

Advancing Causal Discovery in Spatio-Temporal Systems: Methods and Applications

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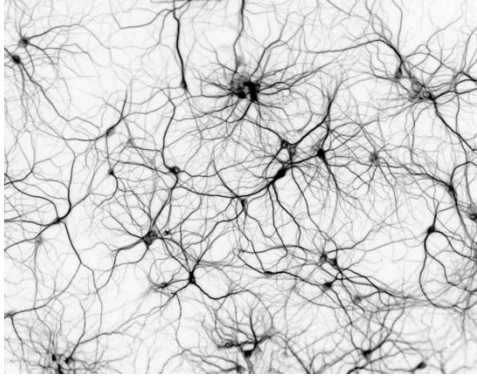




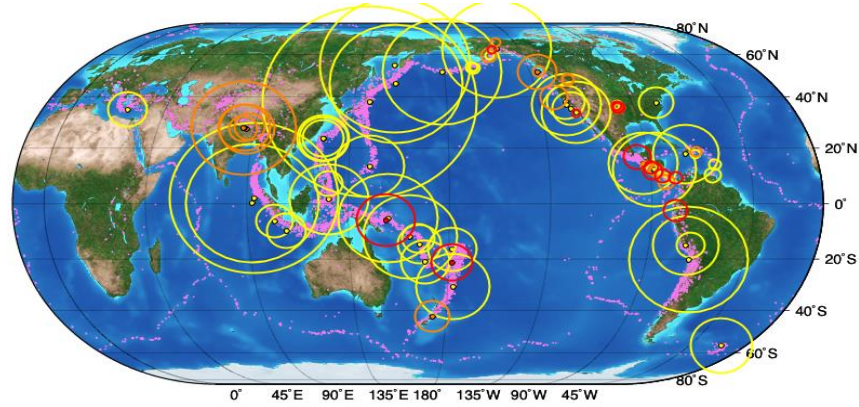
Roadmap

- Basic setup
- Granger network estimation
 - Structural constraints
 - Uncertainty quantification
- General: continuous space
- Other approaches

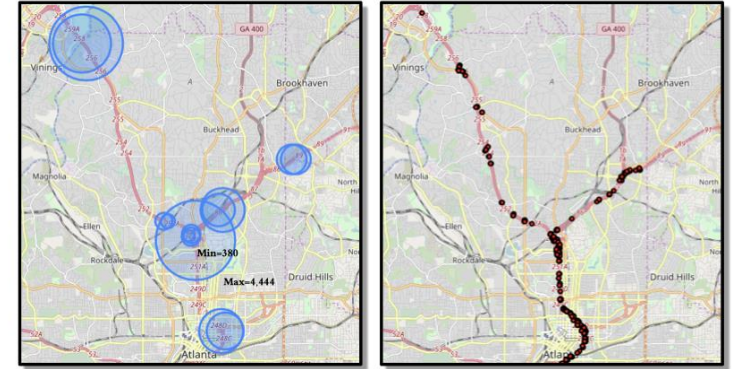
Spatial-temporal data



Neuronal networks

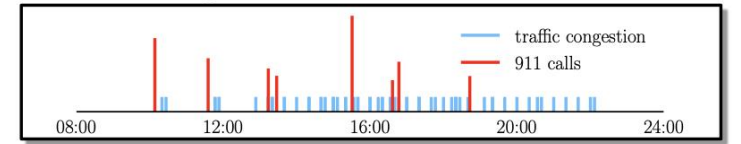


Seismic activities



Traffic congestions

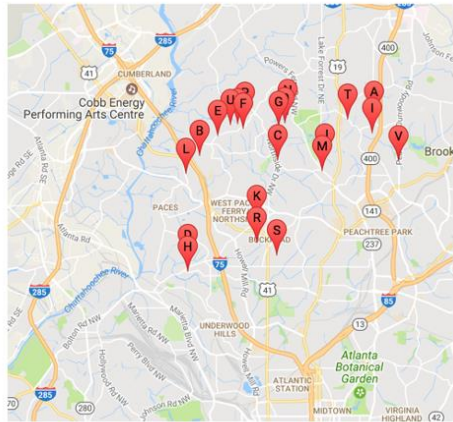
911 calls-for-service



An events series in one day

Traffic incidents

22 cases of Buckhead burglary



Crime activities



COVID spread



40 access hubs

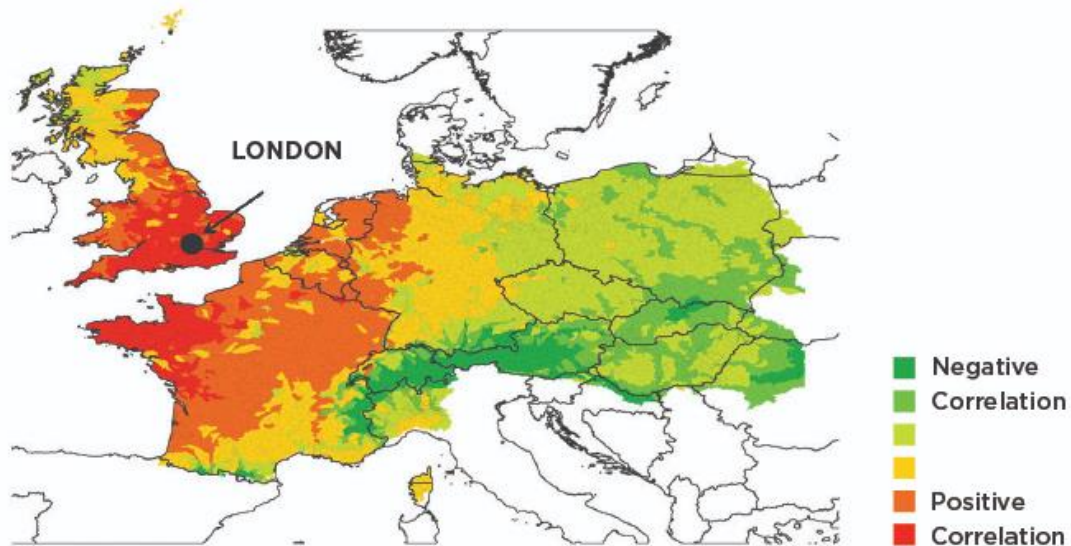
21 local hubs

3 gateway hubs

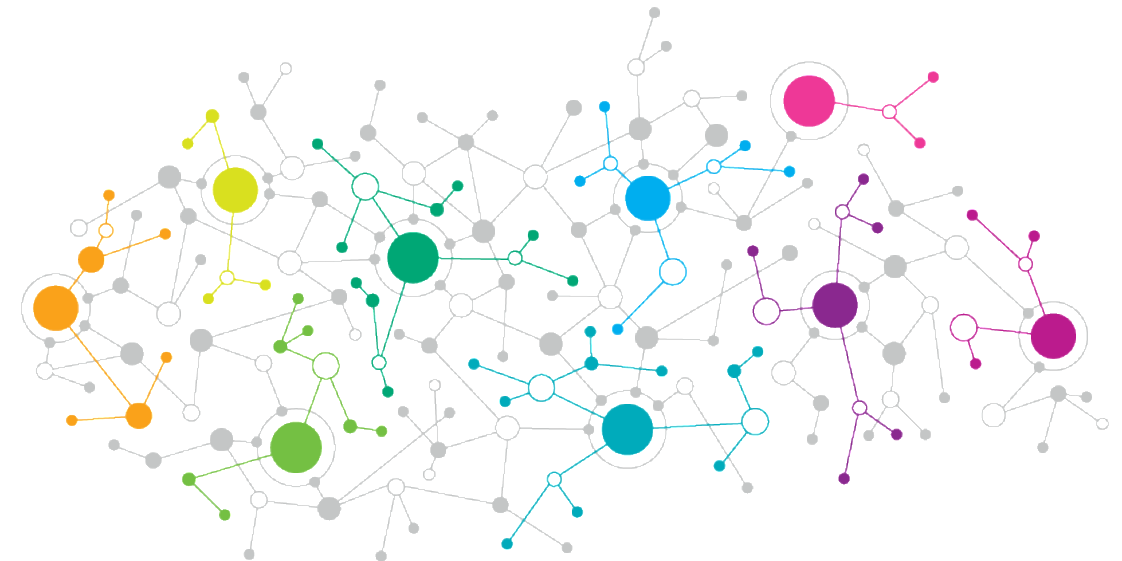
Supply chain networks

Spatial correlation as network connectivity

- Traditional spatial correlation
- Network influence



Underlying space is Euclidean

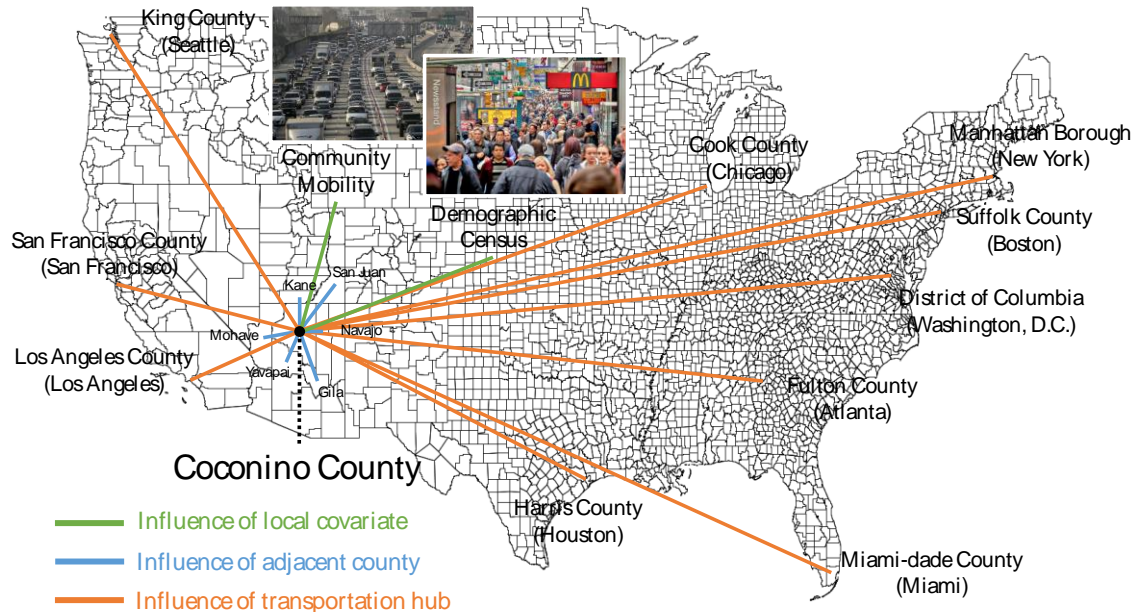


Underlying space is a graph

COVID-19 cases over US counties

- **Influence:**

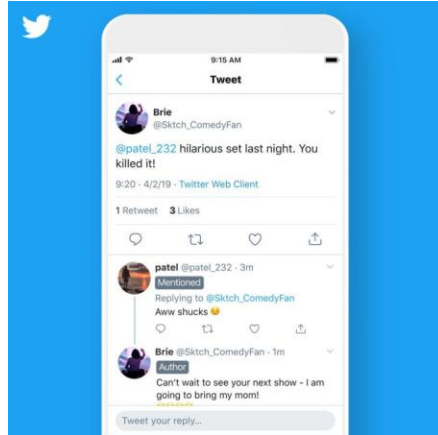
- nearby locations, major cities, and transportation hubs have a larger influence
- Influence may change over time



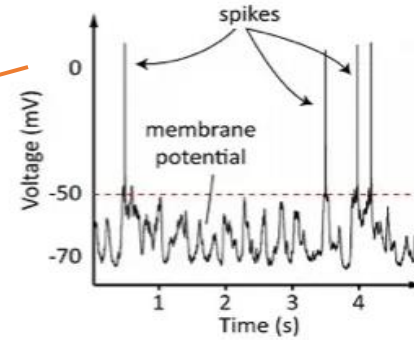
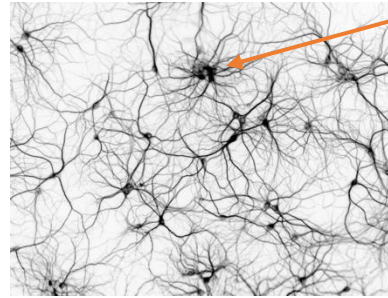
“High-resolution spatio-temporal model for county-level COVID-19 activity in the U.S.” Zhu, Bukharin, Xie, Santillana, Yang, X. *ACM Transactions on Management Information Systems (TMIS)*, 2021.

