# State-space models as graphs (part II) 

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## Outline

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Introduction
Linear-Gaussian model and Kalman filter
A doubly graphical perspective on SSMs
Point-wise estimation: GraphEM and DGLASSO algorithms
Point-wise estimation: extensions
Probabilistic estimation
Experimental evaluation
Conclusion
```


## Motivation

- A large class of problems in statistics, machine learning, and signal processing requires sequential processing of observed data with temporal structure.
- geophysical systems (atmosphere, oceans)
- robotics
- target tracking, positioning, navigation
- communications
- biomedical signal processing
- financial engineering
- ecology
- Goals:
- prediction (with uncertainty quantification)
- parameter estimation (with interpretability)


## Inference in State-Space Models (SSM)

- Let us consider:
- a set of hidden states $\mathbf{x}_{t} \in \mathbb{R}^{N_{x}}, t=1, \ldots, T$.
- a set of observations $\mathbf{y}_{t} \in \mathbb{R}^{N_{y}}, t=1, \ldots, T$.
- An SSM is an underlying hidden process of $\mathbf{x}_{t}$ that evolves and that, partially and noisily, expresses itself through $\mathbf{y}_{t}$.

- Probabilistic notation:
- Hidden state $\rightarrow p\left(\mathbf{x}_{t} \mid \mathbf{x}_{t-1}\right)$
- Observations $\rightarrow p\left(\mathbf{y}_{t} \mid \mathbf{x}_{t}\right)$


## The estimation problem

- We sequentially observe data $\mathbf{y}_{t}$ related to the hidden state $\mathbf{x}_{t}$.
$\rightarrow$ At time $t$, we have accumulated $t$ observations, $\mathbf{y}_{1: t} \equiv\left\{\mathbf{y}_{1}, \ldots, \mathbf{y}_{t}\right\}$.
$\rightarrow$ Interesting problems (when $\theta$ is known):
- Filtering
- State prediction: $p_{\theta}\left(\mathrm{x}_{t+\tau} \mid \mathrm{y} 1: t\right)$,
- Observation prediction: $p_{\theta}\left(\mathrm{y}_{t+\tau} \mid \mathrm{Y}_{1: t}\right), \quad \tau \geq$
- Smoothing: $p_{\theta}\left(\mathbf{x}_{t-\tau} \mid \mathbf{y}_{1: t}\right), \quad \tau \geq 1$
- We want a sequential, efficient, and probabilistic filtering of the observations.
$\rightarrow$ At time $t$, we want to process only $y_{t}$, but not reprocess all $\mathbf{y}_{1: t-1}$ (that were already processed!)



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## The linear-Gaussian Model

- The linear-Gaussian model is arguably the most relevant SSM:
- Functional notation:
- Unobserved state $\rightarrow \mathbf{x}_{t}=\mathbf{A}_{t} \mathbf{x}_{t-1}+\mathbf{q}_{t}$
- Observations $\quad \rightarrow \mathbf{y}_{t}=\boldsymbol{H}_{t} \mathrm{x}_{t}+\mathbf{r}_{t}$
where $\mathbf{q}_{t} \sim \mathcal{N}\left(0, \mathbf{Q}_{t}\right)$ and $\mathbf{r}_{t} \sim \mathcal{N}\left(0, \mathbf{R}_{t}\right)$.
- Probabilistic notation:
- Hidden state $\rightarrow p\left(\mathbf{x}_{t} \mid \mathbf{x}_{t-1}\right) \equiv \mathcal{N}\left(\mathbf{x}_{t} ; \mathbf{A}_{t} \mathbf{x}_{t-1}, \mathbf{Q}_{t}\right)$
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$>$ Kalman filter: obtains the filtering pdfs $p\left(\mathrm{x}_{t} \mid \mathrm{y}_{1: t}\right)$, at each $t$
- Gaussian pdfs, with means and covariances matrices are calculated at each $t$
- Efficient processing of $y_{t}$, obtaining
$>$ Rauch-Tung-Striebel (RTS) smoother: obtains $p\left(\mathrm{x}_{t} \mid \mathbf{y}_{1: T}\right)$
- requires a backward reprocessing, refining the Kalman estimates


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## Kalman summary and RTS smoother

- Hidden state $\rightarrow p\left(\mathbf{x}_{t} \mid \mathbf{x}_{t-1}\right) \equiv \mathcal{N}\left(\mathbf{x}_{t} ; \mathbf{A}_{t} \mathbf{x}_{t-1}, \mathbf{Q}_{t}\right)$
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## Kalman filter

- Initialize: $\mathbf{m}_{0}, \mathbf{P}_{0}$
- For $t=1, \ldots, T$

Predict stage:

$$
\begin{aligned}
& \mathbf{x}_{t}^{-}=\mathbf{A}_{t} \mathrm{~m}_{t-1} \\
& \mathbf{P}_{t}^{-}=\mathbf{A}_{t} \mathbf{P}_{t-1} \mathbf{A}_{t}^{\top}+\mathbf{Q}_{t}
\end{aligned}
$$

Update stage:

$$
\begin{aligned}
& \mathbf{z}_{t}=\mathbf{y}_{t}-\mathbf{H}_{t} \mathbf{x}_{t}^{-} \\
& \mathbf{S}_{t}=\mathbf{H} \mathbf{P}_{t}^{-} \mathbf{H}_{t}^{\top}+\mathbf{R}_{t} \\
& \mathbf{K}_{t}=\mathbf{P}_{t}^{-} \mathbf{H}_{t}^{\top} \mathbf{S}_{t}^{-1} \\
& \mathrm{~m}_{t}=\mathbf{x}_{t}^{-}+\mathbf{K}_{t} \mathbf{z}_{t} \\
& \mathbf{P}_{t}=\mathbf{P}_{t}^{-}-\mathbf{K}_{t} \mathbf{S}_{t} \mathbf{K}_{t}^{\top}
\end{aligned}
$$

$\checkmark$ Filtering distribution: $p\left(\mathbf{x}_{t} \mid \mathbf{y}_{1: t}\right)=\mathcal{N}\left(\mathbf{x}_{t} ; \mathrm{m}_{t}, \mathbf{P}_{t}\right)$
$\checkmark$ Smoothing distribution: $p\left(\mathbf{x}_{t} \mid \mathbf{y}_{1: T}\right)=\mathcal{N}\left(\mathbf{x}_{t} ; \mathbf{m}_{t}^{s}, \mathbf{P}_{t}^{s}\right)$
$X$ How to proceed if some model parameters are unknown ?

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## Goal of the talk

$$
\mathbf{x}_{t}=\mathbf{A} \mathbf{x}_{t-1}+\mathbf{q}_{t}, \quad \mathbf{q} t \sim \mathcal{N}(0, \mathbf{Q})
$$

## This talk: DGLASSO model and inference approach

- Joint estimation of two matrices describing the hidden state dynamics in the linear Gaussian state-space model.
- Sparse graphical model to represent (i) the (Granger) causal dependencies among the states, and (ii) the correlation among the state noises.
- Majorization-minimization methodology for graphical inference.

A graphical perspective on $\mathbf{A}$

- Goal. Estimation of matrix A (a) introducing prior knowledge, and (b) under a novel interpretation of $\mathbf{A}$ :

$$
\mathbf{x}_{t}=\mathbf{A} \mathbf{x}_{t-1}+\mathbf{q}_{t}, \quad \mathbf{q}_{t} \sim \mathcal{N}(0, \mathbf{Q})
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- Graph discovery perspective: A can be seen as sparse directed graph



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- $\mathbf{x}_{t} \in \mathbb{R}^{N_{x}}$ contains $N_{x}$ time-series
- each of them represents the latent process in a node in the graph



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$$
\mathbf{A}=\left(\begin{array}{ccccc}
0.9 & 0.7 & 0 & 0 & 0 \\
0 & 0 & -0.3 & 0 & 0 \\
0 & 0 & 0 & 0 & 0.8 \\
0 & -0.1 & 0 & 0 & 0 \\
0 & 0 & 0.5 & 0 & 0
\end{array}\right)
$$ process in a node in the graph

- $A(i, j)$ is the linear effect from node $j$ at time $t-1$ to node $i$ at time $t$ :

$$
x_{t, i}=\sum_{j=1}^{N_{x}} A(i, j) x_{t-1, j}+q_{t, i}
$$

- $A(i, j) \neq 0 \Rightarrow x_{t-1, j}$ Granger-causes $x_{t, i}$.


A graphical modeling $\mathbf{P}=\mathbf{Q}^{-1}$

$$
\mathbf{x}_{t}=\mathbf{A} \mathbf{x}_{t-1}+\mathbf{q}_{t}, \quad \mathbf{q}_{t} \sim \mathcal{N}(0, \mathbf{Q})
$$

- Gaussian graphical model (GGM) perspective: $\mathbf{P}=\mathrm{Q}^{-1}$ can be seen as an sparse undirected graph.

