# Exact Bayesian inference for off-line change-point detection in tree-structured graphical models

### Loïc Schwaller Statistics for Structures Seminar







March 17, 2017



- 1. Choose an order.
- 2. First player





- 1. Choose an order.
- 2. First player







- 1. Choose an order.
- 2. First player







- 1. Choose an order.
- 2. First player







- 1. Choose an order.
- 2. First player







- 3. Repeat 2 for some time.
- 4. Change order.
- 5. Repeat 2 for some time.

- 3. Repeat 2 for some time.
- 4. Change order.
- 5. Repeat 2 for some time.



- 3. Repeat 2 for some time.
- 4. Change order.
- 5. Repeat 2 for some time.



- 3. Repeat 2 for some time.
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- 5. Repeat 2 for some time.



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- Expression levels of 11 genes involved in wing muscle development
- ▶ 67 time-points



<sup>&</sup>lt;sup>1</sup>Arbeitman et al. 2002.

#### Exact Bayesian Inference in Graphical Models Using Trees



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#### Exact Bayesian Inference in Graphical Models Using Trees

<sup>&</sup>lt;sup>1</sup>Arbeitman et al. 2002.

► Bayesian inference

Exact inference

### **Bayesian** inference

## Requirement

- Providing a full probabilistic construction
  - Prior distributions
- Exact inference

### Bayesian inference

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- Providing a full probabilistic construction
  - Prior distributions
- Exact inference

- ▷ Graphical models
  - Markov property
  - hyper Markov property

Tool

### Bayesian inference

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- Providing a full probabilistic construction
  - Prior distributions

- ▷ Graphical models
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Tool

Exact inference

### Requirement

- Dealing with the combinatorial issue
  - $\binom{N-1}{K-1}$  segmentations
  - $2^{p(p-1)/2}$  undirected graphs

Bayesian inference	
Requirement	Tool
<ul> <li>Providing a full probabilistic construction</li> <li>Prior distributions</li> </ul>	<ul> <li>Graphical models</li> <li>Markov property</li> <li>hyper Markov property</li> </ul>
• Exact inference	
Requirement	Tool

- Dealing with the combinatorial issue
  - $\binom{N-1}{K-1}$  segmentations
  - $2^{p(p-1)/2}$  undirected graphs

- ▷ Algebraic results
  - Segmentations
  - Spanning trees (Meilă and Jaakkola 2007)

### Outline



## Introduction Graphical models

## Graphical models



$$p(\mathbf{\mathring{+}}, \mathbf{\mathring{+}}, \mathbf{\mathring{+}}) = p(\mathbf{\mathring{+}})p(\mathbf{\mathring{+}}|\mathbf{\mathring{+}})p(\mathbf{\mathring{+}}|\mathbf{\mathring{+}})p(\mathbf{\mathring{+}}|\mathbf{\mathring{+}})$$

## Graphical models



 Graphical models extend this reasoning to arbitrary dependence structures.

## Graphical models



 Graphical models extend this reasoning to arbitrary dependence structures.

Directed Acyclic Graphs



Undirected Graphs



## Undirected graphs

- ► **V** = {1, ..., *p*}
- $\mathcal{P}_2(V)$  = subsets of V of size 2



### Definition

For  $E \subseteq \mathcal{P}_2(V)$ ,  $G = (V, E_G)$  is the undirected graph with **vertices** V and **edges**  $E_G$ .

## Undirected graphs

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### Definition

For  $E \subseteq \mathcal{P}_2(V)$ ,  $G = (V, E_G)$  is the undirected graph with vertices V and edges  $E_G$ .

### Definition

A clique is a fully connected subsets of vertices.