“Early detection of COVID-19 hotspots using spatio-temporal data.” Zhu, Bukharin, Xie, Yamin, Yang, Keskinocak, and X. *IEEE Journal Selected Topics in Signal Processing (JSTSP) 2022, ICML Time Series Workshop (Best Paper Award, 2nd Place) 2021.*

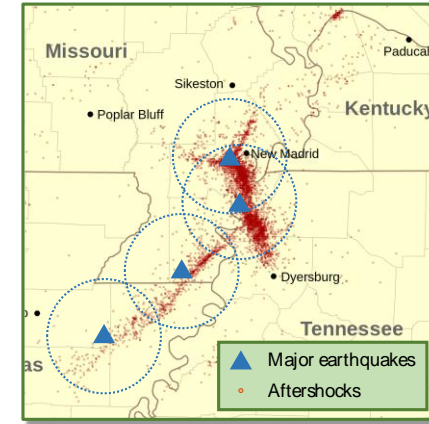
Discrete event data (time, marks)



Tweets



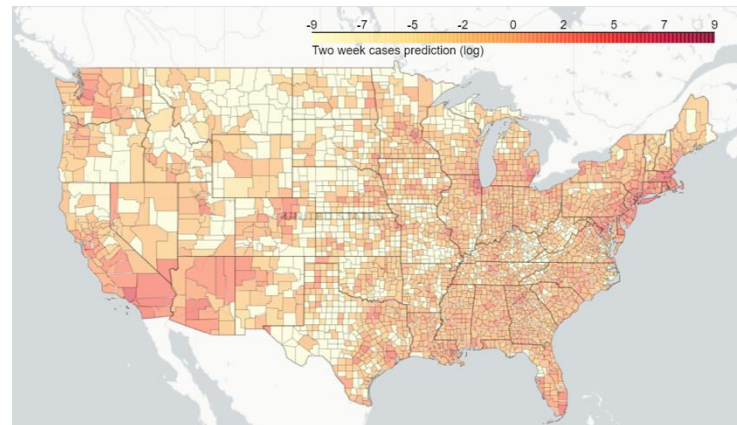
Neural spike trains



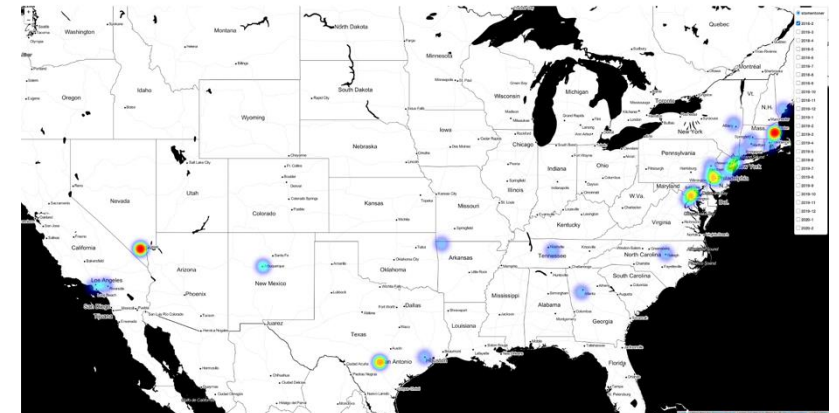
Earthquake catalog



Police reports



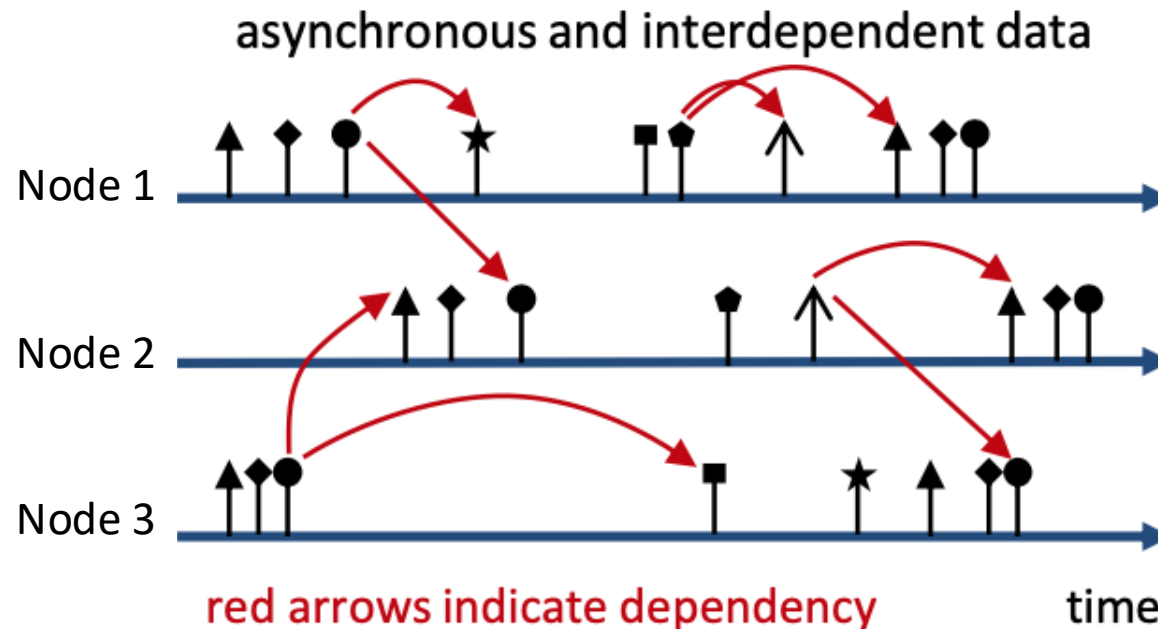
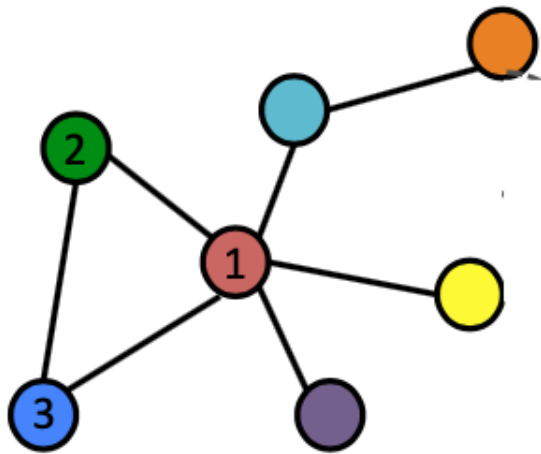
Daily #case at US counties



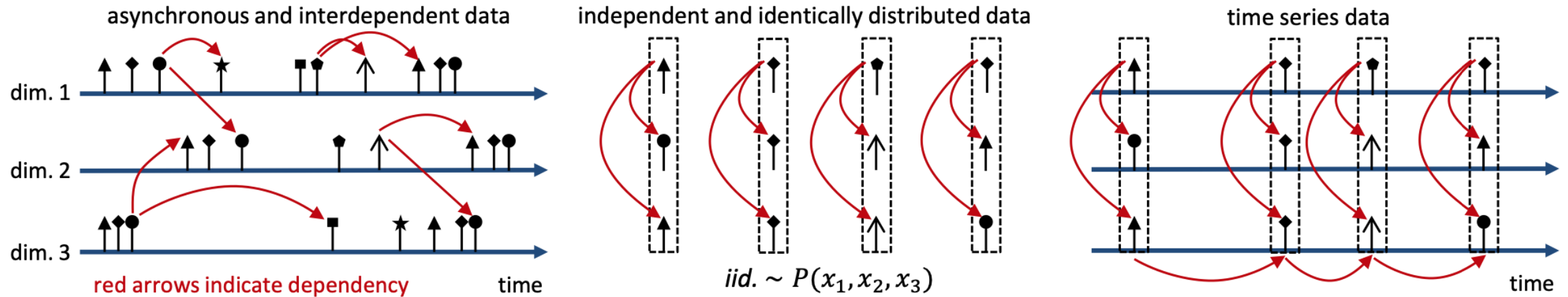
Demand over networks

Discrete events data: “Dots”

- Discrete events data: A sequence of (time, marks)
- Asynchronously occur over time and mark space
- Marks contain additional information: location, category, description-- can be high-dimensional



Different from i.i.d. data and classic time-series



- Asynchronously recorded data
- Interrelated over space and time
- Timing of data point carries information

Influence

- “Triggering” or “inhibition effect” of an event over **space and time**
- Granger causality



Time passes



Zhu, Li, Peng, X. Imitation learning of spatio-temporal point processes.
IEEE-TKDE, 2022. NeurIPS AI for Earth Sciences Workshop, 2020.

Crime data

- “Broken window effect”

Once a neighborhood has a crime incident, similar crime is more likely to happen.

- “Buckhead burglary” in Atlanta, 2017

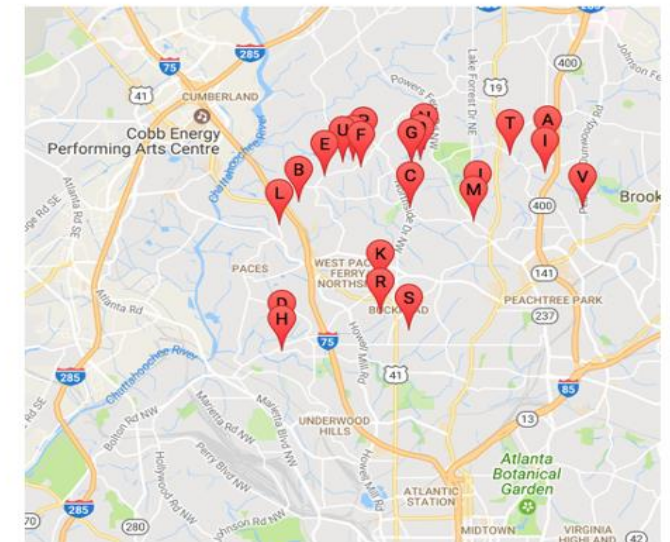
22 cases committed by a serial offender.

(Zhu, and X., *Annals of Applied Statistics*, 2022
Presented at JSM “Best of AOAS, 2021.”)

(Collaboration with *Atlanta Police Department*.)