$$
\mathbf{q}(n) \Perp \mathbf{q}(\ell) \mid\left\{\mathbf{q}(j), j \in 1, \ldots, N_{x} \backslash\{n, \ell\}\right\} \Longleftrightarrow P(n, \ell)=P(\ell, n)=0
$$



## Summary of DGLASSO model



Summary representation of the DGLASSO graphical model, for the example graphs $\mathbf{A}$ and P from the two previous slides.

DGLASSO (dynamic graphical lasso): maximum a posteriori (MAP) estimator of $\mathbf{A}$ and P under lasso sparsity regularization on both matrices, given the observed sequence $\mathbf{y}_{1: T}$.

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## Proposed penalized formulation

## Goal. MAP estimate of $\mathbf{A}$ and $\mathrm{P}\left(\mathrm{P}=\mathrm{Q}^{-1}\right)$ :

$$
\begin{aligned}
\mathbf{A}^{*}, \mathbf{P}^{*} & =\underset{\mathbf{A}, \mathbf{P}}{\operatorname{argmax}} p\left(\mathbf{A}, \mathbf{P} \mid \mathbf{y}_{1: T}\right)=\underset{\mathbf{A}}{\operatorname{argmax}} p(\mathbf{A}, \mathbf{P}) p\left(\mathbf{y}_{1: T} \mid \mathbf{A}, \mathbf{P}\right) \\
& =\underset{\mathbf{A}, \mathbf{P}}{\operatorname{argmin}} \underbrace{-\log p(\mathbf{A}, \mathbf{P})}_{\mathcal{L}_{0}(\mathbf{A}, \mathbf{P})} \underbrace{-\log p\left(\mathbf{y}_{1: T} \mid \mathbf{A}, \mathbf{P}\right)}_{\mathcal{L}_{1: T}(\mathbf{A}, \mathrm{P})}=\mathcal{L}(\mathbf{A}, \mathbf{P})
\end{aligned}
$$

- Lasso penalty (prior): we promote sparse matrices ( $\mathbf{A}, \mathbf{P}$ ) for interpretable and compact network of connections:

- $\log$ likelihood

$\rightarrow$ requires to run KF using $(\mathbf{A}, \mathbf{P})$
Challenges:
- Joint minimization with non-smooth and non-convex implicit loss.
$\rightarrow$ gradient-based solutions are challenging (unrolling KF recursion) and numerically unstable


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## Challenges:

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## Construction of the majorant function

EM-like approach: ${ }^{1}$

- Majorizing approximation (E-step): Run the Kalman filter/RTS smoother by setting $(\widetilde{\mathbf{A}}, \widetilde{\mathbf{P}}) \in \mathbb{R}^{N_{x} \times N_{x}} \times \mathcal{S}_{N_{x}}$ and build the majorizing approximation $(\mathcal{Q}(\mathbf{A}, \mathbf{P} ; \widetilde{\mathbf{A}}, \widetilde{\mathbf{P}}) \geq \mathcal{L}(\mathbf{A}, \mathbf{P}), \forall(\mathbf{A}, \mathbf{P}))$ :

$$
\mathcal{Q}(\mathbf{A}, \mathbf{P} ; \widetilde{\mathbf{A}}, \widetilde{\mathbf{P}})=\frac{T}{2} \operatorname{tr}\left(\mathbf{P}\left(\boldsymbol{\Psi}-\boldsymbol{\Delta} \mathbf{A}^{\top}-\mathbf{A} \boldsymbol{\Delta}^{\top}+\mathbf{A} \mathbf{\Phi} \mathbf{A}^{\top}\right)\right)-\frac{T}{2} \log \operatorname{det}(2 \pi \mathbf{P})
$$

where, for every $t \in\{1, \ldots, T\}, \mathbf{G}_{t}=\boldsymbol{\Sigma}_{t}(\widetilde{\mathbf{A}})^{\top}\left(\widetilde{\mathbf{A}} \boldsymbol{\Sigma}_{t}(\widetilde{\mathbf{A}})^{\top}+\widetilde{\mathbf{P}}^{-1}\right)^{-1}$, and

$$
\begin{aligned}
& \boldsymbol{\Psi}=\frac{1}{T} \sum_{t=1}^{T} \boldsymbol{\Sigma}_{t}^{s}+\boldsymbol{\mu}_{t}^{s}\left(\boldsymbol{\mu}_{t}^{s}\right)^{\top} \\
& \mathbf{\Phi}=\frac{1}{T} \sum_{t=1}^{T} \boldsymbol{\Sigma}_{t-1}^{s}+\boldsymbol{\mu}_{t-1}^{s}\left(\boldsymbol{\mu}_{t-1}^{s}\right)^{\top}, \\
& \boldsymbol{\Delta}=\frac{1}{T} \sum_{t=1}^{T} \boldsymbol{\Sigma}_{t}^{s} \mathbf{G}_{t-1}^{\top}+\boldsymbol{\mu}_{t}^{s}\left(\boldsymbol{\mu}_{t-1}^{s}\right)^{\top},
\end{aligned}
$$

using RTS outputs $\left(\boldsymbol{\mu}_{t}^{s}, \boldsymbol{\Sigma}_{t}^{s}\right)_{1 \leq t \leq T}$ using $(\widetilde{\mathbf{A}}, \widetilde{\mathbf{P}})$.

[^0]
## DGLASSO minimization procedure

- Block alternating majorization-minimization technique:

Set $\left(\mathbf{A}^{(0)}, \mathbf{P}^{(0)}\right)$.
At each iteration $i \in \mathbb{N}$,
(a) Run RTS to build function $\mathcal{Q}\left(\mathbf{A}, \mathbf{P} ; \mathbf{A}^{(i)}, \mathbb{P}^{(i)}\right)$ (E-step)
(b) Update transition matrix (M-step):

$$
\mathbf{A}^{(i+1)}=\underset{\mathbf{A}}{\operatorname{argmin}} \mathcal{Q}\left(\mathbf{A}, \mathbf{P}^{(i)} ; \mathbf{A}^{(i)}, \mathbf{P}^{(i)}\right)+\lambda_{A}\|\mathbf{A}\|_{1}+\frac{1}{2 \theta_{A}}\left\|\mathbf{A}-\mathbf{A}^{(i)}\right\|_{F}^{2}
$$

(c) Run RTS to build function $\mathcal{Q}\left(\mathbf{A}, \mathbf{P} ; \mathbf{A}^{(i+1)}, \mathbf{P}^{(i)}\right)$ (E-step)
(d) Update precision matrix (M-step):

$$
\mathbf{P}^{(i+1)}=\underset{\mathbf{P}}{\operatorname{argmin}} \mathcal{Q}\left(\mathbf{A}^{(i+1)}, \mathbf{P} ; \mathbf{A}^{(i+1)}, \mathbf{P}^{(i)}\right)+\lambda_{P}\|\mathbf{P}\|_{1}+\frac{1}{2 \theta_{P}}\left\|\mathbf{P}-\mathbf{P}^{(i)}\right\|_{F}^{2}
$$

- Proximal terms, with stepsizes $\left(\theta_{A}, \theta_{P}\right)>0$, to stabilize the minimization process and guarantee convergence of iterates.
- Convenient bi-convex structure of $\mathcal{Q}(\cdot, \cdot ; \widetilde{\mathbf{A}}, \widetilde{\mathbf{P}})$
- Step (b) is a lasso-like regression problem
- Step (d) is a GLASSO-like problem.


## Convergence theorem

Consider the sequence $\left\{\mathbf{A}^{(i)}, \mathbf{P}^{(i)}\right\}_{i \in \mathbb{N}}$ generated by DGLASSO, assuming exact resolution of both inner steps (b) and (d). Denote $\mathcal{L}=\mathcal{L}_{0}+\mathcal{L}_{1: T}$ the loss function.

- The sequence $\left\{\mathbf{A}^{(i)}, \mathbf{P}^{(i)}\right\}_{i \in \mathbb{N}}$ produced by DGLASSO algorithm satisfies

$$
(\forall i \in \mathbb{N}) \quad \mathcal{L}\left(\mathbf{A}^{(i+1)}, \mathbf{P}^{(i+1)}\right) \leq \mathcal{L}\left(\mathbf{A}^{(i)}, \mathbf{P}^{(i)}\right) .
$$

- If the sequence $\left\{\mathbf{A}^{(i)}, \mathbf{P}^{(i)}\right\}_{i \in \mathbb{N}}$ is bounded, then $\left\{\mathbf{A}^{(i)}, \mathbf{P}^{(i)}\right\}_{i \in \mathbb{N}}$ converges to a critical point of $\mathcal{L}$.
- Proof based on the recent work. ${ }^{2}$
- In practice, inner mininimization steps (b) and (d) using a Dykstra proximal splitting solver. ${ }^{3}$

[^1]
## Summary of the GraphEM algorithm

- DGLASSO generalises our previous GraphEM, ${ }^{4}$ where only $\mathbf{A}$ is unknown.


## GraphEM algorithm

- Initialization of $\mathbf{A}^{(0)}$.
- For $i=1,2, \ldots$.

E-step Run the Kalman filter and RTS smoother by setting $\mathbf{A}^{\prime}:=\mathbf{A}^{(i-1)}$ and construct $\mathcal{Q}\left(\mathbf{A} ; \mathbf{A}^{(i-1)}\right)$.
M-step Update $\mathbf{A}^{(i)}=\operatorname{argmin}_{\mathbf{A}}\left(\mathcal{Q}\left(\mathbf{A} ; \mathbf{A}^{(i-1)}\right)\right)$ using Douglas-Rachford algorithm (simpler version) or monotone+skew (MS) algorithm (generalized version).

- Flexible approach, valid as long as the proximity operators of $\left(f_{m}\right)_{2 \leq m \leq M}$ are available, with $\mathcal{L}_{0}=\sum_{m=1}^{M} f_{m}$

[^2]
## Outline