Exact Bayesian Inference in Graphical Models Using Trees

## Graph decomposition

- $G = (V, E_G)$
- $A, B \subseteq V$

### Definition

(A, B) is a **decomposition** of G if

- $A \cup B = V$
- $A \cap B$  is a clique
- $A \cap B$  separates A from B



## Markov property

►  $Y = (Y_1, ..., Y_p)$  a random vector taking values in  $\mathcal{Y} = \bigotimes_{i=1}^p \mathcal{Y}_i$ 

• 
$$Y_A := (Y_\alpha)_{\alpha \in A}, A \subseteq V$$



### Definition

A distribution  $\pi$  for Y is **Markov** w.r.t. G, if for all decompositions (A, B) of G,

 $Y_A \perp\!\!\!\perp Y_B | Y_{A \cap B}$ 

 $\mathfrak{M}_{G} = \{ \text{distributions } \pi \text{ Markov w.r.t. } G \}$ 

## Factorisation

- ►  $Y = (Y_1, ..., Y_p)$  a random vector taking values in  $\mathcal{Y} = \bigotimes_{i=1}^p \mathcal{Y}_i$
- $Y_A := (Y_\alpha)_{\alpha \in A}, A \subseteq V$
- $Y \sim \pi$  with positive density

### Proposition

$$(\pi \text{ Markov w.r.t. } G) \Leftrightarrow (\pi(Y) = \prod_{C \in C_G} \psi_C(Y_C))$$

C<sub>G</sub> maximal cliques of G



## Graphical models (formally)

### Definition (Graphical Model)

### An undirected graphical model is a couple $(G, \mathcal{F}_G)$ where

- ▶ G is an undirected graph,
- $\mathcal{F}_G \subseteq \mathfrak{M}_G$  is a family of distributions Markov w.r.t. G.

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### **Bayesian inference**



- Some Markov property for  $\rho$ 

## Strong hyper Markov property

- $(G, \mathcal{F}_G)$  graphical model
- $\rho$  hyperdistribution on  $\mathcal{F}_{G}$
- $\pi \sim \rho$

### Definition

 $\rho$  is said to be **strong hyper Markov** w.r.t. *G* if, for any decomposition (*A*, *B*) of *G*,

 $\pi_A \perp \!\!\!\perp \pi_{B|A}.$ 



## Strong hyper Markov property

- $(G, \mathcal{F}_G)$  graphical model
- $\rho$  hyperdistribution on  $\mathcal{F}_{G}$
- $\pi \sim \rho$

### Proposition (Dawid and Lauritzen 1993)

If  $\rho$  is strong hyper Markov w.r.t. G, then the marginal likelihood

$$p(Y) = \int \pi(Y) \rho(\pi) d\pi$$

is Markov w.r.t. to G.

## Strong hyper Markov property

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## Compatible family

- $\rho$  strong hyper Markov w.r.t. to the **complete graph**
- ► G graph

### Proposition (Dawid and Lauritzen 1993)

There exists a unique hyperdistribution  $\rho^{G}$  on  $\mathfrak{M}_{G}$  that is strong hyper Markov w.r.t. G and s.t.

$$\forall C \in C_G, \ \rho_C^G = \rho_C.$$

- $\rho_C$  hyperdistribution induced by  $\rho$  on  $\pi_C$
- C<sub>G</sub> maximal cliques of G

## Compatible family

- $\mathcal{G} = \{G_1, \ldots, G_u\}$  graph family
- $\rho$  strong hyper Markov w.r.t. to the complete graph

### Definition

The **compatible family** built on  $\mathcal{G}$  from  $\rho$  is given by  $\{\rho^G\}_{G \in \mathcal{G}}$ 

$$C \in C_{G_i} \cap C_{G_j}$$

$$\underbrace{\int \pi_C(Y_C)\rho_C^{G_i}(\pi_C)d\pi_C}_{p(Y_C|G_i)} = \underbrace{\int \pi_C(Y_C)\rho_C^{G_j}(\pi_C)d\pi_C}_{p(Y_C|G_j)}$$
#### In practice

#### • $\rho$ given by a **parametric distribution**

Y	π	ρ
$R^{ ho}$	Normal	(Normal-)Wishart Geiger and Heckerman 2002
$\{1,\ldots,r\}^p$	Multinomial	Dirichlet Dawid and Lauritzen 1993
[0; 1] <sup>p</sup>	Copula	Depends on the copula Schwaller et al. 2015

Introduction
Algebraic magic bag

### Algebraic tricks

# ΣΠ

- Computing sum-products
  - For spanning trees
  - For segmentations

## Spanning Trees

#### Definition

A spanning tree is a connected graph with no cycles.



$$\mathcal{T} := \left\{ T = (V, E_T) \text{ spanning tree on } V \right\}$$

$$|\mathcal{T}| = p^{p-2}$$

$$Maximal cliques = edges$$

#### Summing over $\mathcal{T}$



Theorem (Matrix-Tree, Kirchhoff 1847, Cayley 1889)

$$\Delta_{ij} = \begin{cases} -b_{ij} & \text{if } i \neq j \\ \sum_{k} b_{kj} & \text{if } i = j \end{cases}$$

All cofactors of  $\Delta$  are equal to Z(b).