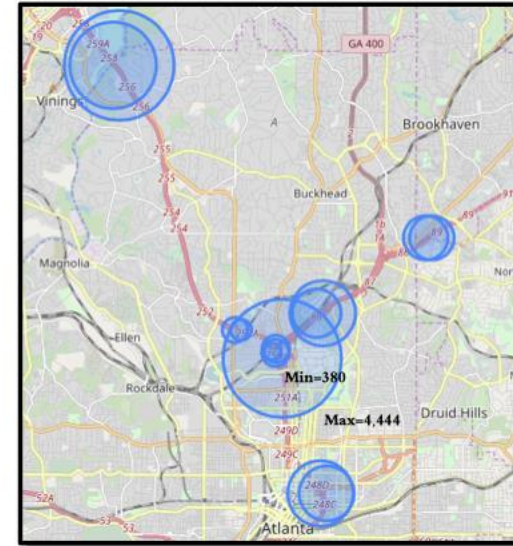


22 cases of Buckhead burglary

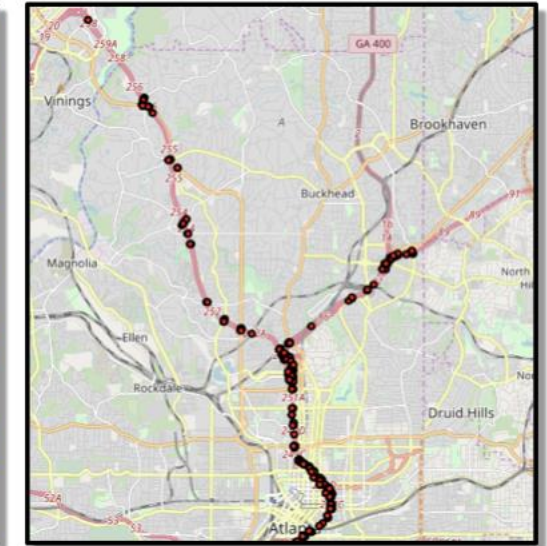


Traffic data

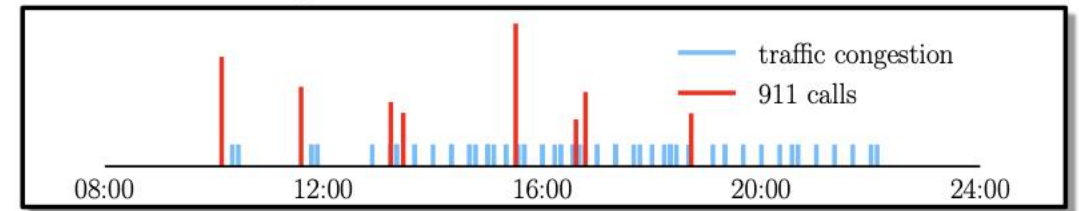
- Traffic congestion events
- Two triggering mechanisms:
 - Traffic congestion triggers future congestion
 - Traffic incidents trigger congestion



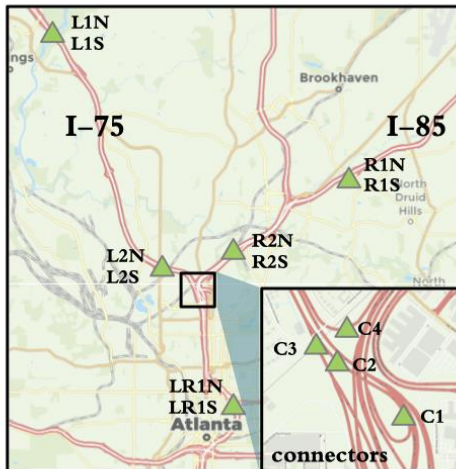
Traffic congestions



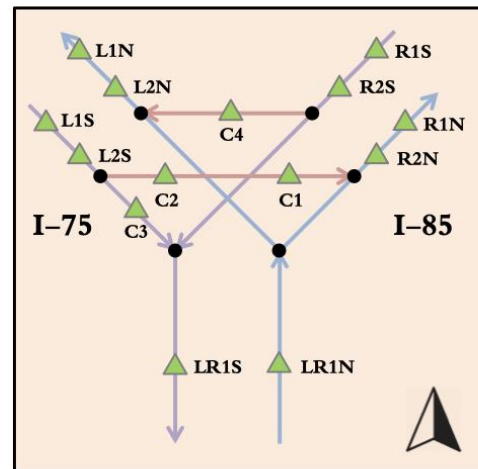
911 calls-for-service



An events series in one day



Traffic sensor map in Atlanta

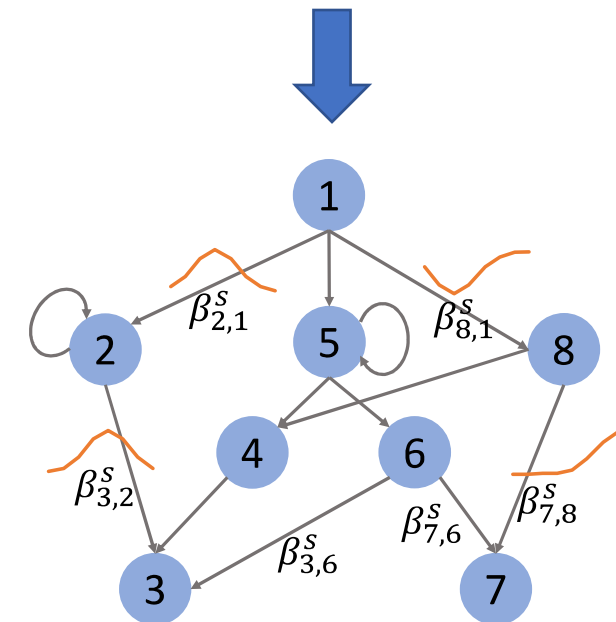
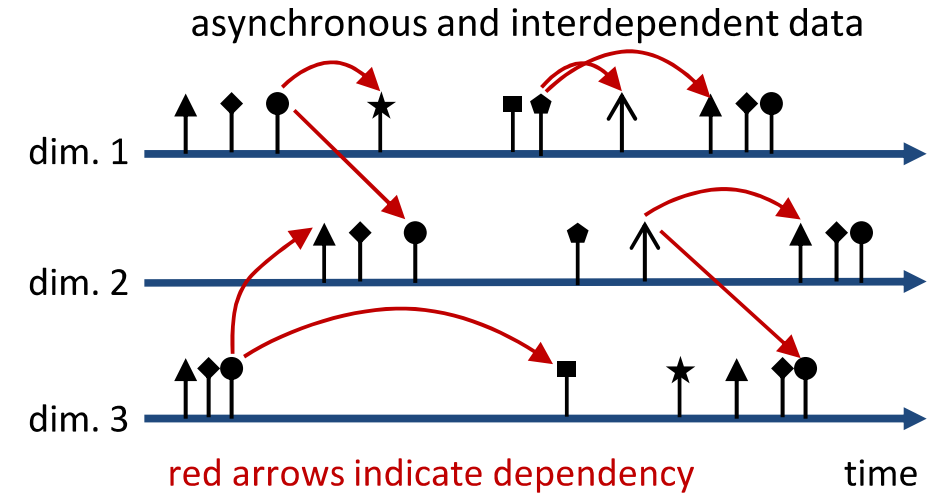


Traffic network

Spatio-temporal point processes with attention for traffic congestion event modeling. Zhu, Ding, Van Hentenryck, and X. *IEEE Transactions on Intelligent Transportation Systems*, 2022.

Goals

- Use discrete event data, recover spatio-temporal influence: **Granger causality**
 - **Interpretation:** Understanding underlying influence network and temporal influence
 - **Prediction:** predicting the chance of a future event
 - **Monitoring:** detecting changes – anomalies and novelty
 - **Decision:** intervention, optimization



How to model influence?

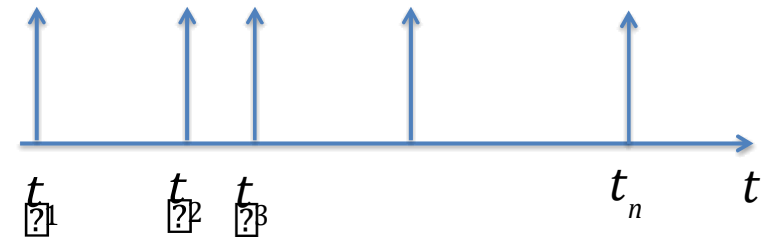
- **Hawkes processes** (Hawkes 1971)
- Point-process: a sequence of random events at times $\{t_1, t_2, \dots\}$

$$\lambda(t)dt = P\{\text{event in } [t, t + dt) | H_t\}$$

$$\lambda(t|H^t) = \lim_{\Delta t \rightarrow 0} \frac{E[N(t + \Delta t) | H_t]}{\Delta t}$$

Hawkes, Alan G. "Spectra of some self-exciting and mutually exciting point processes." *Biometrika* 1971.

history

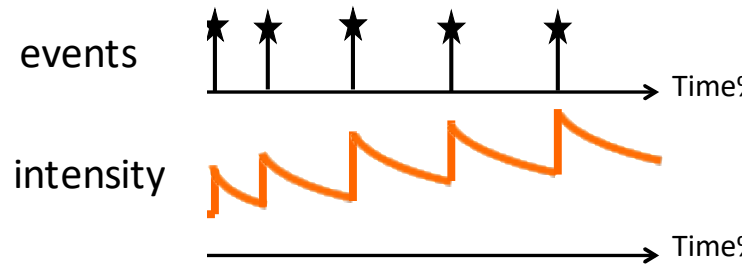


Alan Hawkes

Common point processes

- Poisson process: $\lambda(t) = \mu(t)$ deterministic
- Hawkes process: conditional intensity depends on history

$$\lambda(t) = \mu(t) + \text{influence from past}$$



- Self-correcting process

$$\lambda(t) = \mu(t) - \text{influence from past}$$

Hawkes process

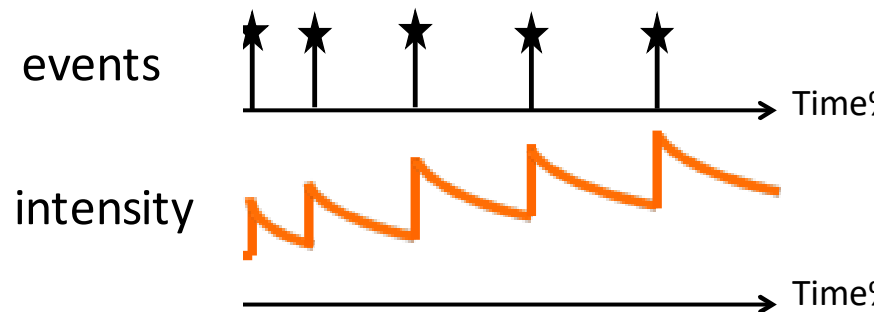
- Conditional intensity function

$$\lambda(t) = \mu(t) + \alpha \sum_{t_k < t} \phi(t - t_k)$$

Baseline intensity

Magnitude of influence

Influence kernel function



Hawkes process over networks

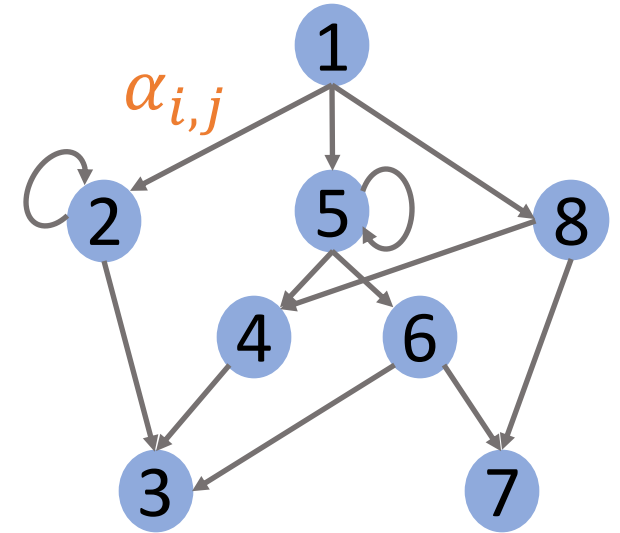
- Events on K nodes $(t_1, u_1), (t_2, u_2), \dots$

$$\lambda_i(t) = \mu_i(t) + \sum_{t_k < t} \alpha_{i,u_k} \phi(t - t_k)$$

Baseline intensity
at node i

Influence between
node α_{ij}

Temporal influence
kernel function



- Commonly assumed: Exponential decay influence

$$\phi(t) = \beta e^{-\beta t}, t \geq 0 \text{ (Markovian)}$$

Hawkes processes literature

- Single and multi-dimensional Hawkes processes

(Alan Hawkes 1971) (review, Reinhart 2018)