```
Introduction
Linear-Gaussian model and Kalman filter
A doubly graphical perspective on SSMs
Point-wise estimation: GraphEM and DGLASSO algorithms
```

Point-wise estimation: extensions

## Probabilistic estimation

## Experimental evaluation

Conclusion

## Ongoing extensions: beyond $\ell_{1}$ norm $(1 / 3)$

- GraphEM requires the penalty term $\mathcal{L}_{0}(\mathbf{A})$ to be convex (e.g., $\ell_{1}$ norm).
- However, for very sparse graphs, non-convex penalties such as SCAD, MCP, CELO have shown to be more suited than $\ell_{1}$ norm (closer to pseudo-norm $\ell_{0}$ ).

- GraphIT algorithm ${ }^{5}$ implements an iterative reweighted (IR) scheme
- MM framework: $\mathcal{L}_{0}(\mathbf{A})$ is approximated by a surrogate convex function
- optimization via modern solvers with strong convergence gurantees

(a) True graph

(b) GraphEM

(c) GraphIT

[^3]
## Ongoing extensions: beyond Markovianity (2/3)

- Non-Markovian LG-SSM:
- Unobserved state $\rightarrow \mathbf{x}_{t}=\sum_{i=1}^{P} \mathbf{A}_{i} \mathbf{x}_{t-i}+\mathbf{q}_{t}$
- Observations $\quad \rightarrow \mathrm{y}_{t}=\boldsymbol{H}_{t} \mathrm{x}_{t}+\mathrm{r}_{t}$
- Standard filtering and smoothing approach with known $\left\{A_{i}\right\}_{i=1}^{P}$
- stacking (columnwise) the $p$ consecutive states into $\mathbf{z}_{t}=\left[\mathbf{x}_{t} ; \mathbf{x}_{t-1} ; \ldots ; \mathbf{x}_{t-p+1}\right] \in \mathbb{R}^{p N_{x}}$
- run KF and RTS in the extended model

$$
\left\{\begin{array}{l}
\mathbf{z}_{t}=\check{\mathbf{A}} \mathbf{z}_{t-1}+\check{\mathbf{q}}_{t}  \tag{1}\\
\mathbf{y}_{t}=\check{\mathbf{H}} \mathbf{z}_{t}+\mathbf{r}_{t}
\end{array}\right.
$$

where we define

$$
\begin{gathered}
\check{\mathbf{A}}=\left[\begin{array}{cccc}
\mathbf{A}_{1} & \cdots & \cdots & \mathbf{A}_{p} \\
\boldsymbol{I} & 0 & \cdots & 0 \\
& \ddots & \ddots & \vdots \\
(0) & & \boldsymbol{I} & 0
\end{array}\right] \in \mathbb{R}^{p N_{x} \times p N_{x}}, \\
\check{\mathbf{H}}=[\mathbf{H}(0)] \in \mathbb{R}^{N_{y} \times p N_{x}}, \check{\mathbf{Q}}=\left[\begin{array}{cc}
\mathbf{Q} & (0) \\
(0) & (0)
\end{array}\right] \in \mathbb{R}^{p N_{x} \times p N_{x}}, \\
\check{\mathbf{q}}_{t} \sim \mathcal{N}(0, \check{\mathbf{Q}}), \text { and } \mathbf{r}_{t} \sim \mathcal{N}(0, \mathbf{R})
\end{gathered}
$$

Ongoing extensions: beyond Markovianity (2/3)

$$
\mathbf{A}_{1}=\left(\begin{array}{ccc}
0.9 & 0.7 & 0 \\
0 & 0 & -0.3 \\
0 & 0 & 0
\end{array}\right), \mathbf{A}_{2}=\left(\begin{array}{lll}
0 & 0 & 0 \\
0 & 0 & 0 \\
0 & 0.8 & 0
\end{array}\right)
$$



## Ongoing extensions: beyond Markovianity (2/3)

- LaGrangEM (ICASSP 2024): a GraphEM-type algorithm that operates in non-Markovian models including desirable properties and interpretability, e.g.,
- acyclic graph
- sparsity
- only one-lag interaction at maximum betwen nodes (more sparsity!)
- reasonable in some physical models
- one input arrow at maximum at each node (even more sparsity!)
- strong connection with modern Granger causality models ${ }^{6}$

- So far, great results but with intermediate/post-processing mapping steps which may compromise the theoretical guarantees (?)
- ongoing work in bridging the gap between well-perorming methods and solid theory

[^4]
## Ongoing extensions: beyond linearity $(3 / 3)$

- Models of this type:

$$
\mathbf{x}_{t}=\sum_{j=1}^{J} \mathbf{A}_{j} \boldsymbol{\Phi}_{j}\left(\mathbf{x}_{t-1}\right)+\mathbf{q}_{t}
$$

e.g., with $J=3$ :

$$
\mathbf{x}_{t}=\mathbf{A}_{1} \mathbf{x}_{t-1}+\mathbf{A}_{2} \mathbf{x}_{t-1}^{2}+\mathbf{A}_{3} \mathbf{x}_{t-1}^{2}+\mathbf{q}_{t}
$$

- possible to include cross-terms
- Functional learning (Taylor-expansion perspective)
- Ongoing work with several challenges:
- too high-dimensional space
- identifiability issues
- even more complicated for fully Bayesian approaches


## Outline

```
Introduction
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## SpaRJ algorithm

- $\mathrm{SpaRJ}^{7}$ (sparse reversible jump) is a fully probabilistic algorithm for the estimation of $\mathbf{A}$, i.e., obtains samples from $p\left(\mathbf{A} \mid \mathbf{y}_{1: T}\right)$.
- The sparsity is imposed by transitioning among models of different complexity, defined hierarchically:
- $M_{n} \in\{0,1\}^{N_{x} \times N_{x}}$ : sparsity pattern sample
- $A_{n}$ : matrix $\mathbf{A}$ sample, with non-zero elements, $A(i, j)$ for
- We use reversible jump MCMC (RJ-MCMC) to explore $p\left(\mathbf{A} \mid \mathrm{y}_{1: T}\right) .^{8}$
- MCMC algorithm to simulate in spaces of varying dimension, e.g., the number of ones in the sparsity pattern, $\left|M_{n}\right|$
- It requires to define:
- transition kernels for the model jumps
- mechanism to set values when jumping to a more complex model.

