## W

## Flexibility, interpretability, and scalability in time series modeling

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## Modern sources of time series



## Until recently, ML (mostly) ignored time series

## It's hard!

\# parameters (naively) grows rapidly with

- \# of series
- complexity of dynamics captured


## More data

Algorithms more computationally intensive

Theory not applicable because typically assume no time dependencies

## Now time series are "in"



## But, success also relies on...

## Lots of replicated <br> 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

## But, success also relies on...

Lots of replicated<br>series<br>- Lots of correspondence data<br>Lots of trials of a robot navigating every part of the maze<br>- Lots of transcribed audio



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

## But, success also relies on...

Lots of replicated<br>series<br>- Lots of correspondence data<br>- Lots of trials of a robot navigating every part of the maze<br>- Lots of transcribed audio



Rare disease (or event) modeling:
Need to focus on tails of distribution

## But, success also relies on...




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

## But, success also relies on...



Few, low-trustworthy labels

No clear prediction metric


Interpretable interactions

Modeling
sparsely sampled, nonstationary time series

Handling bias in stochastic gradients of sequential data

## Granger causality: <br> 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 jiff $A_{\mathrm{ji}, \mathrm{k}}=0 \quad \forall \mathrm{k}$

## Granger causality selection - Linear model


$\begin{array}{lll}x_{t} & A_{1} & x_{t-1}\end{array}$
$A_{2} \quad X_{t-2}$
$\mathrm{e}_{\mathrm{t}}$

$$
\min _{A_{1}, \ldots, A_{K}} \underbrace{\sum_{t=K}^{T}\left(x_{t}-\sum_{k=1}^{K} A_{k} x_{t-k}\right)^{2}}_{\text {reconstruction error }}+\lambda \underbrace{\sum_{i j}\left\|\left(A_{j i, 1}, \ldots, A_{j i, K}\right)\right\|_{2}}_{\text {group lasso penalty }}
$$

## The issue with a linear approach

## maintain



Functional networks in the brain
Gene regulatory networks

## Modeling nonlinear dynamics



## Identifying Granger causality



## Using penalized neural networks



## 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:

( K lags of series j )


## Penalized multilayer perceptron (MLP)



## Lag selection via hierarchical group lasso

$$
\min _{\mathbf{w}} \sum_{t=K}^{T}\left(x_{i t}-g_{i}\left(x_{(t-1):(t-K)}\right)\right)^{2}
$$


hierarchical
group lasso penalty


## Weights of the LSTM

$W=\left(\left(W^{f}\right)^{T},\left(W^{i n}\right)^{T},\left(W^{o}\right)^{T},\left(W^{c}\right)^{T}\right)$ define effect of input on prediction

forget gate $\quad f_{t}=\sigma\left(W^{f} x_{t}+U^{f} h_{(t-1)}\right)$
input gate $\quad i_{t}=\sigma\left(W^{i n} x_{t}+U^{i n} h_{(t-1)}\right)$
output gate $\quad o_{t}=\sigma\left(W^{o} x_{t}+U^{o} h_{(t-1) i}\right)$
$\begin{gathered}\text { cell state } \\ \text { evolution }\end{gathered} \quad c_{t}=f_{t} \odot c_{t-1}+i_{t} \odot \sigma\left(W^{c} x_{t}+U^{c} h_{(t-1)}\right)$
hidden state $h_{t}=o_{t} \odot \sigma\left(c_{t}\right)$
evolution

## A penalized LSTM

$W=\left(\left(W^{f}\right)^{T},\left(W^{i n}\right)^{T},\left(W^{o}\right)^{T},\left(W^{c}\right)^{T}\right)$ define effect of input on prediction

series j does not Granger cause series if $j$ th column of weights $W$ is 0

$$
\min _{W, U, w^{O}} \underbrace{\sum_{t=2}^{T}\left(x_{i t}-g_{i}\left(x_{<t}\right)\right)^{2}}_{\text {reconstruction error }}+\lambda \underbrace{\lambda \sum_{j=1}^{p}\left\|W_{: j}\right\|_{2}}_{\text {group lasso penalty }}
$$