- Continuous spatio-temporal modeling with diffusion kernel (ETAS)

(Ogata 1999) (Zhu et al. 2020)

- Asymptotic convergence results of linear and non-linear processes

(Bacry, Dayri, Muzy 2012) (L. Zhu 2013) (L. Zhu 2015)

- Estimate network interactions, assuming known influence function:

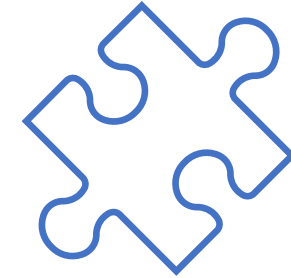
(Stomakhin, Short, Bertozzi 2011), (Myers, Leskovec, 2014), (Rodriguez et al. 2011) (Yang, Zha 2013) (Hall, Willett 2016) (Chen et al. 2017) (Li et al. 2018) (Yuan et al. 2019)

- Causal inference and testing for purely temporal process

(Chen, Witten, Shojaie 2017) (Xu, Farajtabar, Zha, 2016) (Achab et al. 2017)

- Bayesian model

(Rasmussen 2013) (Linderman, Wang Blei 2017) (Donnet, Rivoriard, Rosseau 2020)



- Uncertainty quantitation
- Structural assumptions
- General influence kernel



Roadmap

- Basic setup
- Granger network estimation
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- Other approaches

Maximum likelihood

- Parameters are solved by maximum likelihood

$$\max_{\theta} \ell(\theta)$$

- Property of the optimization problem
 - When $\theta = \{\mu, \alpha_{ij}\}$, and β is fixed, it can be shown that $\ell(\theta)$ is **convex** in θ
 - When $\theta = \{\mu, \alpha_{ij}, \beta\}$, problem is **non-convex**
 - When influence \neq exponential decay, may not have closed-form integration

Maximum likelihood estimate for α_i

- Define coefficient for i -th node as α_i

$$\max_A \ell(A) = \sum_{i=1}^K \ell_i(\alpha_i)$$

Decoupled in nodes, enable decentralized estimation

- Log-likelihood for the i -th node

$$\ell_i(\alpha_i) = - \int_0^T \lambda_i(t) dt + \int_0^T \log(\lambda_i(t)) dN_t^i$$

- Assuming known influence function $\phi(t)$, $\ell_i(\alpha_i)$ convex function in α_i
- Can be solved efficiently to global solution (e.g., gradient descent)

Likelihood function for Hawkes networks

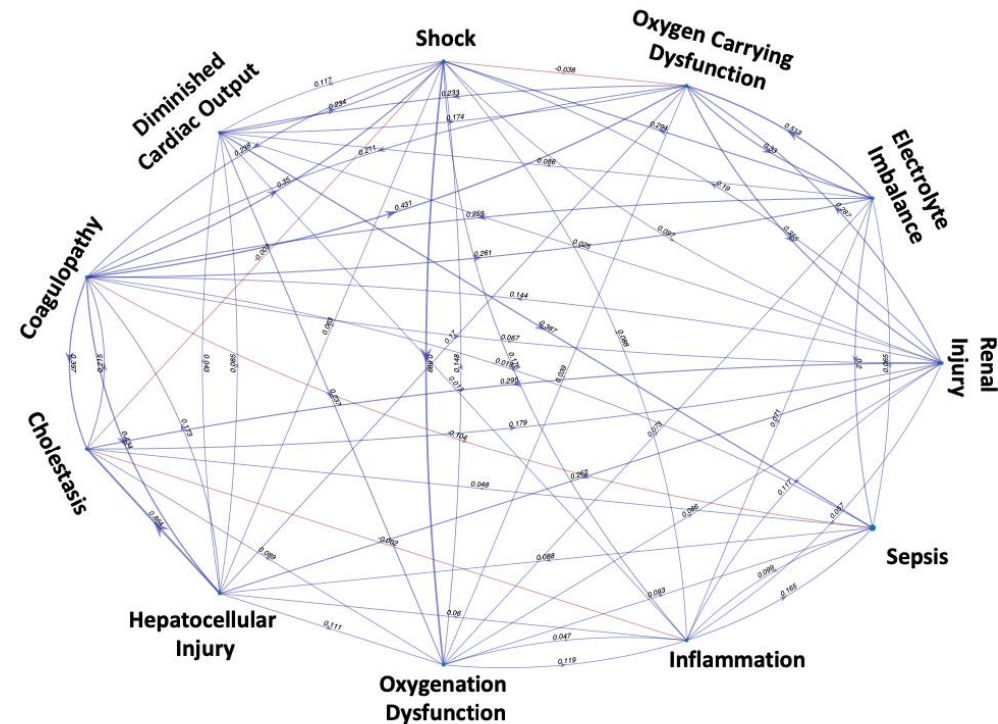
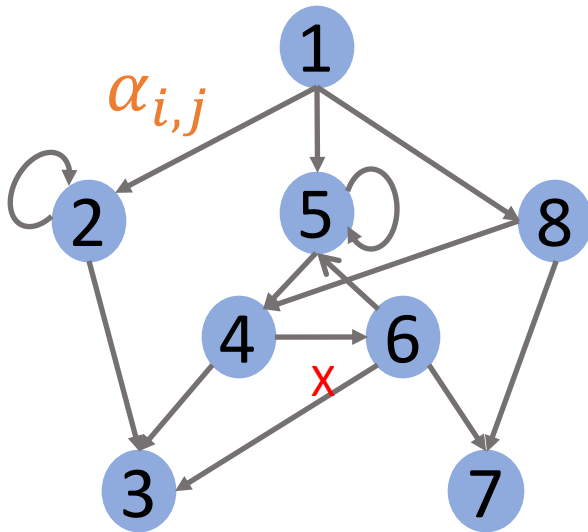
- Log-likelihood function for Hawkes network, exponential influence
- Data $(t_i, u_i), i = 1, \dots, n$

$$\begin{aligned} \ell(\theta) = & \sum_{i=1}^n \log \left[\mu_{u_i} + \sum_{t_j < t_i} \alpha_{u_i, u_j} \beta e^{-\beta(t_i - t_j)} \right] - \sum_{j=1}^K \mu_j t \\ & - \sum_{j=1}^K \sum_{t_i < t} \alpha_{u_i, j} [1 - e^{-\beta(t - t_i)}] \end{aligned}$$

- Parameters $\theta = (A, \mu)$ are solved by maximum likelihood: $\max_{\theta} \ell(\theta)$
- Convex

Granger causality: Real-time sepsis prediction

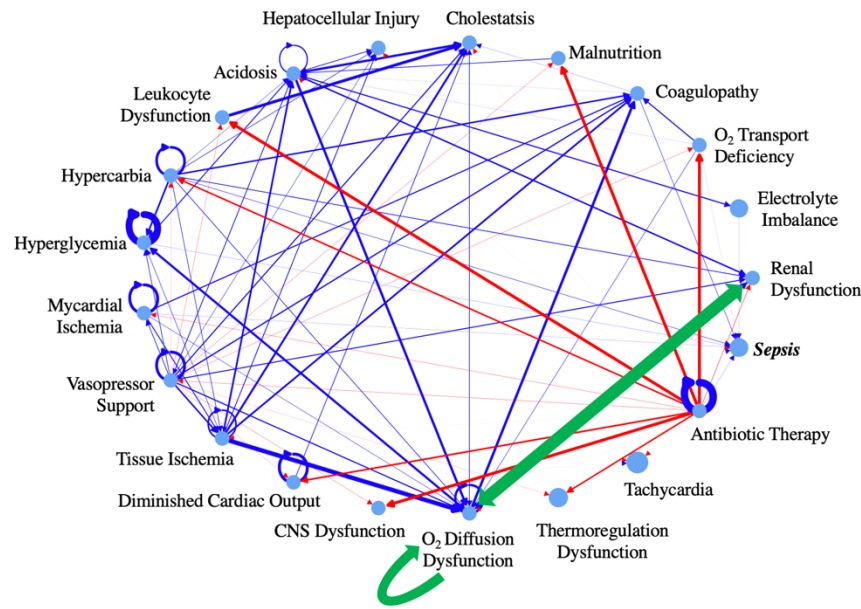
- Add Directed Acyclic Graph (DAG) constraints to remove cycles



- Granger causal chain discovery for sepsis-associated derangements via multivariate Hawkes processes. Wei, Xie, Josef, Kamaleswaran. KDD 2023.
- Causal graph discovery from self and mutually exciting time series. Wei, Xie, Josef, and Kamaleswaran. IEEE Selected Areas in Information Theory (JSAIT). Vol. 4, pp. 747-761. 2023.

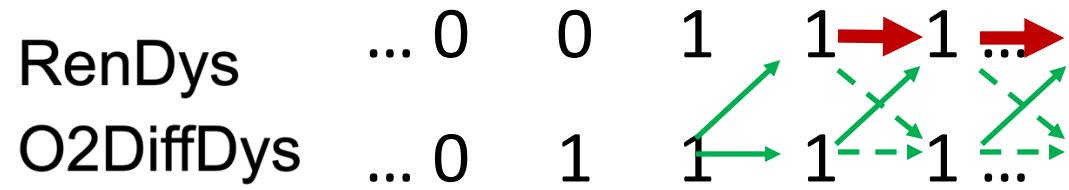
Why need structural assumption

- Our first attempt on Granger causal graph discovery [2] returns **cyclic** patterns, and therefore less reasonable causal interpretations



Ambiguity on the cause

Miss natural & important info



0: no event;
1: event

DAG-encouraging regularization

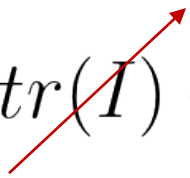
Graph adjacency matrix A constant d

Motivation

[Zheng et al. (2018)]

$$tr(e^A) = tr(I) + tr(A) + \frac{1}{2}tr(A^2) + \dots$$

Length-1 cycles **Length-2 cycles** ...



DAG-encouraging regularization

Graph adjacency matrix A

constant d

Motivation

[Zheng et al. (2018)]

$$tr(e^A) = tr(I) + tr(A) + \frac{1}{2}tr(A^2) + \dots$$



Linear relaxation
(convex!)

[No penalty on length-1 cycles]

$$\alpha_{12} + \alpha_{21} \leq \delta_1 \quad \dots$$

$$\alpha_{23} + \alpha_{32} \leq \delta_2$$

... ..

DAG-encouraging regularization

Graph adjacency matrix A constant d

Motivation
[Zheng et al. (2018)]

$$tr(e^A) = tr(I) + tr(A) + \frac{1}{2}tr(A^2) + \dots$$

Length-1 cycles
Length-2 cycles
...



Linear relaxation
(convex!)