[^5]
## SpaRJ algorithm

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- $M_{n} \in\{0,1\}^{N_{x} \times N_{x}}$ : sparsity pattern sample
- $A_{n}$ : matrix $\mathbf{A}$ sample, with non-zero elements, $A(i, j)$ for $\left\{(i, j): M_{n}(i, j)=1\right\}$
- We use reversible jump MCMC (RJ-MCMC) to explore $p\left(\mathbf{A} \mid \mathrm{y}_{1: T}\right) .^{8}$
- MCMC algorithm to simulate in spaces of varying dimension, e.g., the number of ones in the sparsity pattern, $\left|M_{n}\right|$
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- It requires to define:
- transition kernels for the model jumps
- mechanism to set values when jumping to a more complex model.

[^8]
## Pseudocode of SpaRJ

Input: Known SSM parameters $\left\{\overline{\mathbf{x}}_{0}, \mathbf{P}_{0}, \mathbf{Q}, \mathbf{R}, \mathbf{H}\right\}$, observations $\left\{y_{t}\right\}_{t=1}^{T}$, hyper-parameters, number of iterations $N$, initial value $\mathbf{A}_{0}$ Output: Set of sparse samples $\left\{\mathbf{A}_{n}\right\}_{n=1}^{N}$

```
Initialization
    Initialize }\mp@subsup{M}{0}{}\mathrm{ as fully dense (all ones) and }\mp@subsup{\mathbf{A}}{0}{
    Run Kf obtaining lo }\mp@subsup{l}{0}{}:=\operatorname{log}(\textrm{p}(\mp@subsup{\mathbf{y}}{1:T}{}|\mp@subsup{\mathbf{A}}{0}{}))p(\mp@subsup{\mathbf{A}}{0}{}
    for }n=1,\ldots,N d
    Step 1: Propose model
    Propose a new sparsity pattern }\mp@subsup{M}{}{\prime}\mathrm{ , obtaining a symmetry correction of c.
    Step 2: Propose A
    Propose A' using an MCMC sampler conditional on M'
    Step 3: MH accept-reject
    Evaluate Kalman filter with A:= \mathbf{A}
    Set l}\mp@subsup{l}{}{\prime}:=\operatorname{log}(p(\mp@subsup{\mathbf{y}}{1:T}{}|\mp@subsup{\mathbf{A}}{}{\prime}))p(\mp@subsup{\mathbf{A}}{}{\prime}
    Compute log}(\mp@subsup{a}{T}{}):=\mp@subsup{l}{}{\prime}-\mp@subsup{l}{n-1}{}+c\mathrm{ and Accept w.p. }\mp@subsup{a}{T}{}
    if Accept then
    Set }\mp@subsup{M}{n}{}:=\mp@subsup{M}{}{\prime},\mp@subsup{\mathbf{A}}{n}{}:=\mp@subsup{\mathbf{A}}{}{\prime},\mp@subsup{l}{n}{}:=\operatorname{log}(p(\mp@subsup{\textrm{y}}{1:T}{}|\mp@subsup{\mathbf{A}}{}{\prime}))p(\mp@subsup{\mathbf{A}}{}{\prime}
    else
    Set }\mp@subsup{M}{n}{}:=\mp@subsup{M}{n-1}{},\mp@subsup{\mathbf{A}}{n}{}:=\mp@subsup{\mathbf{A}}{n-1}{},\mp@subsup{l}{n}{}:=\mp@subsup{l}{n-1}{
    end if
    end for
```


## Pseudocode of SpaRJ

Input: Known SSM parameters $\left\{\overline{\mathbf{x}}_{0}, \mathbf{P}_{0}, \mathbf{Q}, \mathbf{R}, \mathbf{H}\right\}$, observations $\left\{y_{t}\right\}_{t=1}^{T}$, hyper-parameters, number of iterations $N$, initial value $\mathbf{A}_{0}$
Output: Set of sparse samples $\left\{\mathbf{A}_{n}\right\}_{n=1}^{N}$
Initialization
Initialize $M_{0}$ as fully dense (all ones) and $\mathbf{A}_{0}$
Run Kf obtaining $l_{0}:=\log \left(\mathrm{p}\left(\mathbf{y}_{1: T} \mid \mathbf{A}_{0}\right)\right) p\left(\mathbf{A}_{0}\right)$
for $n=1, \ldots, N$ do
Step 1: Propose model
Propose a new sparsity pattern $M^{\prime}$, obtaining a symmetry correction of $c$.
Step 2: Propose $\mathbf{A}^{\prime}$
Propose $\mathbf{A}^{\prime}$ using an $M C M C$ sampler conditional on $M^{\prime}$
Step 3: MH accept-reject
Evaluate Kalman filter with $\mathbf{A}:=\mathbf{A}^{\prime}$
Set $\ddot{l}^{\prime}:=\log \left(p\left(\mathbf{y}_{1: T} \mid \mathbf{A}^{\prime}\right)\right) p\left(\mathbf{A}^{\prime}\right)$
Compute $\log \left(a_{r}\right):=l^{\prime}-l_{n-1}+c$ and Accept w.p. $a_{r}$ :
if Accept then
else
end if
end for

## Pseudocode of SpaRJ

Input: Known SSM parameters $\left\{\overline{\mathbf{x}}_{0}, \mathbf{P}_{0}, \mathbf{Q}, \mathbf{R}, \mathbf{H}\right\}$, observations $\left\{y_{t}\right\}_{t=1}^{T}$, hyper-parameters, number of iterations $N$, initial value $\mathbf{A}_{0}$
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for $n=1, \ldots, N$ do
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Step 2: Propose $\mathrm{A}^{\prime}$
Propose $\mathbf{A}^{\prime}$ using an MCMC sampler conditional on $M^{\prime}$
Step 3: MH accept-reject
Evaluate Kalman filter with $\mathbf{A}:=\mathbf{A}^{\prime}$
Set $l^{\prime}:=\log \left(p\left(\mathbf{y}_{1: T} \mid \mathbf{A}^{\prime}\right)\right) p\left(\mathbf{A}^{\prime}\right)$
Compute $\log \left(a_{r}\right):=l^{\prime}-l_{n-1}+c$ and Accept w.p. $a_{r}$
if Accept then
else
end if
end for

## Pseudocode of SpaRJ

Input: Known SSM parameters $\left\{\overline{\mathbf{x}}_{0}, \mathbf{P}_{0}, \mathbf{Q}, \mathbf{R}, \mathbf{H}\right\}$, observations $\left\{y_{t}\right\}_{t=1}^{T}$, hyper-parameters, number of iterations $N$, initial value $\mathbf{A}_{0}$
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Run Kf obtaining $l_{0}:=\log \left(\mathrm{p}\left(\mathbf{y}_{1: T} \mid \mathbf{A}_{0}\right)\right) p\left(\mathbf{A}_{0}\right)$
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Propose $\mathbf{A}^{\prime}$ using an MCMC sampler conditional on $M^{\prime}$
Step 3: MH accept-reject
Evaluate Kalman filter with $\mathbf{A}:=\mathbf{A}^{\prime}$
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Compute $\log \left(a_{r}\right):=l^{\prime}-l_{n-1}+c$ and Accept w.p. $a_{r}$ :
if Accept then
else
end if
end for

