid \theta)} = \Pr(\mathcal{S})^{-1} \cdot \sum_{t \in \mathcal{S}} \mathbb{E}_{u \mid y, \theta} \left[\nabla_{\theta} \log \Pr(y_t, u_t \mid u_{t-1}, \theta) \right]$$
Requires message passing over full sequence O(|T|)

Buffering for approximate unbiasedness



"Buffered" gradient estimator:

$$\widetilde{\nabla_{\theta} \log \Pr(y \mid \theta)} = \Pr(\mathcal{S})^{-1} \cdot \sum_{t \in \mathcal{S}} \mathbb{E}_{\substack{u \mid y_{\mathcal{S}^*, \theta}}} [\nabla_{\theta} \log \Pr(y_t, u_t \mid u_{t-1}, \theta)]$$

Computation $\mathcal{O}(|\mathcal{S}^*|)$
(and memory)

Aicher, Ma, Foti, Fox, to appear in SIAM Journal on Mathematics of Data Science.

Error analysis

exact posterior $\gamma(u) = \Pr(u \mid y_T, \theta)$ approx posterior $\widetilde{\gamma}(u) = \Pr(u \mid y_{S^*}, \theta)$

Theorem 1. Let $\epsilon_1 = \max\{\mathcal{W}_1(\gamma_{-B}, \tilde{\gamma}_{-B}), \mathcal{W}_1(\gamma_{S+B}, \tilde{\gamma}_{S+B})\}$. If the gradient is Lipschitz in u with constant L_U and the forward and backward smoothing kernels are contractions with constant L < 1, then



Aicher, Ma, Foti, Fox, to appear in SIAM Journal on Mathematics of Data Science.

LGSSM example:
$$\begin{aligned} x_t &= Ax_{t-1} + \mathcal{N}(0, Q) \\ y_t &= x_t + \mathcal{N}(0, R) \end{aligned} \begin{cases} A &= 0.9 \cdot \operatorname{Rot}(\pi/10) \\ Q &= 0.1 \cdot \mathbb{I}_2 \\ R &= \mathbb{I}_2 \end{aligned}$$



Canine iEEG analysis



16 channels, 90 seizures

grab out 4 mins @ 200Hz per channel per seizure \rightarrow 70 million time points

AR-HMM + MCMC







Example SGRLD segmentation (zoomed in around a seizure)

SLDS + MCMC







Example SGRLD segmentation (zoomed in around a seizure)

Handling stochastic gradient bias in training RNNs

Goal: Low-bias training of RNNs



Unrolled recurrent neural network (RNN)

Backpropagation through time (BPTT)



Backpropagation through time (BPTT)

Stochastic gradient:

$$\widehat{g}(\theta) = \sum_{k=0}^{\infty} \frac{dL_t}{dh_{t-k}} \cdot \frac{\partial h_{t-k}}{\partial \theta}$$

SGD using BPTT:

$$\theta_{n+1} = \theta_n - \gamma_n \cdot \hat{g}(\theta_n)$$



O(T) computation time and memory

Expensive for long sequences

Truncated backpropagation through time (TBPTT)

Stochastic gradient:

$$\widehat{g}_{K}(\theta) = \sum_{k=0}^{K} \frac{dL_{t}}{dh_{t-k}} \cdot \frac{\partial h_{t-k}}{\partial \theta}$$

SGD using TBPTT:

$$\theta_{n+1} = \theta_n - \gamma_n \cdot \hat{g}_K(\theta_n)$$





Truncate after K steps of BPTT

O(K) computation time and memory

What's the effect of this bias, and can we bound it?

How to choose K?

How does the bias affect learning?



Truncate after K steps of BPTT

Gradient decay assumptions



Existing Work: Restrict RNN weights such that

$$\left\|\frac{\partial h_{t-r+1}}{\partial h_{t-r}}\right\| \le \lambda < 1 \quad \longrightarrow \quad \left\|\frac{dL_t}{dh_{t-k-1}}\right\| \le \lambda \cdot \left\|\frac{dL_t}{dh_{t-k}}\right\|$$

"Stable" or "Chaos Free" RNN [Laurent & von Brecht '16, Miller & Hardt '19]

Gradient decay assumptions





Our relaxed assumption:

Example: LSTM on language modeling task Penn Treebank dataset



Decay on average, but individual traces do not
Error analysis: Bound on relative bias

RNN notation: $h_t = H(x_t, h_{t-1}; \theta)$ $y_t = F(h_t)$

Assuming:

- Our gradient decay bound holds: $\mathbb{E}_t \left\| \frac{dL_t}{dh_{t-k-1}} \right\| \le \beta \cdot \mathbb{E}_t \left\| \frac{dL_t}{dh_{t-k}} \right\|$ for all $k \ge \tau$
- $\partial H/\partial \theta$ is bounded

Then TBPTT has *bounded relative bias*:

$$\delta = \frac{\|\mathbb{E}[\hat{g}_{K}(\theta)] - g(\theta)\|}{\|g(\theta)\|} \leq \mathcal{O}(\beta^{K-\tau}) \checkmark \text{Geometric in K}$$
Relative bias

Error analysis: Convergence rate of SGD with biased grads

Assuming:

- Relative bias at each step bounded by $\delta < 1$
- Loss is L-smooth and \hat{g} has bounded variance

Then SGD with decaying stepsize $\gamma_n = \gamma \cdot n^{-1/2}$ converges at a rate:

$$\min_{\substack{n=1,...,N}} \|g(\theta_n)\|^2 = \mathcal{O}\left((1-\delta)^{-1} \cdot N^{-1/2}\log N\right)$$
Convergence to
stationary point

Example: LSTM on language modeling task Penn Treebank dataset



For fixed K, relative bias increases during training (in this example)

Estimated



Adaptive TBPTT algorithm $\mathbb{E}_t \left\| \frac{dL_t}{dh_{t-k-1}} \right\| \le \beta \cdot \mathbb{E}_t \left\| \frac{dL_t}{dh_{t-k}} \right\|$ for all $k \ge \tau$

Slope = $\hat{\beta}$

lag k



Target bias δ

 $\log k$

level

 $\leftarrow K_n(\delta)$

TBPTT: Text Example

Data: "... no it was n't black monday 2 but while the new york stock exchange did n't fall apart friday as the dow jones industrial average plunged ..."

Penn Treebank, 1-Layer LSTM*



Perplexity vs. K – comparison

	Penn treebank			
К	Valid PPL	Test PPL		
10	99.7 (0.6)	99.9 (0.8)		
50	110.4 (0.4)	110.8(0.8)		
100	116.2(0.5)	116.9(0.5)		
200	125.2(1.2)	126.1 (0.9)		
300	161.5(0.5)	161.2(0.3)		
$\delta = 0.9$	100.1 (0.5)	99.0~(0.5)		
$\delta = 0.5$	90.1 (0.4)	89.5(0.3)		
$\delta = 0.1$	88.1(0.2)	87.2 (0.2)		
300				
250 -				
200		\sim		

Epoch

Truncation Length K

Wikitext-2

	Κ	Valid PPL	Test PPL
	10	144.2(0.4)	136.5(1.3)
	50	133.4(2.9)	127.2(2.8)
	100	134.4(0.3)	127.8(0.5)
	200	130.3(1.1)	124.6(0.7)
	300	129.6(1.4)	$124.0\ (2.2)$
	$\delta = 0.9$	130.0(1.3)	$124.1 \ (2.2)$
	$\delta = 0.5$	$127.2 \ (0.7)$	121.7 (0.6)
	$\delta = 0.1$	$127.5 \ (0.6)$	$121.9\ (1.2)$
100			
±00 -			
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$\frac{1}{100} - \frac{1}{100} - \frac{1}$			

Truncation Length K

Summary

1. Deep learning offers **tremendous opportunities** for modeling complex dynamics, but problems much vaster than prediction + large corpora

OF HOMELESS PERSONS

2. Scaling learning is possible, but have to think carefully about broken dependencies (bias)

Interpretable

interactions



Credit for the hard work...



Chris Aicher (Stat PhD)



Sam Ainsworth (CSE PhD)



Ian Covert (CSE PhD)



Nick Foti (Research Scientist, now at Apple)











Chris Glynn (Postdoc, Asst Prof at UNH) postdoc at Berkeley)



Yian Ma Alex Tank (Stat PhD, (AMath PhD, now at Voleon)



Shirley You Ren (Stat PhD, now at Apple)