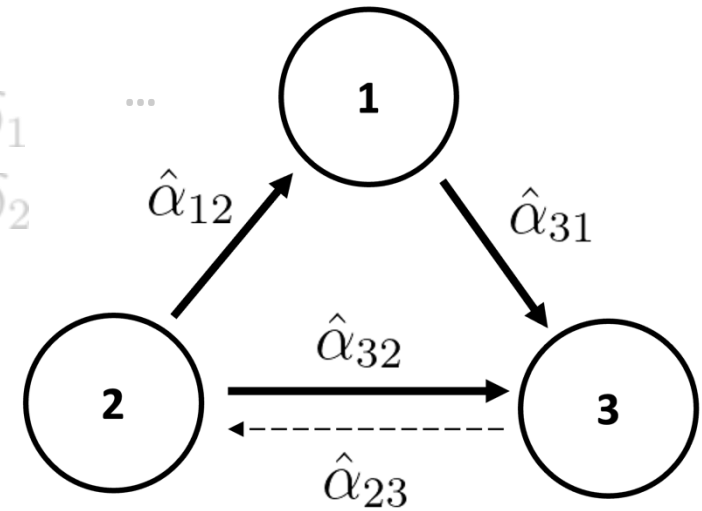
Proposed data-adaptive
modification [3]

[No penalty on length-1 cycles]

$$\alpha_{12} + \alpha_{21} \leq \delta_1$$

$$\alpha_{23} + \alpha_{32} \leq \delta_2$$

...



Step 1: Rough estimation $\hat{A} = (\hat{\alpha}_{ij})$

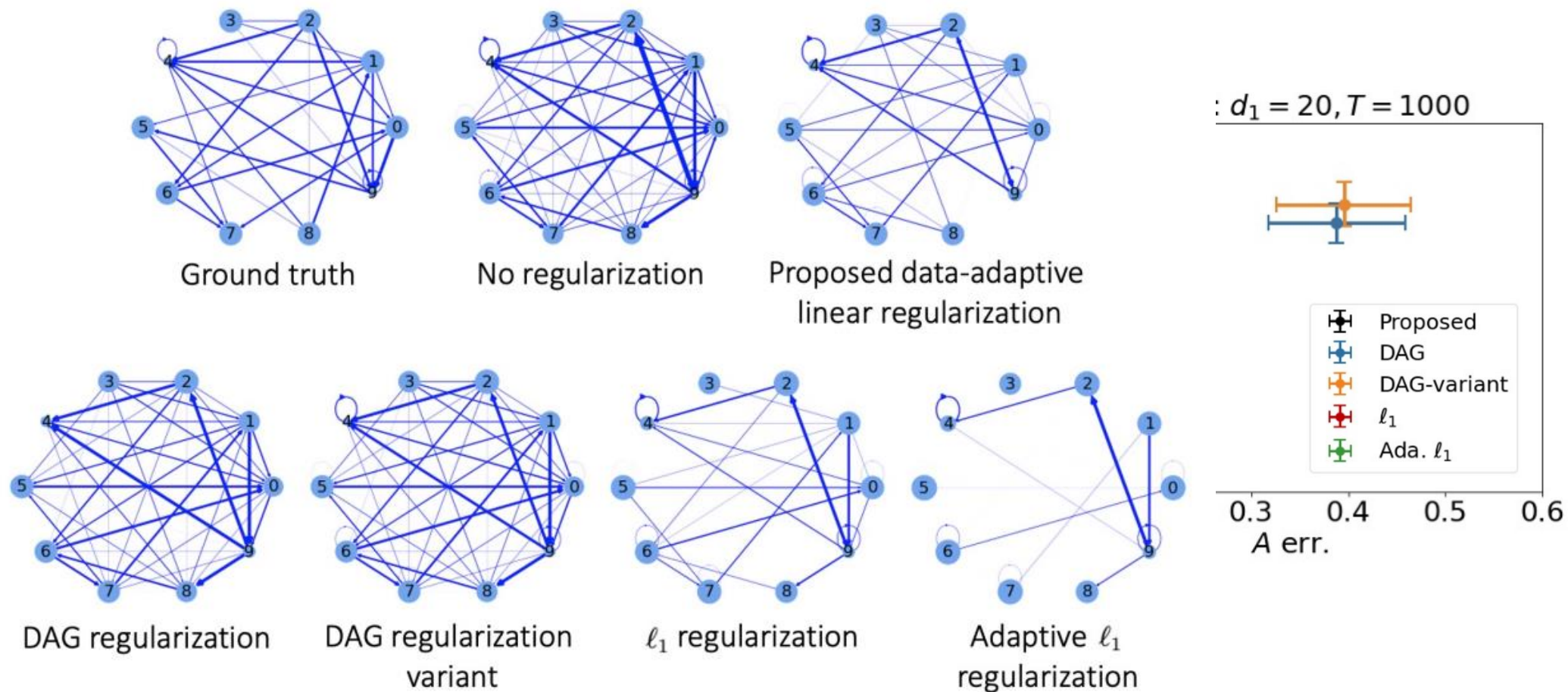
Step 2: Data-adaptive linear DAG-encouraging constraints

$$\alpha_{23} + \alpha_{32} \leq \hat{\alpha}_{32} \quad \& \quad \alpha_{12} + \alpha_{23} + \alpha_{31} \leq \hat{\alpha}_{12} + \hat{\alpha}_{31}$$

Simulation

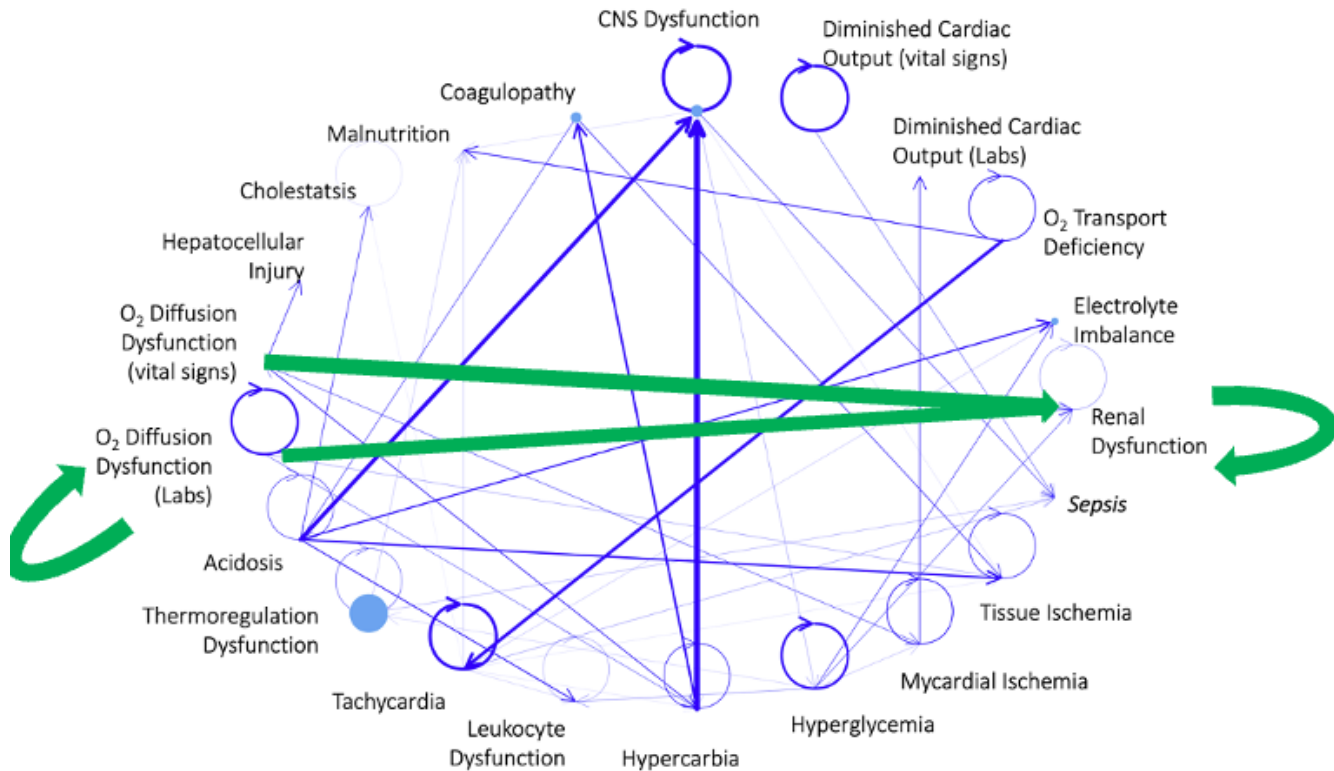
Regularization	None	Proposed	DAG	DAG-Variant	ℓ_1	Ada. ℓ_1
A err.	.3874	.2094	.3541	.2949	.2501	.3022
ν err.	.1175	.0775	.0895	.0841	.0884	.1251
$h(A_0)$.1223	.0308	.0337	.0242	.0274	.0232
SHD	41	25	32	34	41	29

- DAG regularization removes suspicious links and helps parameter recovery



Real-data experiment

- Resulting Causal DAG



RenDys ... 0 0 1 → 1 → 1 ...
 O2DiffDys ... 0 1 → 1 → 1 → 1 ...

0: no event;
1: event



Roadmap

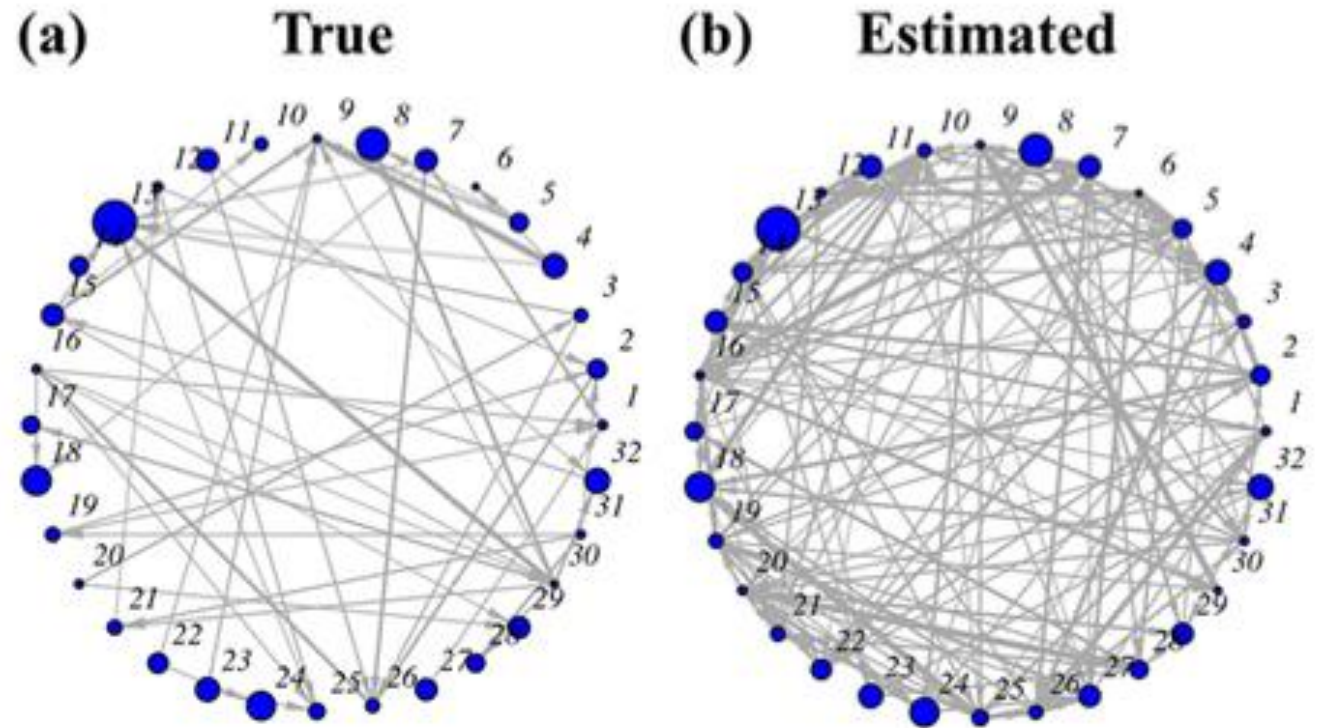
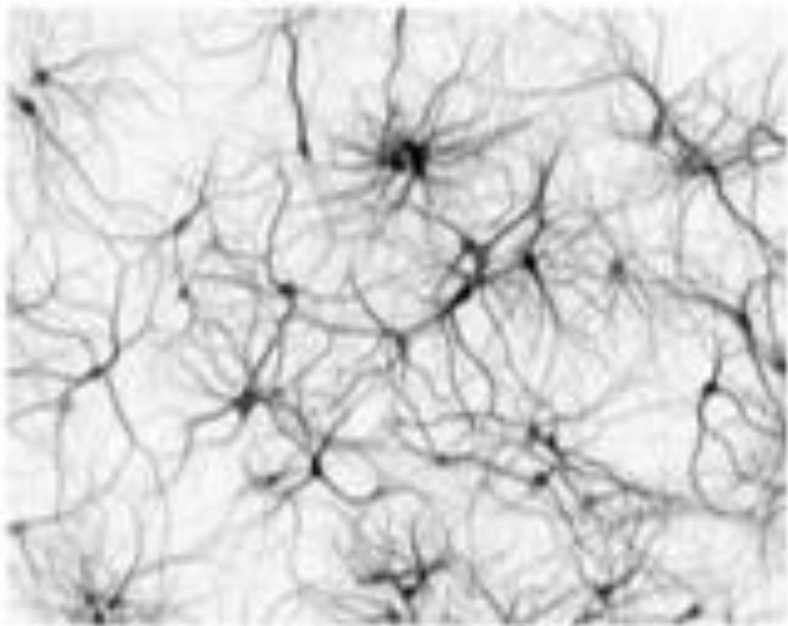
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Why need uncertainty quantification?