## Pseudocode of SpaRJ

Input: Known SSM parameters $\left\{\overline{\mathbf{x}}_{0}, \mathbf{P}_{0}, \mathbf{Q}, \mathbf{R}, \mathbf{H}\right\}$, observations $\left\{y_{t}\right\}_{t=1}^{T}$, hyper-parameters, number of iterations $N$, initial value $\mathbf{A}_{0}$
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Initialize $M_{0}$ as fully dense (all ones) and $\mathbf{A}_{0}$
Run Kf obtaining $l_{0}:=\log \left(\mathrm{p}\left(\mathbf{y}_{1: T} \mid \mathbf{A}_{0}\right)\right) p\left(\mathbf{A}_{0}\right)$
for $n=1, \ldots, N$ do
Step 1: Propose model
Propose a new sparsity pattern $M^{\prime}$, obtaining a symmetry correction of $c$.
Step 2: Propose $\mathrm{A}^{\prime}$
Propose $\mathbf{A}^{\prime}$ using an MCMC sampler conditional on $M^{\prime}$
Step 3: MH accept-reject
Evaluate Kalman filter with $\mathbf{A}:=\mathbf{A}^{\prime}$
Set $l^{\prime}:=\log \left(p\left(\mathbf{y}_{1: T} \mid \mathbf{A}^{\prime}\right)\right) p\left(\mathbf{A}^{\prime}\right)$
Compute $\log \left(a_{r}\right):=l^{\prime}-l_{n-1}+c$ and Accept w.p. $a_{r}$ :
if Accept then
Set $M_{n}:=M^{\prime}, \mathbf{A}_{n}:=\mathbf{A}^{\prime}, l_{n}:=\log \left(p\left(\mathbf{y}_{1: T} \mid \mathbf{A}^{\prime}\right)\right) p\left(\mathbf{A}^{\prime}\right)$
else
Set $M_{n}:=M_{n-1}, \mathbf{A}_{n}:=\mathbf{A}_{n-1}, l_{n}:=l_{n-1}$
end if
end for