## 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


## Very different structures

- 21 time points

Structure extracted from currently established gene regulatory networks

## DREAM3 results

\% AUROC


# Capturing contemporaneous interactions via structured deep generative models 



Interpretable interactions

Modeling
sparsely sampled, nonstationary time series

Handling bias in stochastic gradients of sequential data



# Census tracts in Seattle, WA 

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

## Challenge: Spatiotemporally sparse data



Average \# of monthly house sales

## Challenge: Spatiotemporally sparse data

Tract 281980


Tract 340184




## Single census tract model



$$
\begin{aligned}
& x_{t, i}^{\text {tract } i}=a_{i} x_{t-1, i}+\epsilon_{t, i} \quad \epsilon_{t, i} \sim \mathcal{N}\left(0, \sigma_{i}^{2}\right) \\
& y_{t, i, l}=x_{t, i}+\sum_{h=1}^{H} \beta_{i, h} U_{l, r}+v_{t, i, l} \quad v_{t, i, l} \sim \mathcal{N}\left(0, R_{i}\right) \\
&{ }_{\text {th }} \text { sales } \\
& \text { house-level features }
\end{aligned}
$$



## 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 <br> in predictive <br> performance!

## Another data-scarce study: Dynamics of homelessness

## 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

Data challenges:

- Counts occur on single night
- Count method varies from metro to metro and across time
- Observe most in shelters and Ponly fraction on the streets ${ }^{1} T$ OF HOMELESS PERSONS \% sheltered varies widely between metros


## Per-metro count-based dynamical model



## Benefits over past approaches...



## Benefits over past approaches...


(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)

## Benefits over past approaches...



## Benefits over past approaches...



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


If rent increases x\%, do \# homeless increase?


## Typically weak relationship + wide uncertainty intervals

Past methods overly confident. . .ignore noise in homeless count and census data

Interpretable interactions

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## Recap: Mechanisms for coping with limited data


clusters and hierarchies

low-dimensional embeddings

sparse directed interactions

switching between simpler dynamics

Interpretable interactions

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## Discrete-time state space models



Smoothing/ Filtering

Forecasting


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

## Learning challenge for SSMs

$$
\log \operatorname{Pr}(y, u \mid \theta)=\sum_{t} \underbrace{\log \operatorname{Pr}\left(y_{t} \mid u_{t}, \theta\right.}_{\text {Emissions }})+\underbrace{\log \operatorname{Pr}\left(u_{t} \mid u_{t-1}\right.}_{\text {Transitions }}, \theta)
$$



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



Fisher's Identity:

$$
\nabla_{\theta} \log \operatorname{Pr}(y \mid \theta)=\underbrace{\mathbb{E}_{u \mid y, \theta}}_{\text {Expectation conditioned on full sequence }}\left[\nabla_{\theta} \log \operatorname{Pr}(y, u \mid \theta)\right]
$$

## Algorithms for SSMs



## Stochastic gradients + SSMs



## Issue with naïve approach...



## A naïve stochastic gradient for SSMs

Fisher's Identity:

$$
\begin{aligned}
\nabla_{\theta} \log \operatorname{Pr}(y \mid \theta) & =\mathbb{E}_{u \mid y, \theta}\left[\nabla_{\theta} \log \operatorname{Pr}(y, u \mid \theta)\right] \\
& =\sum_{t=1}^{T} \underbrace{\mathbb{E}_{u \mid y, \theta}}_{\underbrace{}}\left[\nabla_{\theta} \log \operatorname{Pr}\left(y_{t}, u_{t} \mid u_{t-1}, \theta\right)\right]
\end{aligned}
$$

Naive gradient estimator:

$$
\nabla_{\theta} \widehat{\log \operatorname{Pr}}(y \mid \theta)=\operatorname{Pr}(\mathcal{S})^{-1} \cdot \sum_{t \in \mathcal{S}} \mathbb{E}_{\underbrace{u \mid y_{\mathcal{S}}, \theta}}\left[\nabla_{\theta} \log \operatorname{Pr}\left(y_{t}, u_{t} \mid u_{t-1}, \theta\right)\right]
$$