# **Complexity** = $O(p^3)$

#### Segmentations

#### Definition

A segmentation of [[1; N]] is a partition of [[1; N]] into sets of consecutive elements called segments.



### Summing over $\mathcal{M}_{\mathcal{K}}$



Proposition (Rigaill et al. 2012)

 $C_K(a) = [a^K]_{1,N+1}$ 

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## Model & Inference

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•  $Y = \{Y^t\}_{t=1}^N$  multivariate random process of dimension p

$$\mathbf{Y}^{\mathsf{t}} \qquad \mathbf{Y}^{\mathsf{t}_{s,s,l}}$$

$$\mathbf{Y}_{2} \qquad \mathcal{N}_{1} \qquad \mathcal{N}_{2} \qquad \mathcal{N}_{1} \qquad \mathcal{N}_{2} \qquad \mathcal{N}_{2} \qquad \mathcal{N}_{1} \qquad \mathcal{N}_{2} \qquad \mathcal{N}_{$$













#### Model



#### Model



#### Inference

Marginal likelihood

$$p(Y|K) = \sum_{m \in \mathcal{M}_K} \sum_{\mathbf{T} \in \mathcal{T}^K} \int p(Y, \Pi, \mathbf{T}, m|K) d\Pi$$

$$|\mathcal{M}_{K}| \cdot |\mathcal{T}^{K}| = \binom{N-1}{K-1} \cdot p^{K(p-2)} \approx \left(\frac{Np^{p-2}}{K}\right)^{K}$$

# ExampleN = 200 $|\mathcal{M}_4| \approx 1.3 \cdot 10^6$ p = 10 $|\mathcal{T}| = 10^8$

#### A complexity result

#### Proposition (Schwaller and Robin 2016)

Under some assumptions on prior distributions, the marginal likelihood p(Y|K) can be computed in  $O(\max(K, p^3)N^2)$  time from locally integrated quantities on  $\Pi$ .

## Prior distributions

"Under some assumptions on prior distributions"
'
• On segmentations m
• On trees $T = (T_1, \dots, T_K)$
• On <b>distributions</b> $\Pi = (\pi_1,, \pi_K)$

Prior distribution on m



$$p(m|\mathcal{K}) = \frac{1}{C_{\mathcal{K}}(a)} \prod_{[s;t] \in m} a_{st}$$

$$C_{\mathcal{K}}(a) = \sum_{m \in \mathcal{M}_{\mathcal{K}}} \prod_{[s;t] \in m} a_{st}$$



### Prior distribution on m



$$p(Y|K) = \sum_{m} p(m|K)p(Y|m) = \frac{1}{C_{\mathcal{K}}(a)} \sum_{m} p(Y|m) \prod_{[s;t] \in m} a_{st}$$

### Prior distribution on m



$$p(Y|K) = \sum_{m} p(m|K)p(Y|m) = \frac{1}{C_{K}(a)} \underbrace{\sum_{m} p(Y|m) \prod_{[s;t] \in m} a_{st}}_{C_{K}(A)}$$

# Factorising p(Y|m)

$$p(Y|m) = \sum_{\mathbf{T}\in\mathcal{T}^{K}} \int \underbrace{p(Y,\Pi,\mathbf{T}|m)}_{p(\mathbf{T})p(\Pi|\mathbf{T})p(Y|\Pi,m)} d\Pi$$

$$= \sum_{\mathbf{T}\in\mathcal{T}^{K}}\prod_{k}p(T_{k})\int\prod_{k}p(Y^{r_{k}}|\pi_{k})\prod_{k}p(\pi_{k}|T_{k})d\pi_{k}$$

$$=\prod_{k}\underbrace{\sum_{T\in\mathcal{T}}p(T)\int p(Y^{r_{k}}|\pi_{k})p(\pi_{k}|T)d\pi_{k}}_{(M_{k})}$$