## Outline

```
Introduction
Linear-Gaussian model and Kalman filter
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Point-wise estimation: GraphEM and DGLASSO algorithms
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```

Data description and numerical settings

- Four synthetic datasets with $\mathbf{H}=\mathbf{I d}$ and block-diagonal matrix $\mathbf{A}$, composed with $b$ blocks of size $\left(b_{j}\right)_{1 \leq j \leq b}$, so that $N_{y}=N_{x}=\sum_{j=1}^{b} b_{j}$. We set $T=10^{3}$, $\mathbf{Q}=\sigma_{\mathbf{Q}}^{2} \mathbf{l d}, \mathbf{R}=\sigma_{\mathbf{R}}^{2} \mathbf{l d}, \mathbf{P}_{0}=\sigma_{\mathbf{P}}^{2} \mathbf{l d}$.

| Dataset | $N_{x}$ | $\left(b_{j}\right)_{1 \leq j \leq b}$ | $\left(\sigma_{\mathbf{Q}}, \sigma_{\mathbf{R}}, \sigma_{\mathbf{P}}\right)$ |
| :---: | :---: | :---: | :---: |
| A | 9 | $(3,3,3)$ | $\left(10^{-1}, 10^{-1}, 10^{-4}\right)$ |
| B | 9 | $(3,3,3)$ | $\left(1,1,10^{-4}\right)$ |
| C | 16 | $(3,5,5,3)$ | $\left(10^{-1}, 10^{-1}, 10^{-4}\right)$ |
| D | 16 | $(3,5,5,3)$ | $\left(1,1,10^{-4}\right)$ |

- GraphEM is compared with:
- Maximum likelihood EM (MLEM) ${ }^{9}$ conditional Granger Causality (CGC) ${ }^{10}$

[^9]
## Data description and numerical settings

- Four synthetic datasets with $\mathbf{H}=\mathbf{I d}$ and block-diagonal matrix $\mathbf{A}$, composed with $b$ blocks of size $\left(b_{j}\right)_{1 \leq j \leq b}$, so that $N_{y}=N_{x}=\sum_{j=1}^{b} b_{j}$. We set $T=10^{3}$, $\mathbf{Q}=\sigma_{\mathbf{Q}}^{2} \operatorname{ld}, \mathbf{R}=\sigma_{\mathbf{R}}^{2} \operatorname{ld}, \mathbf{P}_{0}=\sigma_{\mathbf{P}}^{2} \backslash \mathrm{~d}$.

| Dataset | $N_{x}$ | $\left(b_{j}\right)_{1 \leq j \leq b}$ | $\left(\sigma_{\mathbf{Q}}, \sigma_{\mathbf{R}}, \sigma_{\mathbf{P}}\right)$ |
| :---: | :---: | :---: | :---: |
| A | 9 | $(3,3,3)$ | $\left(10^{-1}, 10^{-1}, 10^{-4}\right)$ |
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| C | 16 | $(3,5,5,3)$ | $\left(10^{-1}, 10^{-1}, 10^{-4}\right)$ |
| D | 16 | $(3,5,5,3)$ | $\left(1,1,10^{-4}\right)$ |

- GraphEM is compared with:
- Maximum likelihood EM (MLEM) ${ }^{9}$
- Granger-causality approaches: pairwise Granger Causality (PGC) and conditional Granger Causality (CGC) ${ }^{10}$

[^10]
## Experimental results of GraphEM



True graph (left) and GraphEM estimate (right) for dataset C.

## Experimental results of GraphEM

|  | method | RMSE | accur. | prec. | recall | spec. | F1 |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| A | GraphEM | 0.081 | 0.9104 | 0.9880 | 0.7407 | 0.9952 | 0.8463 |
|  | MLEM | 0.149 | 0.3333 | 0.3333 | 1 | 0 | 0.5 |
|  | PGC | - | 0.8765 | 0.9474 | 0.6667 | 0.9815 | 0.7826 |
|  | CGC | - | 0.8765 | 1 | 0.6293 | 1 | 0.7727 |
| B | GraphEM | 0.082 | 0.9113 | 0.9914 | 0.7407 | 0.9967 | 0.8477 |
|  | MLEM | 0.148 | 0.3333 | 0.3333 | 1 | 0 | 0.5 |
|  | PGC | - | 0.8889 | 1 | 0.6667 | 1 | 0.8 |
|  | CGC | - | 0.8889 | 1 | 0.6667 | 1 | 0.8 |
| C | GraphEM | 0.120 | 0.9231 | 0.9401 | 0.77 | 0.9785 | 0.8427 |
|  | MLEM | 0.238 | 0.2656 | 0.2656 | 1 | 0 | 0.4198 |
|  | PGC | - | 0.9023 | 0.9778 | 0.6471 | 0.9949 | 0.7788 |
|  | CGC | - | 0.8555 | 0.9697 | 0.4706 | 0.9949 | 0.6337 |
| D | GraphEM | 0.121 | 0.9247 | 0.9601 | 0.7547 | 0.9862 | 0.8421 |
|  | MLEM | 0.239 | 0.2656 | 0.2656 | 1 | 0 | 0.4198 |
|  | PGC | - | 0.8906 | 0.9 | 0.6618 | 0.9734 | 0.7627 |
|  | CGC | - | 0.8477 | 0.9394 | 0.4559 | 0.9894 | 0.6139 |

## Experimental results: Realistic weather datasets



True


GRAPHEM


DGLASSO


PGC


MLEM


CGC

Graph inference results on an example from WeathN5a dataset. ${ }^{11}$

[^11]
## Computational complexity of DGLASSO



Figure 6: Evolution of the complexity time (left), $\operatorname{RMSE}\left(\mathbf{A}^{*}, \widehat{\mathbf{A}}\right)$ (middle) and $\operatorname{cNMSE}\left(\boldsymbol{\mu}^{*}, \widehat{\boldsymbol{\mu}}\right)$ (right) metrics, as a function of the time series length $K$, for experiments on dataset A averaged over 50 runs.

## Performance of DGLASSO (toy example)

|  |  | Estimation of A |  |  | Estimation of P |  |  | Estim. Q | State distrib. |  | Predictive distrib. |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  | Method | RMSE | AUC | F1 | RMSE | AUC | F1 | RMSE | $\mathrm{cNMSE}\left(\boldsymbol{\mu}^{*}, \widehat{\boldsymbol{\mu}}\right)$ | cNMSE $\left(\boldsymbol{\mu}^{5 \pi}, \hat{\boldsymbol{\mu}}^{3}\right)$ | cNMSE $\left(\nu^{*}, \hat{\nu}\right)$ | $\mathcal{L}_{1: K}(\mathbf{A}, \mathbf{P})$ |
|  | DGLASSO | 0.061 | 0.843 | 0.641 | 0.082 | 0.778 | 0.698 | 0.083 | $6.394 \times 10^{-}$ | $1.050 \times 10^{-}$ | $2.984 \times 10^{-4}$ | 12307.169 |
|  | MLEM | 0.076 | 0.817 | 0.500 | 0.105 | 0.857 | 0.500 | 0.102 | $1.095 \times 10^{-7}$ | $1.803 \times 10^{-7}$ | $4.843 \times 10^{-4}$ | 12341.205 |
|  | GLASSO | NA | NA | NA | 0.818 | 0.804 | 0.496 | 1073.510 | $4.485 \times 10^{-6}$ | $7.180 \times 10^{-6}$ | 1.000 | 28459.294 |
|  | rGLASSO | NA | NA | NA | 0.764 | 0.924 | 0.598 | 31.689 | $2.826 \times 10^{-6}$ | $5.492 \times 10^{-6}$ | 1.000 | 22957.693 |
|  | GRAPHEM | 0.045 | 0.895 | 0.847 | NA | NA | NA | NA | $4.364 \times 10^{-6}$ | $6.944 \times 10^{-6}$ | $2.980 \times 10^{-4}$ | 29035.030 |
|  | DGLASSO | 0.068 | 0.833 | 0.603 | 0.070 | 0.893 | 0.835 | 0.071 | $7.490 \times 10^{-8}$ | $1.236 \times 10^{-}$ | $3.281 \times 10^{-}$ | 11806.744 |
|  | MLEM | 0.080 | 0.815 | 0.500 | 0.106 | 0.898 | 0.500 | 0.100 | $1.299 \times 10^{-7}$ | $2.133 \times 10^{-7}$ | $4.619 \times 10^{-4}$ | 11833.448 |
|  | GLASSO | NA | NA | NA | 0.827 | 0.826 | 0.505 | 341.873 | $5.069 \times 10^{-6}$ | $8.072 \times 10^{-6}$ | 1.000 | 27744.964 |
|  | rGLASSO | NA | NA | NA | 0.734 | 0.930 | 0.608 | 33.896 | $3.215 \times 10^{-6}$ | $6.187 \times 10^{-6}$ | 1.000 | 22530.036 |
|  | GRAPHEM | 0.047 | 0.893 | 0.848 | NA | NA | NA | NA | $5.158 \times 10^{-6}$ | $8.036 \times 10^{-6}$ | $2.912 \times 10^{-4}$ | 29031.412 |
|  | DGLASSO | 0.070 | 0.829 | 0.581 | 0.090 | 0.954 | 0.830 | 0.078 | $1.896 \times 10^{-}$ | $2.994 \times 10^{-}$ | $3.956 \times 10^{-}$ | 10311.104 |
|  | MLEM | 0.081 | 0.810 | 0.500 | 0.097 | 0.974 | 0.500 | 0.094 | $2.583 \times 10^{-7}$ | $4.180 \times 10^{-7}$ | $5.053 \times 10^{-4}$ | 10326.410 |
|  | GLASSO | NA | NA | NA | 0.901 | 0.805 | 0.489 | $3.926 \times 10^{17}$ | 0.012 | 0.012 | 1.000 | 26634.892 |
|  | rGLASSO | NA | NA | NA | 0.805 | 0.928 | 0.614 | 29.530 | $7.195 \times 10^{-6}$ | $1.320 \times 10^{-5}$ | 1.000 | 21322.247 |
|  | GRAPHEM | 0.049 | 0.892 | 0.857 | NA | NA | NA | NA | $1.055 \times 10^{-5}$ | $1.641 \times 10^{-5}$ | $3.912 \times 10^{-4}$ | 29023.369 |
|  | DGLASSO | 0.073 | 0.835 | 0.575 | 0.083 | 1.000 | 0.598 | 0.080 | $5.127 \times 10^{-7}$ | $8.243 \times 10^{-7}$ | $3.373 \times 10^{-4}$ | 7911.943 |
|  | MLEM | 0.098 | 0.808 | 0.500 | 0.095 | 1.000 | 0.500 | 0.084 | $6.296 \times 10^{-7}$ | $1.027 \times 10^{-6}$ | $4.219 \times 10^{-4}$ | 7923.850 |
|  | GLASSO | NA | NA | NA | 0.964 | 0.941 | 0.550 | 187.823 | $2.348 \times 10^{-5}$ | $3.701 \times 10^{-5}$ | 1.000 | 23684.178 |
|  | rGLASSO | NA | NA | NA | 0.882 | 0.956 | 0.645 | 28.703 | $1.886 \times 10^{-5}$ | $3.239 \times 10^{-5}$ | 1.000 | 20100.491 |
|  | GRAPHEM | 0.061 | 0.892 | 0.864 | NA | NA | NA | NA | $2.503 \times 10^{-5}$ | $3.839 \times 10^{-5}$ | $3.743 \times 10^{-4}$ | 29016.321 |

## Performance of DGLASSO (climate model)

|  | method | RMSE | accur. | prec. | recall | spec. | F1 | Time (s.) |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| WeathN5a | DGLASSO | 0.108 | 0.937 | 0.894 | 0.998 | 0.894 | 0.937 | 0.608 |
|  | MLEM | 0.140 | 0.413 | 0.413 | 1.000 | 0.000 | 0.584 | 0.596 |
|  | GRAPHEM | 0.127 | 0.703 | 0.595 | 1.000 | 0.496 | 0.742 | 0.606 |
|  | PGC | - | 0.772 | 0.902 | 0.515 | 0.953 | 0.652 | 0.019 |
|  | CGC | - | 0.672 | 0.828 | 0.285 | 0.945 | 0.415 | 0.026 |
| WeathN5b | DGLASSO | 0.166 | 0.773 | 0.668 | 0.992 | 0.619 | 0.788 | 0.630 |
|  | MLEM | 0.197 | 0.413 | 0.413 | 1.000 | 0.000 | 0.584 | 0.376 |
|  | GRAPHEM | 0.186 | 0.629 | 0.536 | 1.000 | 0.368 | 0.694 | 0.470 |
|  | PGC | - | 0.675 | 0.677 | 0.469 | 0.819 | 0.544 | 0.017 |
|  | CGC | - | 0.634 | 0.659 | 0.263 | 0.895 | 0.369 | 0.023 |
| WeathN10a | DGLASSO | 0.202 | 0.948 | 0.898 | 0.925 | 0.954 | 0.890 | 1.363 |
|  | MLEM | 0.264 | 0.219 | 0.219 | 1.000 | 0.000 | 0.359 | 0.834 |
|  | GRAPHEM | 0.224 | 0.511 | 0.311 | 1.000 | 0.374 | 0.473 | 1.445 |
|  | PGC | - | 0.879 | 0.904 | 0.504 | 0.983 | 0.644 | 0.232 |
|  | CGC | - | 0.773 | 0.539 | 0.211 | 0.932 | 0.278 | 0.358 |
| WeathN10b | DGLASSO | 0.192 | 0.866 | 0.633 | 0.994 | 0.829 | 0.769 | 0.557 |
|  | MLEM | 0.342 | 0.219 | 0.219 | 1.000 | 0.000 | 0.359 | 0.989 |
|  | GRAPHEM | 0.219 | 0.855 | 0.620 | 0.994 | 0.816 | 0.757 | 0.655 |
|  | PGC | - | 0.799 | 0.558 | 0.473 | 0.890 | 0.506 | 0.154 |
|  | CGC | - | 0.750 | 0.407 | 0.218 | 0.900 | 0.265 | 0.178 |

## Convergence of SpaRJ and GarphEM with data



Figure: $3 \times 3$ system with known isotropic state covariance.

## Convergence of SpaRJ with iterations



Figure: Progression of sample metrics in a $12 \times 12$.

## Real-world applications

- cardiology application of finding rotors in atrial fibrillation
- topology discovery is the key
- climate models
- already tested over realistic climate synthetic data (the Causality for Climate Competition, NeurIPS 2019)
- preliminary work "Graphs in State-Space Models for Granger Causality in Climate Science" at CausalStats 2023
- networks, neuroscience, ..., ideas? :-)


## Outline