- Causal inference: with statistical significance there exists an edge?

Granger causality graph $G(U, E)$, then $j \rightarrow i \notin E$, iff $\alpha_{ij} = 0$.

Example: Recovery neuronal networks



“Uncertainty quantification for inferring Hawkes networks.” Wang, Xie, Cuzzo, Mak, X. *NeurIPS* 2020.

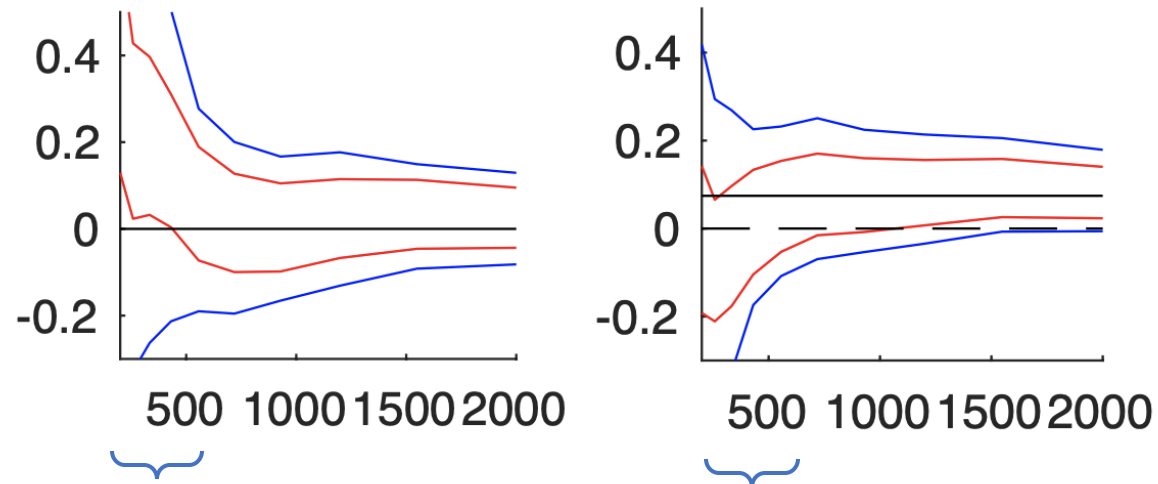
Asymptotic properties of MLE

- (Rathbun 1996) MLE is consistent with asymptotically normal as $T \rightarrow \infty$

$$\sqrt{T}(\hat{\alpha}_i - \alpha_i) \rightarrow N(0, I_i^{*-1})$$

- How good is asymptotic?

I_i^* : Fisher information



Red: asymptotic CI

Blue: Non-asymptotic CI

Can we do better than asymptotic?

- Challenge:

Continuous time non-i.i.d. data

$$\lambda(t) = \mu(t) + \text{influence from past}$$

Standard Hoeffding or Bernstein type of concentration bound does not apply

- New approach:

- Recent advances concentration inequality for continuous-time martingale
- Develop more precise general **sequential confidence set** adaptive to data

“Time-uniform Chernoff bounds via nonnegative supermartingales”,
Howard et al., *Prob. Surveys* 2020.

UQ for estimating $\hat{\alpha}_{ij}$: Main idea

- Recall: Delta method (mean-value theorem)

$$S_i(\alpha_i) - S_i(\hat{\alpha}_i) = \underbrace{H_i(\alpha_i')}_{=0} (\alpha_i - \hat{\alpha}_i) \underbrace{\quad}_{\rightarrow TI_i^*}$$

$$\Rightarrow \alpha_i - \hat{\alpha}_i \approx \frac{1}{T} I_i^{*-1} S_i(\alpha_i)$$

score function is a continuous-time martingale

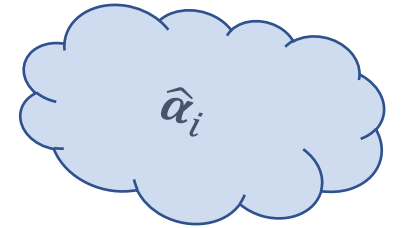
- Concentration bound for entries of $I_i^{*-1} S_i(\alpha_i) \in R^K$

Sequential confidence set

Theorem (Uncertain sets for each α_i)

For any α_i , $t \in [0, T]$, let $\hat{I}_i(\alpha_i, t)$ be estimator for the Fisher Information given data up to time t . Then

$$C_{i,\varepsilon} = \{\alpha_i \in R^K: g_k(\alpha_i) \leq \ln(2K/\varepsilon), k = 1, \dots, 2K\}$$



is a confidence set for α_i at level $1 - \varepsilon$.

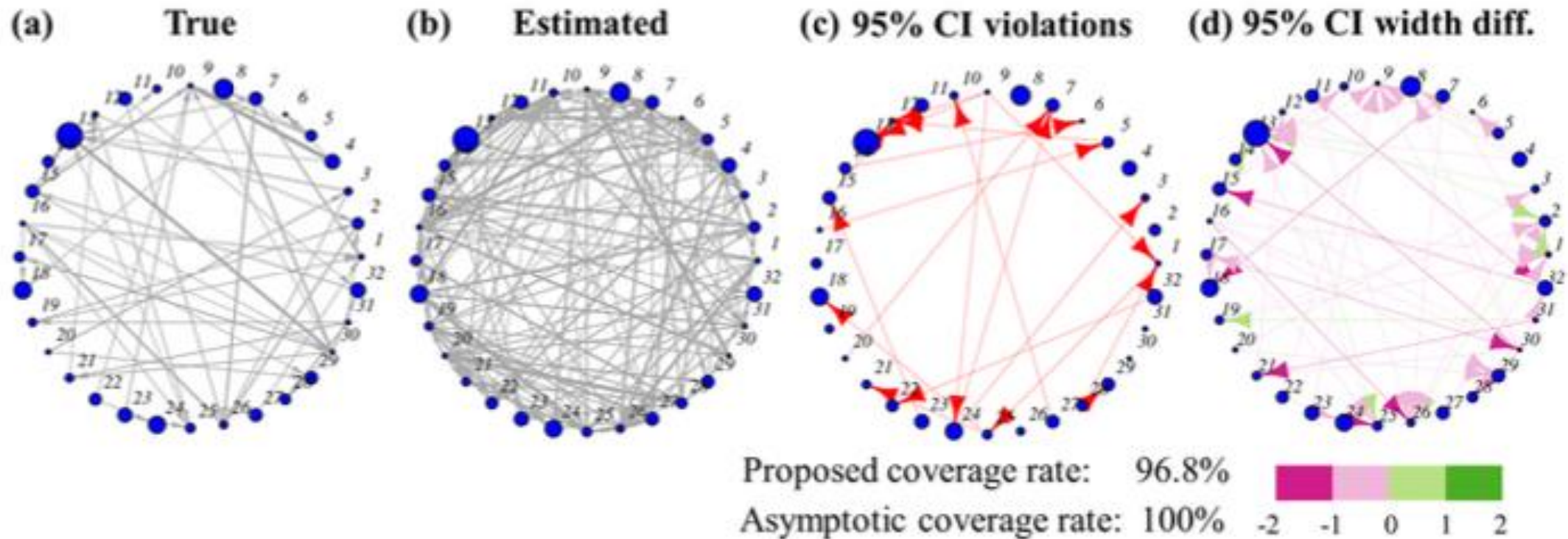
Corollary (Width of confidence interval, asymptotically optimal)

Width of $C_{i,\varepsilon}$ in the direction of $\alpha_{ij} \rightarrow 2\sqrt{2\ln(2K/\varepsilon)\sigma_{ij}^2/T}$.

$$g_k(\alpha_i) = \int_0^T \mathbf{z}_k^T(H_{t^-}, \alpha_i) dS_{i,t}(\alpha_i) - V_i(\mathbf{z}_k, \alpha_i), \quad \mathbf{z}_k(H_{t^-}, \alpha_i) \in \left\{ \pm \sqrt{\frac{2\ln(2K/\varepsilon)}{T\mathbf{e}_j^T \hat{I}_i^{-1}(\alpha_i, t)\mathbf{e}_j}}, j = 1, \dots, K \right\}$$

Intrinsic variance: $V_i(\mathbf{z}_k, \alpha_i) = \int_0^T (\lambda_i(t) \exp(\lambda_i^{-1}(t)\mathbf{z}^T \eta_i(t)) - \mathbf{z}^T \eta_i(t) - \lambda_i(t)) dt$

Results



- Asymptotic CI is over-covering
- Non-asymptotic CI achieves targeted coverage and has narrower bandwidth



Roadmap

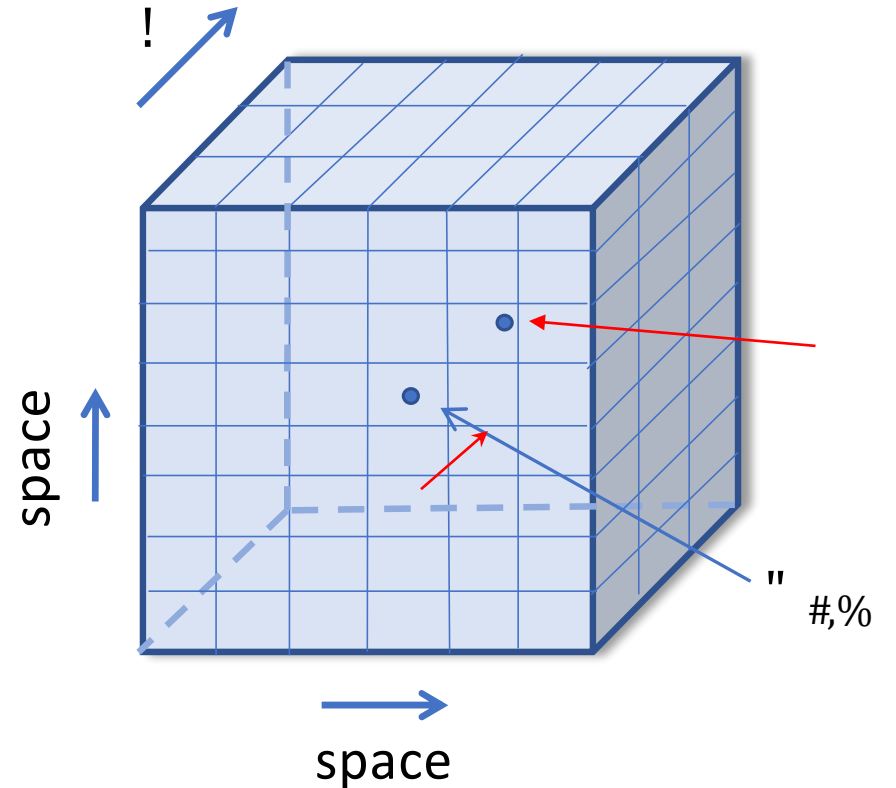
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General influence kernel: Continuous space, non-stationary

- Events $x_i = (t_i, u_i), u_i \in M$

$$\lambda(x) = \mu(x) + \sum_{x': t' < t} K(x, x')$$

Can we build general model for $K(x', x)$?