## An unbiased, but impractical alternative

Fisher's Identity:

$$
\begin{aligned}
\nabla_{\theta} \log \operatorname{Pr}(y \mid \theta) & =\mathbb{E}_{u \mid y, \theta}\left[\nabla_{\theta} \log \operatorname{Pr}(y, u \mid \theta)\right] \\
& =\sum_{t=1}^{T} \mathbb{E}_{u \mid y, \theta}\left[\nabla_{\theta} \log \operatorname{Pr}\left(y_{t}, u_{t} \mid u_{t-1}, \theta\right)\right]
\end{aligned}
$$

Unbiased gradient estimator:

$$
\nabla_{\theta} \widehat{\log \operatorname{Pr}(y \mid \theta)=\operatorname{Pr}(\mathcal{S})^{-1} \cdot \sum_{t \in \mathcal{S}} \underbrace{}_{\substack{\text { Requires message } \\
\mathbb{E}_{u \mid y, \theta}}}\left[\nabla_{\theta} \log \operatorname{Pr}\left(y_{t}, u_{t} \mid u_{t-1}, \theta\right)\right]} \text { passing over full } \begin{aligned}
& \text { sequence } \bigcirc(|T|)
\end{aligned}
$$

## Buffering for approximate unbiasedness


"Buffered" gradient estimator:

$$
\begin{aligned}
& \nabla_{\theta}\widetilde{\log \operatorname{Pr}(y} \mid \theta)=\operatorname{Pr}(\mathcal{S})^{-1} \cdot \sum_{t \in \mathcal{S}} \\
& \underbrace{}_{\begin{array}{c}
\text { Computation } \mathcal{O} \\
\mathbb{E}_{u \mid y_{S^{*}, \theta}}
\end{array}}\left[\nabla_{\theta} \log \operatorname{Pr}\left(y_{t}, u_{t} \mid u_{t-1}, \theta\right)\right]
\end{aligned}
$$

## Error analysis

exact posterior $\quad \gamma(u)=\operatorname{Pr}\left(u \mid y_{\mathcal{T}}, \theta\right)$ approx posterior $\widetilde{\gamma}(u)=\operatorname{Pr}\left(u \mid y_{\mathcal{S}^{*}}, \theta\right)$

Theorem 1. Let $\epsilon_{1}=\max \left\{\mathcal{W}_{1}\left(\gamma_{-B}, \tilde{\gamma}_{-B}\right), \mathcal{W}_{1}\left(\gamma_{S+B}, \tilde{\gamma}_{S+B}\right)\right\}$. 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

$$
\left\|\mathbb{E}_{\gamma}\left[\nabla_{\theta} \log \operatorname{Pr}\left(y_{\mathcal{S}}, u_{\mathcal{S}} \mid \theta\right)\right]-\mathbb{E}_{\tilde{\gamma}}\left[\nabla_{\theta} \log \operatorname{Pr}\left(y_{\mathcal{S}}, u_{\mathcal{S}} \mid \theta\right)\right]\right\|_{2} \leq
$$

$$
4 L_{U} \cdot \frac{1-L^{S}}{1-L} \cdot L^{B} \cdot \epsilon_{1}
$$

## Geometrically in B



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

## 



## Canine iEEG analysis



## 16 channels, 90 seizures

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



## 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)

Stochastic gradient.


$$
\theta_{n+1}=\theta_{n}-\gamma_{n} \cdot \hat{g}\left(\theta_{n}\right)
$$



## Backpropagation through time (BPTT)

Stochastic gradient:

$$
\hat{g}(\theta)=\sum_{k=0}^{\infty} \frac{d L_{t}}{d h_{t-k}} \cdot \frac{\partial h_{t-k}}{\partial \theta}
$$

## SGD using BPTT:

$$
\theta_{n+1}=\theta_{n}-\gamma_{n} \cdot \hat{g}\left(\theta_{n}\right)
$$

O(T) computation time and memory

## Truncated backpropagation through time (TBPTT)

Stochastic gradient:
$\hat{g}_{K}(\theta)=\sum_{k=0}^{K} \frac{d L_{t}}{d h_{t-k}} \cdot \frac{\partial h_{t-k}}{\partial \theta}$

SGD using TBPTT:

$$
\theta_{n+1}=\theta_{n}-\gamma_{n} \cdot \hat{g}_{K}\left(\theta_{n}\right)
$$