```
Introduction
Linear-Gaussian model and Kalman filter
A doubly graphical perspective on SSMs
Point-wise estimation: GraphEM and DGLASSO algorithms
Point-wise estimation: extensions
Probabilistic estimation
Experimental evaluation
```

Conclusion

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- Novel graphical interpretation on matrices $\mathbf{A}$ and $\mathbf{Q}$ in LG-SSMs.
- Algorithms to estimate only a sparse A: GraphEM (point-wise) and SpaRJ (fully Bayesian).
- GraphEM is faster and allows explicit penalty functions (prior knowledge) beyond sparsity.
- SpaRJ provides samples of the posterior allowing for uncertainty quantification.
- Algorithm to estimate both sparse A and Q: DGLASSO (point-wise)
$\rightarrow$ strong model interpretation
- sophisticated optimization scheme
- All have solid theoretical guarantees and show good performance.
$\rightarrow$ This is a challenging problem with many exciting ongoing methodological and applied avenues ahead!


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## Thank you for your attention!

GraphEM paper: V. Elvira, É. Chouzenoux, "Graphical Inference in Linear-Gaussian State-Space Models", IEEE Transactions on Signal Processing, Vol. 70, pp. 4757-4771, 2022.

SpaRJ: B. Cox and V. Elvira, "Sparse Bayesian Estimation of Parameters in Linear-Gaussian State-Space Models", IEEE Transactions on Signal Processing, vol. 71, pp. 1922-1937, 2023.

GraphIT paper: E. Chouzenoux and V. Elvira, "Iterative reweighted $\ell_{1}$ algorithm for sparse graph inference in state-space models", IEEE International Conf. on Acoustics, Speech, and Signal Processing (ICASSP 2023), Rhodes, Greece, June, 2023.

Non-Markovian models: E. Chouzenoux and V. Elvira, "Graphical Inference in Non-Markovian Linear-Gaussian State-space Models", IEEE International Conf. on Acoustics, Speech, and Signal Processing (ICASSP 2024), Seoul, Korea, April, 2024.

## Under review:

- DGLASSO: E. Chouzenoux and V. Elvira, "Sparse Graphical Linear Dynamical Systems, submitted, 2023. https://arxiv.org/abs/2307.03210
- Application to climate: V. Elvira, E. Chouzenoux, J. Cerda, and G. Camps-Valls "Graphs in State-Space Models for Granger Causality in Climate Science", CausalStats Workshop, 2023.
- Community detection paper: B. Cox and V. Elvira, "Community Detection for structural Parameter Estimation in Linear-Gaussian State-Space Models", 2024.

GraphEM in a nutshell

- Goal. MAP estimate of A:

$$
\mathbf{A}^{*}=\operatorname{argmax}_{\mathbf{A}} p\left(\mathbf{A} \mid \mathbf{y}_{1: T}\right)=\operatorname{argmax}_{\mathbf{A}} p(\mathbf{A}) p\left(\mathbf{y}_{1: T} \mid \mathbf{A}\right)
$$

- Equivalent to minimizing $\mathcal{L}(\mathbf{A})=-\log p(\mathbf{A})-\log p\left(\mathbf{y}_{1: T} \mid \mathbf{A}\right)$.
$\Rightarrow$ Challenges: evaluating $\mathcal{L}_{1: T}(\mathbf{A}) \equiv-\log p\left(\mathbf{y}_{1: T} \mid \mathbf{A}\right)$ requires to run the $K F$ :

- Function $\mathcal{L}_{0}(\mathbf{A}) \equiv-\log p(\mathbf{A})$ might be complicated (e.g., non smooth)
- Non tractable minimization.
$\rightarrow$ Simplest version of GraphEM: ${ }^{12}$ an EM strategy to minimize a sequence of (tractable) majorizing approximations of $\mathcal{L}$.
- Lasso regularization (Laplace prior) to promote a sparse matrix A. $\left(\forall \mathbf{A} \in \mathbb{R}^{N_{x} \times N_{x}}\right) \quad \mathcal{L}_{0}(\mathbf{A})=\gamma\|\mathbf{A}\|_{1}, \quad \gamma>0$.

[^12]
## GraphEM in a nutshell

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[^15]
## Expression of EM steps

- Majorizing approximation (E-step): Run the Kalman filter/RTS smoother by setting the state matrix to $\mathbf{A}^{\prime}$ and define ${ }^{13}$

$$
\begin{aligned}
& \boldsymbol{\Sigma}=\frac{1}{T} \sum_{t=1}^{T} \mathbf{P}_{t}^{s}+\mathbf{m}_{t}^{s}\left(\mathbf{m}_{t}^{s}\right)^{\top} \\
& \mathbf{\Phi}=\frac{1}{T} \sum_{t=1}^{T} \mathbf{P}_{t-1}^{s}+\mathbf{m}_{t-1}^{s}\left(\mathbf{m}_{t-1}^{s}\right)^{\top} \\
& \mathbf{C}=\frac{1}{T} \sum_{t=1}^{T} \mathbf{P}_{t}^{s} \mathbf{G}_{t-1}^{\top}+\mathbf{m}_{t}^{s}\left(\mathbf{m}_{t-1}^{s}\right)^{\top}
\end{aligned}
$$

and build

$$
\mathcal{Q}\left(\mathbf{A} ; \mathbf{A}^{\prime}\right)=\frac{T}{2} \operatorname{tr}\left(\mathbf{Q}^{-1}\left(\boldsymbol{\Sigma}-\mathbf{C} \mathbf{A}^{\top}-\mathbf{A} \mathbf{C}^{\top}+\mathbf{A} \boldsymbol{\Phi} \mathbf{A}^{\top}\right)\right)+\mathcal{L}_{0}(\mathbf{A})+\mathrm{ct} / \mathbf{A}
$$

such that, for every $\mathbf{A} \in \mathbb{R}^{N_{x} \times N_{x}}$ :

$$
\mathcal{Q}\left(\mathbf{A} ; \mathbf{A}^{\prime}\right) \geq \mathcal{L}(\mathbf{A}), \quad \text { and } \quad \mathcal{Q}\left(\mathbf{A}^{\prime} ; \mathbf{A}^{\prime}\right)=\mathcal{L}\left(\mathbf{A}^{\prime}\right)
$$

- Upper bound optimization (M-step): The M-step consists in searching for a minimizer of $\mathcal{Q}\left(\mathbf{A} ; \mathbf{A}^{\prime}\right)$ with respect to $\mathbf{A}\left(\mathbf{A}^{\prime}\right.$ being fixed).

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[^17]
## Computation of the M-step

- Convex non-smooth minimization problem
$\operatorname{argmin}_{\mathbf{A}} \underbrace{\mathcal{Q}\left(\mathbf{A} ; \mathbf{A}^{\prime}\right)}_{f(\mathbf{A})}=\operatorname{argmin}_{\mathbf{A}} \underbrace{\frac{T}{2} \operatorname{tr}\left(\mathbf{Q}^{-1}\left(\boldsymbol{\Sigma}-\mathbf{C} \mathbf{A}^{\top}-\mathbf{A} \mathbf{C}^{\top}+\mathbf{A} \boldsymbol{\Phi} \mathbf{A}^{\top}\right)\right)}_{f_{1}(\mathbf{A})=\text { upper bound of }-\log \left(p\left(\mathbf{y}_{1: T} \mid \mathbf{A}\right)\right)}+\underbrace{\gamma\|\mathbf{A}\|_{1}}_{\substack{f_{2}(\mathbf{A})=-\log p(\mathbf{A}) \\ \text { (prior) }}}$

Proximal splitting approach: The proximity operator of $f: \mathbb{R}^{N_{x} \times N_{x}} \rightarrow \mathbb{R}$ is
defined

$$
\operatorname{prox}_{f}(\tilde{\mathbf{A}})=\operatorname{argmin}_{\mathbf{A}}\left(f(\mathbf{A})+\frac{1}{2}\|\mathbf{A}-\widetilde{\mathbf{A}}\|_{F}^{2}\right)