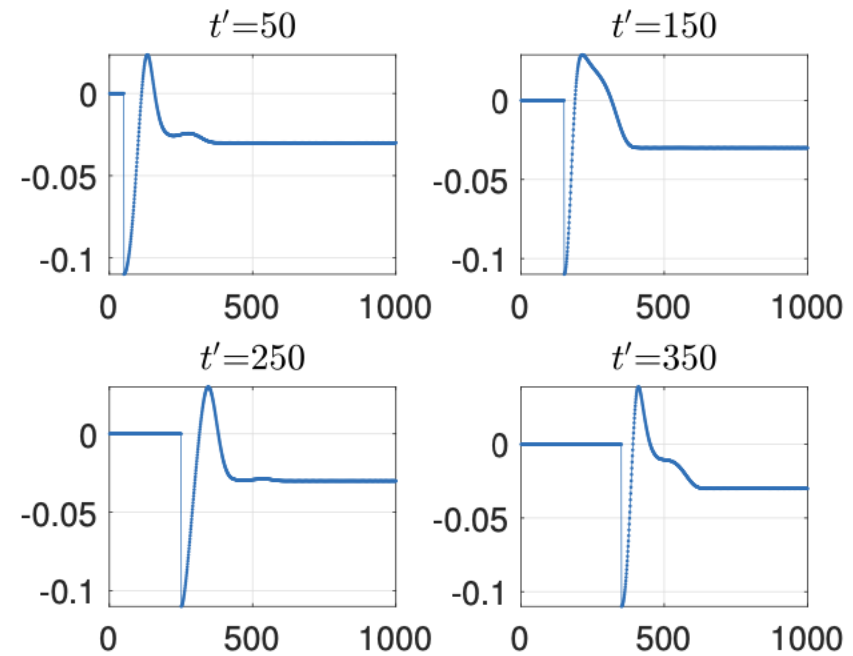
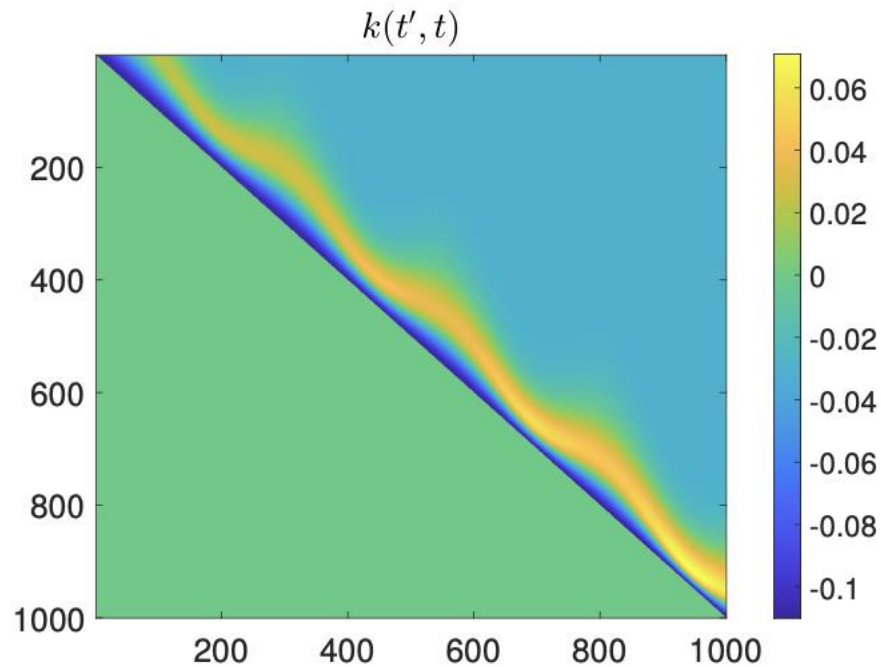
"Neural Spectral Marked Point Processes." Zhu, Wang, Cheng, and X. *ICLR 2022*.

"Spatio-temporal point processes with deep non-stationary kernels". Dong, Cheng, X. *ICLR 2023*.

Kernel representation using deep neural networks

- Kernel representation (Mercer's theorem)

$$k(x, x') = \sum_{r=1}^R v_r \psi_r(x') \phi_r(x)$$

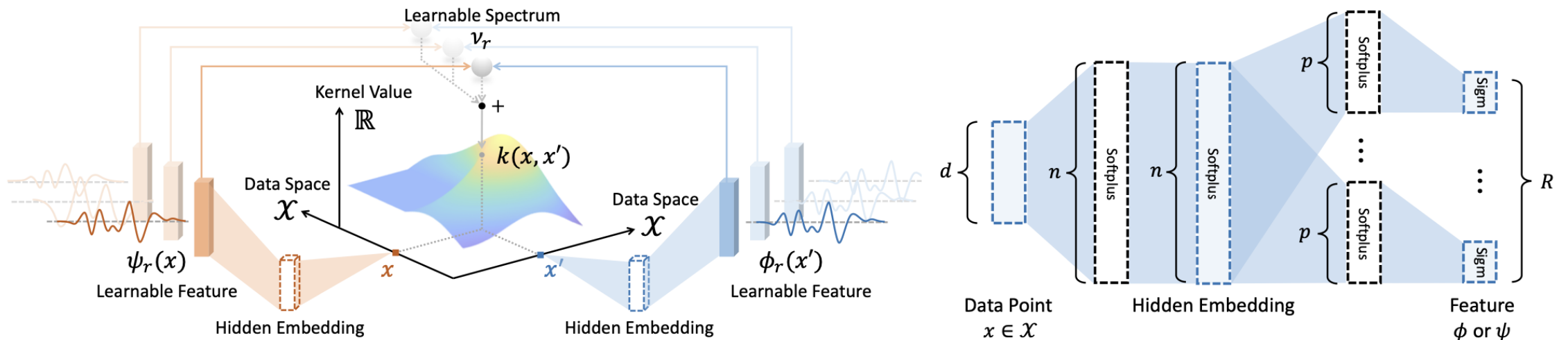


Kernel representation using deep neural networks

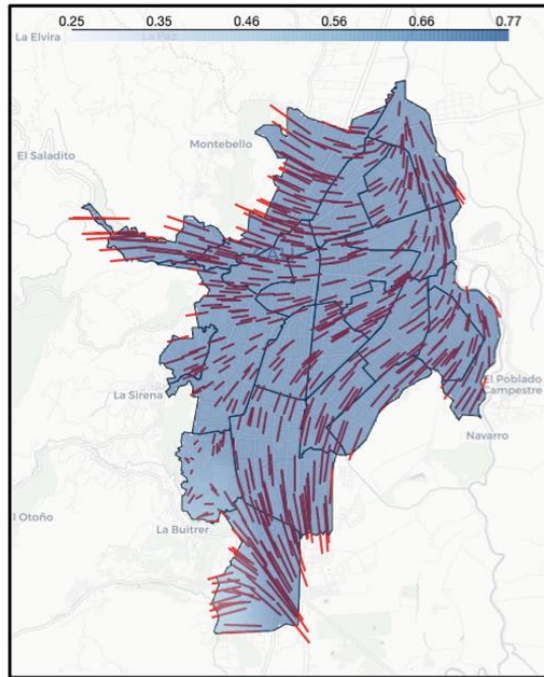
- Kernel representation (Mercer's theorem)

$$k(x, x') = \sum_{r=1}^R v_r \psi_r(x') \phi_r(x)$$

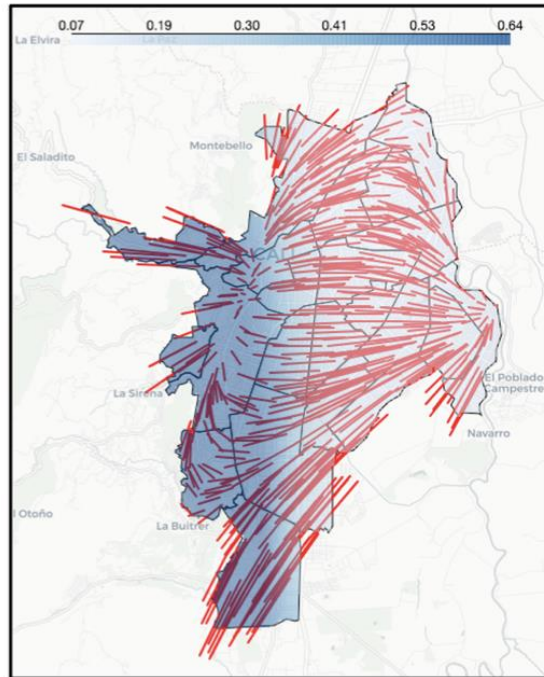
- Feature maps represented by neural networks