 $p(Y^{r_k}) =$  marginal likelihood on  $r_k$ 

#### Integrating on m



## Integrating on m



$$p(m) = \frac{1}{C_{\mathcal{K}}(a)} \prod_{[s;t] \in m} a_{st}$$

$$p(Y|K) = \frac{1}{C_{K}(a)} \sum_{m \in \mathcal{M}_{K}} \prod_{\llbracket s; t \rrbracket \in m} a_{st} \cdot p(Y^{\llbracket s; t \rrbracket})$$

#### Integrating on m



#### Marginal likelihood on a segment

$$p(Y^r) = \sum_{T \in \mathcal{T}} p(T) \int p(Y^r | \pi) p(\pi | T) d\pi$$



#### Prior distribution on T

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$$p(T) = \frac{1}{Z(b)} \prod_{\{i,j\} \in E_T} b_{ij}$$

$$Z(b) = \sum_{T \in \mathcal{T}} \prod_{\{i,j\} \in E_T} b_{ij}$$



### Prior distribution on T

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$$p(T) = \frac{1}{Z(b)} \prod_{\{i,j\} \in E_T} b_{ij}$$

$$p(Y^r) = \frac{1}{Z(b)} \sum_{T \in \mathcal{T}} \int p(Y^r | \pi) p(\pi | T) d\pi \prod_{\{i, j\} \in E_T} b_{ij}$$

### Prior distribution on T

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$$p(T) = \frac{1}{Z(b)} \prod_{\{i,j\} \in E_T} b_{ij}$$

$$p(Y^r) = \frac{1}{Z(b)} \underbrace{\sum_{T \in \mathcal{T}} \int p(Y^r | \pi) p(\pi | T) d\pi \prod_{\{i, j\} \in E_T} b_{ij}}_{\propto Z(B)}$$

## Prior distribution on $\pi$

- $\rho$  strong hyper Markov w.r.t. to the complete graph
- $\{\rho^T\}_{T \in \mathcal{T}}$  compatible family built from  $\rho$  on  $\mathcal{T}$

$$p(\pi|T) = \rho^{T}(\pi) \qquad \forall T \in \mathcal{T}$$

## Prior distribution on $\pi$

 $\begin{array}{l} \bullet \quad \rho \quad \mbox{ strong hyper Markov w.r.t. to the complete graph} \\ \bullet \quad \{\rho^{T}\}_{T \in \mathcal{T}} \quad \mbox{ compatible family built from } \rho \mbox{ on } \mathcal{T} \end{array}$ 

$$p(\pi|T) = \rho^T(\pi) \qquad \forall T \in \mathcal{T}$$

$$p(Y^r|T) = \underbrace{\prod_i p(Y_i^r)}_{U^{(r)}} \prod_{\{i,j\}\in E_T} \frac{p(Y_i^r, Y_j)}{p(Y_i^r)p(Y_j^r)}$$

$$p(Y_i^r, Y_j^r) = \int \pi_{ij}(Y_i^r, Y_j^r) \rho_{ij}(\pi_{ij}) d\pi_{ij}$$
$$p(Y_i^r) = \int \pi_i(Y_i^r) \rho_i(\pi_i) d\pi_i$$

### Integrating on T

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 $p(T) = \frac{1}{Z(b)} \prod_{\{i,j\} \in E_T} b_{ij}$ 

#### Integrating on T

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 $p(T) = \frac{1}{Z(b)} \prod_{\{i,j\}\in F_T} b_{ij}$ 

 $p(Y^r) = \frac{1}{Z(b)} U^{(r)} \sum_{T \in \mathcal{T}} \prod_{\{i,i\} \in F_{\mathcal{T}}} b_{ij} \frac{p(Y_i^r, Y_j^r)}{p(Y_i^r) p(Y_i^r)}$ 

## Integrating on T

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$$p(T) = \frac{1}{Z(b)} \prod_{\{i,j\} \in E_T} b_{ij}$$

$$p(Y^r) = U^{(r)} \cdot \frac{Z(B^{(r)})}{Z(b)}$$

$$B_{ij}^{(r)} = b_{ij} \cdot \frac{p(Y_i^r, y_j^r)}{p(Y_i^r)p(Y_j^r)}$$

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## In a nutshell



# In a nutshell

### Proposition (Schwaller and Robin 2016)

Under some assumptions on prior distributions, the marginal likelihood p(Y|K) can be computed in  $O(\max(K, p^3)N^2)$  time from locally integrated quantities on  $\Pi$ .