Truncate after K steps of BPTT

Biased!
$\mathrm{O}(\mathrm{K})$ 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

Stochastic gradient:

$$
\hat{g}(\theta)=\sum_{k=0}^{\infty} \frac{d L_{t}}{d h_{t-k}} \cdot \frac{\partial h_{t-k}}{\partial \theta} \quad \frac{\partial L_{t}}{\partial h_{t-k}}=\frac{\partial L_{t}}{\partial h_{t}} \prod_{r=1}^{k} \underbrace{\frac{\partial h_{t-r+1}}{\partial h_{t-r}}}_{\text {key term }}
$$

Existing Work: Restrict RNN weights such that

$$
\left\|\frac{\partial h_{t-r+1}}{\partial h_{t-r}}\right\| \leq \lambda<1 \longrightarrow\left\|\frac{d L_{t}}{d h_{t-k-1}}\right\| \leq \lambda \cdot\left\|\frac{d L_{t}}{d h_{t-k}}\right\|
$$

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

## Gradient decay assumptions

Previously:

$$
\left\|\frac{d L_{t}}{d h_{t-k-1}}\right\| \leq \lambda \cdot\left\|\frac{d L_{t}}{d h_{t-k}}\right\|
$$

 vanishing memory

$$
\operatorname{lag} k
$$

Implies uniform bound on $\hat{g}-\hat{g}_{K}$

Our relaxed assumption:
$\mathbb{E}_{t}\left\|\frac{d L_{t}}{d h_{t-k-1}}\right\| \leq \beta \cdot \mathbb{E}_{t}\left\|\frac{d L_{t}}{d h_{t-k}}\right\|$ for all $k \geq \tau$


Implies bound on gradient bias... will see

## Example: LSTM on language modeling task

 Penn Treebank dataset

Decay on average, but individual traces do not

## Error analysis: <br> Bound on relative bias

Assuming:

- Our gradient decay bound holds: $\mathbb{E}_{t}\left\|\frac{d L_{t}}{d h_{t-k-1}}\right\| \leq \beta \cdot \mathbb{E}_{t}\left\|\frac{d L_{t}}{d h_{t-k}}\right\|$ for all $k \geq \tau$
- $\partial H / \partial \theta$ is bounded

Then TBPTT has bounded relative bias:

$$
\delta=\frac{\left\|\mathbb{E}\left[\hat{g}_{K}(\theta)\right]-g(\theta)\right\|}{\|g(\theta)\|} \leq \mathcal{O ( \beta ^ { K - \tau } )}
$$

Relative
bias

## Error analysis: <br> 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:


## Example: LSTM on language modeling task

 Penn Treebank dataset

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

## Adaptive TBPTT algorithm

$\mathbb{E}_{t}\left\|\frac{d L_{t}}{d h_{t-k-1}}\right\| \leq \beta \cdot \mathbb{E}_{t}\left\|\frac{d L_{t}}{d h_{t-k}}\right\|$ for all $k \geq \tau$



## 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 |  |  |
| :--- | ---: | ---: |
| K | 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 | $161.5(0.5)$ | $161.2(0.3)$ |
| $\delta=0.9$ | $100.1(0.5)$ | $99.0(0.5)$ |
| $\delta=0.5$ | $90.1(0.4)$ | $89.5(0.3)$ |
| $\delta=0.1$ | $88.1(0.2)$ | $\mathbf{8 7 . 2}(0.2)$ |


| Wikitext-2 |  |  |
| :--- | :--- | ---: |
| K | 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 | $129.6(1.4)$ | $124.0(2.2)$ |
| $\delta=0.9$ | $130.0(1.3)$ | $124.1(2.2)$ |
| $\delta=0.5$ | $127.2(0.7)$ | $121.7(0.6)$ |
| $\delta=0.1$ | $127.5(0.6)$ | $121.9(1.2)$ |




## Summary

1. Deep learning offers tremendous opportunities for modeling complex dynamics, but problems much vaster than prediction + large corpora
2. Scaling learning is possible, but have to think carefully about broken dependencies (bias)


Modeling sparsely sampled nonstationary time series

Handling bias in
stochastic gradients
of sequential data


## Credit for the hard work...



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