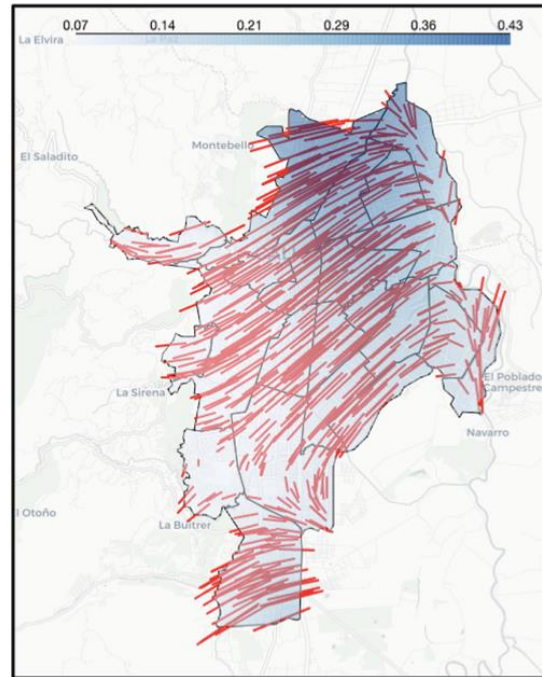
Highly interpretable influence kernels



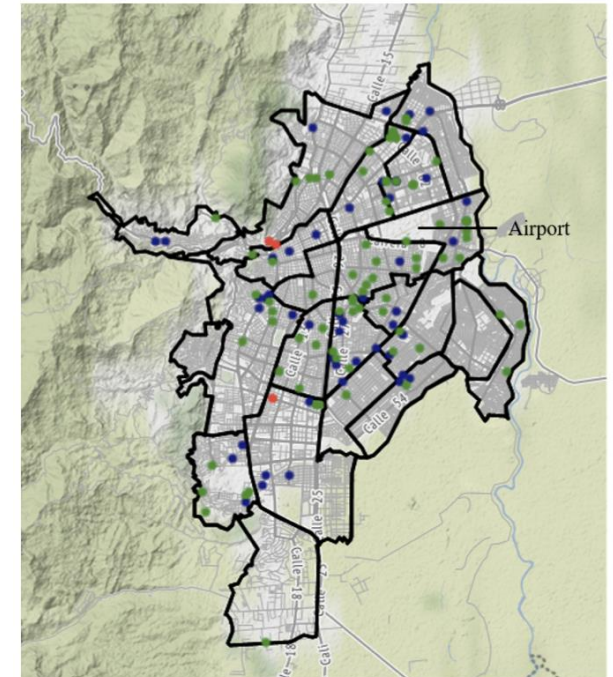
(a) $\kappa_S^{(1)}$



(b) $\kappa_S^{(2)}$



(c) $\kappa_S^{(3)}$

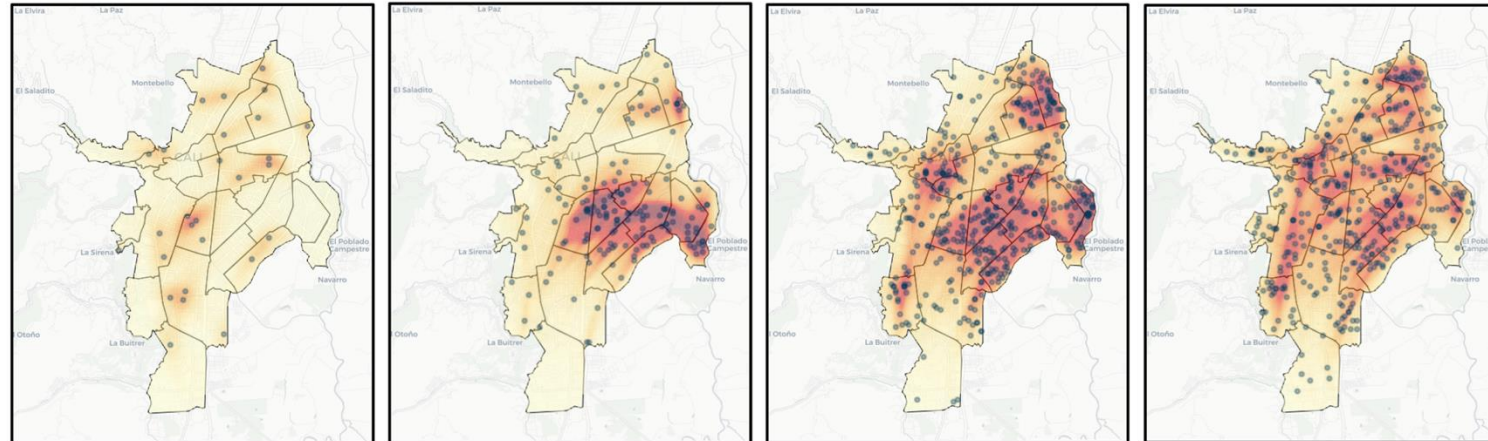


(b) Landmarks

Data: 38,611 cases from March 15 to Sept. 30, 2020.
Exact location of case (residence) and date.

Red: city hall
Blue: church
Green: school

Hotspot prediction

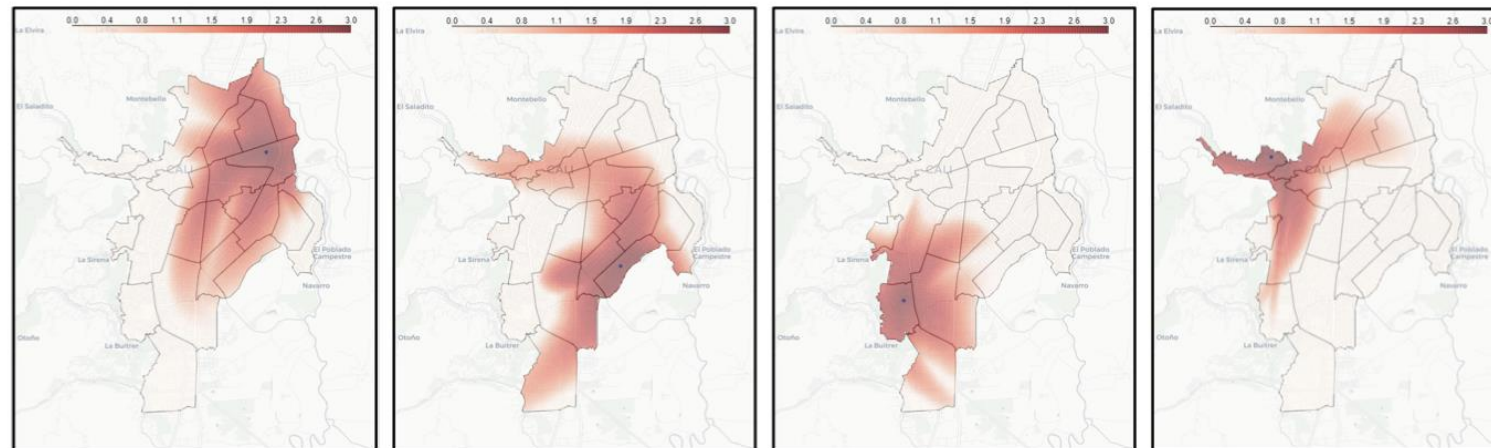


(a) March 22, 2020

(b) May 17, 2020

(c) June 28, 2020

(d) August 30, 2020



(a) Airport

(b) Center of Comuna 15

(c) Center of Comuna 18

(d) Center of Comuna 1

Table 2: Out-of-sample estimation performance.

Models	MAE $Q_{0.25}^{out}$	MAE $Q_{0.5}^{out}$	MAE $Q_{0.75}^{out}$
Random	5.190	8.660	14.900
SIR	2.253	5.713	8.554
AR(3)	2.219	3.776	8.915
ETAS	4.413	8.234	14.153
NSSTPP-Exo ($R=1$)	1.732	6.051	8.779
NSSTPP-Exo ($R=2$)	1.962	5.151	8.575
NSSTPP-Exo ($R=3$)	1.762	5.190	8.342
NSSTPP ($R=3$)	2.051	4.702	7.450

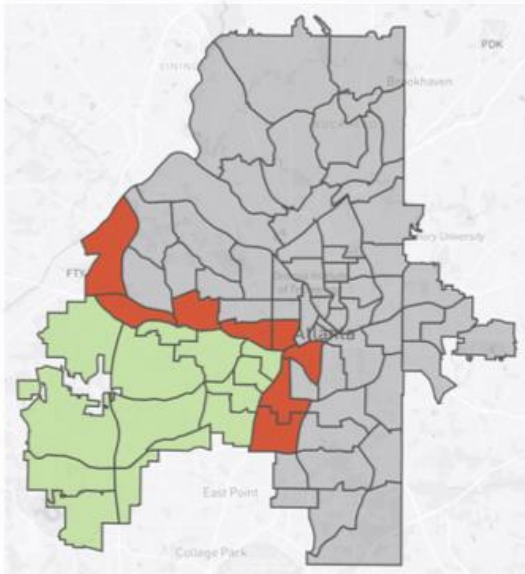


Roadmap

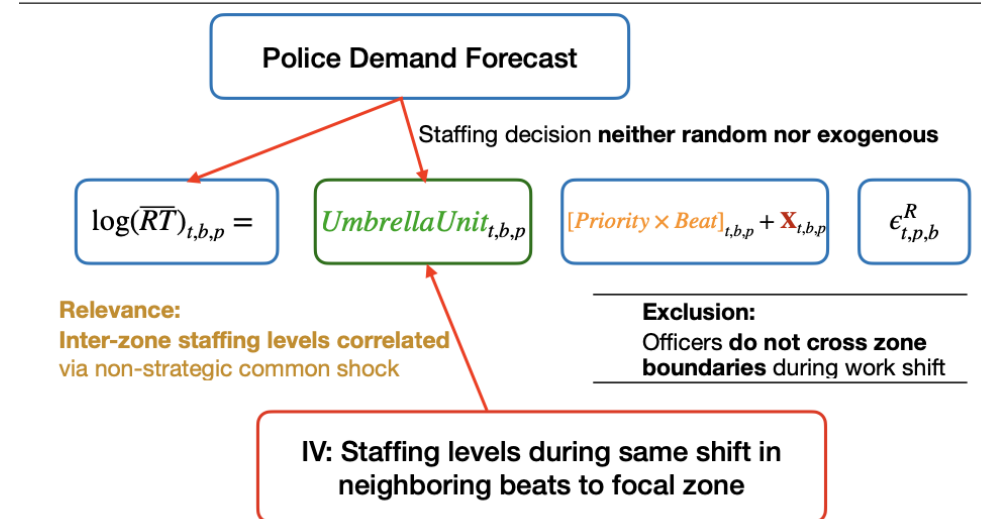
- Basic setup
- Granger network estimation
 - Structural constraints
 - Uncertainty quantification
- General: continuous space
- Other approaches

Police staffing and response time

- How does police staffing contribute to response time disparity and its causal impact on service quality?
- Treatment: staffing, Response: Response time
- Confounding factors: Weather, traffic, service priority....



Instrumental Variables Estimation



Summary

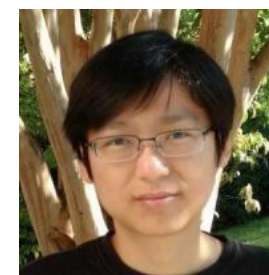
- Granger **causal graph** estimation from spatio-temporal discrete events
 - Structural assumptions, uncertainty quantification
- General: **continuous space** "influence kernel"
- Other possible approaches



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Duke



Xiuyuan Cheng
Duke



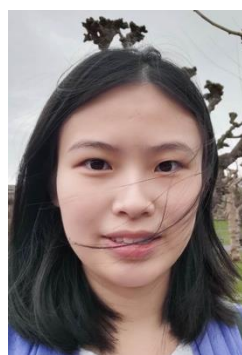
Song Wei
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Jonathan Zhou
GT



Zheng Dong
GT



Haoyun Wang
GT



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Jorge Mateu
UJI Castellon



Qiuping Yu
Georgetown

Main References

1. [Causal graph discovery from self and mutually exciting time series](#). Wei, Xie, Josef, Kamaleswaran. IEEE Selected Areas in Information Theory (JSAIT). 2023.
2. [Granger causal chain discovery for sepsis-associated derangements via multivariate Hawkes processes](#). Wei, Xie, Josef, Kamaleswaran. KDD 2023.
3. [Causal structural learning from time series: A convex optimization approach](#). Wei, Xie. Asilomar 2023.
4. [Uncertainty quantification for inferring Hawkes networks](#). Wang, Xie, Cuzzo, Mak, and Xie. NeurIPS 2020.
5. [Spatio-temporal point processes with deep non-stationary kernels](#). Dong, Cheng, Xie. ICLR 2023.
6. [Non-stationary spatio-temporal point process modeling for high-resolution COVID-19 data](#). Dong, Zhu, Xie, Mateu, Rodriguez-Cortes. Journal of the Royal Statistical Society: Series C. 2023.
7. Police staffing and fairness: Evidence from Atlanta Police. Zhou, Xie, Yu. Working paper. 2024.