$$

## Douglas-Rachford algorithm in GraphEM

Set $Z_{0} \in \mathbb{R}^{N_{x} \times N_{x}}$ and $\theta \in(0,2)$.
$\rightarrow$ For $n=1,2$,

$\checkmark\left\{\mathbf{A}_{n}\right\}_{n \in \mathbb{N}}$ guaranteed to converge to a minimizer of $\mathcal{Q}\left(\mathbf{A} ; \mathbf{A}^{\prime}\right)=f_{1}+f_{2}$
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$$
\begin{aligned}
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& \mathbf{Z}_{n+1}=\mathbf{Z}_{n}+\theta\left(\mathbf{V}_{n}-\mathbf{A}_{n}\right)
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[^18]
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## Generic GraphEM algorithm

- generic GraphEM allows for a larger family of priors (and several): ${ }^{14}$

$$
\begin{equation*}
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\end{equation*}
$$

- $f_{1}(\mathbf{A})$ is still an upper bound of $-\log \left(p\left(\mathbf{y}_{1: T} \mid \mathbf{A}\right)\right)$
- $f_{M}(\mathbf{A})=\gamma\|\mathbf{A}\|_{1}$ (sparsity promoter)
- other losses $\left\{f_{m}(\mathbf{A})\right\}_{m=2}^{M-1}$ promote properties in $\mathbf{A}$ (e.g., stability)


## $\rightarrow$ The inference now requires a more sophisticated optimization algorithm in the $M$-step, the monotone+skew algorithm

## MS algonthm for a generic GraphelMs (M-step)

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MS algorithm for a generic GraphEMs (M-step)

[^20] Models". In: IEEE Transactions on Signal Processing 70 (2022), pp. 4757-4771.

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- $f_{1}(\mathbf{A})$ is still an upper bound of $-\log \left(p\left(\mathbf{y}_{1: T} \mid \mathbf{A}\right)\right)$
- $f_{M}(\mathbf{A})=\gamma\|\mathbf{A}\|_{1}$ (sparsity promoter)
- other losses $\left\{f_{m}(\mathbf{A})\right\}_{m=2}^{M-1}$ promote properties in $\mathbf{A}$ (e.g., stability)
- The inference now requires a more sophisticated optimization algorithm in the $M$-step, the monotone+skew algorithm.


## MS algorithm for a generic GraphEMs (M-step)

- Set $\mathbf{V}_{0}^{m}=\mathbf{A}^{\prime} \forall m \in\{1, \ldots, M\}$, and stepsizes $\lambda \in\left(0, \frac{1}{M}\right), \gamma \in\left[\lambda, \frac{1-\lambda}{M-1}\right]$.
- For $n=1,2, \ldots$.

$$
\begin{aligned}
& \mathbf{W}_{n}^{m}=\mathbf{V}_{n}^{m}+\gamma \mathbf{V}_{n}^{M}(\forall m \in\{1, \ldots, M-1\}) \\
& \mathbf{W}_{n}^{M}=\mathbf{V}_{n}^{M}-\gamma \sum_{m=1}^{M-1} \mathbf{V}_{n}^{m} \\
& \mathbf{A}_{n}^{m}=\mathbf{W}_{n}^{m}-\gamma \operatorname{prox}_{f m} / \mathbf{p r}_{n}^{m}(\forall m \in\{1, \ldots, M-1\}) \\
& \mathbf{A}_{n}^{M}=\operatorname{prox}_{\gamma f_{M}}\left(\mathbf{W}_{n}^{M}\right) \\
& \mathbf{Z}_{n}^{m}=\mathbf{A}_{n}^{m}+\gamma \mathbf{A}_{n}^{M}(\forall m \in\{1, \ldots, M-1\}) \\
& \mathbf{Z}_{n}^{M}=\mathbf{A}_{n}^{M}-\gamma \sum_{m-1}^{M=1} \mathbf{A}_{n}^{m} \\
& \mathbf{V}_{n+1}^{m}=\mathbf{V}_{n}^{m}-\mathbf{W}_{n}^{m}+\mathbf{Z}_{n}^{m}(\forall m \in\{1, \ldots, M\})
\end{aligned}
$$

[^21]
## Theoretical guarantees

## Theorem

Assume that the prior term $\mathcal{L}_{0}$ is proper, convex, lower semicontinuous. Under mild technical assumptions (qualification conditions),

- $\left\{\mathcal{L}\left(\mathbf{A}^{(i)}\right)\right\}_{i \in \mathbb{N}}$ is a decreasing sequence converging to a finite limit $\mathcal{L}^{*}$.
- The sequence of iterates $\left\{\mathbf{A}^{(i)}\right\}_{i \in \mathbb{N}}$ has a cluster point (i.e., one can extract a converging subsequence)
- Let $\mathbf{A}^{*}$ a cluster point (i.e., the limit of a converging subsequence) of $\left\{\mathbf{A}^{(i)}\right\}_{i \in \mathbb{N}}$. Then, $\mathcal{L}\left(\mathbf{A}^{*}\right)=\mathcal{L}^{*}$ and $\mathbf{A}^{*}$ is a critical point of $\mathcal{L}$, i.e., $\nabla \mathcal{L}_{1: T}\left(\mathbf{A}^{*}\right) \in \partial \mathcal{L}_{0}\left(\mathbf{A}^{*}\right)$.


## Data description and numerical settings

- Four synthetic datasets with $\mathbf{H}=\mathbf{I d}$, size $N_{x}=N_{y}=9$, and randomly generated ground truth sparse matrices $\mathbf{A}^{*}$ and $\mathbf{P}^{*}$ (block diagonal $3 \times 3$ ) with varying conditioning for $\mathbf{Q}^{*}=\left(\mathbf{P}^{*}\right)^{-1}$. We set $K=10^{3}$ and $\mathbf{R}=\sigma_{\mathbf{R}}^{2} \mathbf{I d}, \mathbf{P}_{0}=\sigma_{0}^{2} \mathbf{I d}$ with $\left(\sigma_{\mathbf{R}}, \sigma_{0}\right)=\left(10^{-1}, 10^{-4}\right)$.
- Goal: (i) Given $\left\{\mathbf{y}_{k}\right\}_{k=1}^{K}$, and $\left(\mathbf{H}, \mathbf{R}, \mathbf{P}_{0}\right)$, provide estimates $(\widehat{\mathbf{A}}, \widehat{\mathbf{P}})$ of ( $\mathbf{A}^{*}, \mathbf{P}^{*}$ ), evaluated by RMSE and $\mathbf{F}_{1}$ metrics, (ii) Given a new test data, compute the the predictive distribution means by KF/RTS using the estimated model parameters, evaluated by cNMSE and loss metrics.
- DGLASSO, is compared with:
- Maximum likelihood EM (MLEM): DGLASSO model with $\lambda_{A}=\lambda_{P}=0$.
- GRAPHEM approach [Elvira et al., 2022]: MAP estimate of A, while fixing $\widehat{\mathbf{Q}}=\sigma_{Q}^{2}$ Id with finetuned $\sigma_{Q}$.
- GLASSO approach [Friedman et al., 2008]: MAP estimate of $\mathbf{P}$, fixing $\widehat{\mathbf{A}}=\mathbf{0}$ and neglecting $\mathbf{R}$.
- rGLASSO approach [Benfenati et al., 2020]: MAP estimate of $\mathbf{P}$, fixing $\widehat{\mathrm{A}}=\mathbf{0}$.
- Pairwise Granger Causality (PGC) / conditional Granger Causality (CGC) based on sparse vector autoregressive (VAR) models [Luengo et al., 2019].
- Manual finetuning of hyperparameters (e.g., $\ell_{1}$ penalty weight) on a single realization (see more details in paper). Results are averaged on 50


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[^18]:    $\checkmark\left\{\mathbf{A}_{n}\right\}_{n \in \mathbb{N}}$ guaranteed to converge to a minimizer of $\mathcal{Q}\left(\mathbf{A} ; \mathbf{A}^{\prime}\right)=f_{1}+f_{2}$
    \& Both involved proximity operators have closed form solution

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