# Other quantities

Posterior probability of events

{there is a change-point at time t}
{m contains segment [[s; t[]]}



Posterior distribution of K

$$p(K|Y) \propto \frac{p(K)[A^K]_{1,N+1}}{[a^K]_{1,N+1}}$$







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# Data generation

- ▶ *p* = 10 variables
- Time-series of size N = 70, 140 and 210
- Four segments of lengths  $\frac{3}{7}N$ ,  $\frac{1}{7}N$ ,  $\frac{2}{7}N$



- Three structure scenarios
  - spanning trees
  - Erdös-Rényi, p<sub>C</sub> = 2/p
  - Erdös-Rényi, p<sub>C</sub> = 4/p
- For each sample size and structure series, 100 datasets with centered Gaussian observations were generated.

# Inference

## Tree model

Number of segments	K	$K \sim \mathcal{P}(4)$
Segmentation	т	$m \sim \mathcal{U}(\mathcal{M}_{\mathcal{K}})$
Trees	$\{T_k\}_{k=1}^K$ i.i.d.	$T_k \sim \mathcal{U}(\mathcal{T})$
Precision matrices	$\{\Lambda_r\}_{r\in m}$ ind.	$\Lambda_r \sim h \mathcal{W}(\alpha, \phi, T_{\kappa(r m)})$
Observations	$\{Y_t\}_{t=1}^N$ ind.	$Y^t \sim \mathcal{N}(0_p, \Lambda_r)  \forall t \in r$

# Inference

#### Full model \_\_\_\_\_

Number of segments	K	$K \sim \mathcal{P}(4)$
Segmentation	т	$m \sim \mathcal{U}(\mathcal{M}_K)$
Precision matrices	$\{\Lambda_r\}_{r\in m}$ i.i.d	$\Lambda_r \sim \mathcal{W}(\alpha, \phi)$
Observations	$\{Y_t\}_{t=1}^N$ ind.	$Y^t \sim \mathcal{N}(0_p, \Lambda_r)  \forall t \in r$



Posterior probability of a change-point occurring at time t, integrated on K

### ER, low density scenario



Posterior probability of a change-point occurring at time t, integrated on K

### ER, high density scenario



Posterior probability of a change-point occurring at time t, integrated on K



# Applications



▶ Expression levels of 11 genes involved in wing muscle development







- 5 segments selected by p(K|Y)
- Best segmentation found by Neighbourhood Search algorithm (Auger and Lawrence 1989)



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# fMRI Data<sup>2</sup>

- Averaged blood flow of 5 regions
- 20 participants
- 215 images at 2s intervals



<sup>&</sup>lt;sup>2</sup>Cribben et al. 2012.

# fMRI data<sup>3</sup>



<sup>&</sup>lt;sup>3</sup>Cribben et al. 2012.

# Extensions

## Covariates

- ▷ Easy to take into account in a Gaussian setting
- ▷ Not so much generally



# Extensions

- Temporal dependence
  - ▷ Within segments
  - ▶ Based on Temporal Interaction Models (Siracusa 2009)



**Conclusion & Perspectives** 

# Conclusion & Perspectives

Problem at hand					
<ul> <li>Segmentation of the dependence structure in a multivariate time-series</li> </ul>					
So far					
• Exact & Bayesian inference in $O(\max(p^3, K)N^2)$ time					
Using algebraic results on					
Spanning Trees					
<ul> <li>Segmentations</li> </ul>					
Using (hyper) Markov properties					
Perspectives					
► Numerical issues					
► R package					

## References

⊨	Michelle N Arbeitman Fileen F M Furlong Farhad Imam Fric Johnson Brian
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