Hawkes process as models for some genomic data

P. Reynaud-Bouret

CNRS - LJAD University of Nice

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Motifs

= words in the DNA-alphabet \{actg\}. 
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- Unexpected frequency → Markov models (see for a review Reinert, Schbath, Waterman (2000))
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- If two motifs are part of a common biological process, the space between their occurrences (not necessarily consecutive) should be somehow fixed $\rightarrow$ favored or avoided distances (Gusto, Schbath (2005))
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Several examples

TRE

Transcription Regulatory Elements = ”everything” that may enhance or repress gene expression
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- promoter, enhancer, silencer, histone modifications on the DNA.... They should interact but how? Can we have a statistical guess?
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- There are methods (ChIP-chip experiments, ChIP-seq experiments) where after preprocessing the data one has access to the (almost exact) positions of several type of TREs at one time, and this under different experimental conditions. (ENCODE)
### Biological motivation

#### The probabilistic model(s)

- **Parametric estimation**
- **Adaptive estimation**

### Several examples

#### TRE

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- → analysis of dependance between the different positions (see Carstensen, Sandelin, Winther, Hansen (2010)), based on favored or avoided distances.
Several examples

**TRE**

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- There are methods (ChIP-chip experiments, ChIP-seq experiments) where after preprocessing the data one has access to the (almost exact) positions of several type of TREs at one time, and this under different experimental conditions. (ENCODE)
  → analysis of dependance between the different positions (see Carstensen, Sandelin, Winther, Hansen (2010)), based on favored or avoided distances.

Why just DNA ? RNA etc ...
A simplified/informal vision

How can we explain the positions of the occurrences of one event (motifs, TRE, etc) wrt the others and itself?
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- Spontaneous apparition
A simplified/informal vision

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Maximal sensible interaction distance: 5 000 - 10 000 bases because of the 3d DNA structure
Point process on the real line

Point process

\( N = \) random countable set of points of \( \mathbb{R} \) (here).
Point process on the real line

Point process

\( \mathcal{N} = \) random countable set of points of \( \mathbb{R} \) (here).

\( N_A \) number of points of \( \mathcal{N} \) in \( A \), \( N_t = N_{[0,t]} \),

\[
dN_t = \sum_T \delta_T. \int f(t) dN_t = \sum_{T \in \mathcal{N}} f(T)
\]
## Point process on the real line

### Point process

- $\mathcal{N}$ = random countable set of points of $\mathbb{R}$ (here).

- $\mathcal{N}_A$ number of points of $\mathcal{N}$ in $A$, $N_t = \mathcal{N}_{[0,t]}$,

- $dN_t = \sum_T \text{point de } \mathcal{N} \delta_T$. Usually $\mathbb{R}$ is thought as time

### Intensity

- $t \rightarrow \lambda(t)$ represents the probability to have a point at time $t$ conditionnally to the past before $t$ ($s < t$)
Point process on the real line

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Intensity

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"Past" contains in particular the previous occurrences of points.
Point process on the real line

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**Intensity**

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conditionnally to the past before \( t \) \( (s < t) \)

"Past" contains in particular the previous occurrences of points.

NB : here \( \mathbb{R} \) is the DNA strand. The "past" may be interpreted as what has already been read in a prescribed direction (e.g. 5’-3’ or 3’-5’).
The simple Hawkes process

The intensity $\lambda(t)$ is given by
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$$\nu$$

Spontaneous
The simple Hawkes process

The intensity $\lambda(t)$ is given by

$$\nu + \sum_{T \in \mathbb{N}} h(t - T)$$

Spontaneous  Self-exciting
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Spontaneous  Self-exciting

The most classical case corresponds to $h > 0$ (see Hawkes (1971)) and a stationary version exists if $\int h < 1$. There is also in this specific case a branching / cluster process representation (see Hawkes and Oakes (1974)).
The simple Hawkes process

The intensity $\lambda(t)$ is given by

$$
\left( \nu + \sum_{T \in N} h(t - T) \right)_+
$$

Spontaneous  Self-exciting

The most classical case corresponds to $h > 0$ (see Hawkes (1971)) and a stationary version exists if $\int h < 1$. There is also in this specific case a branching / cluster process representation (see Hawkes and Oakes (1974)).

One can actually consider any 1-Lipschitz modification, there is still a stationary version of it if $\int |h| < 1$ (Brémaud and Massoulié (1996)).
The Hawkes process interaction with itself + an additional interaction

\[ \lambda(t) = \]
The Hawkes process interaction with itself + an additional interaction

\[ \lambda(t) = \nu \]

Spontaneous
The Hawkes process interaction with itself + an additional interaction

\[ \lambda(t) = \nu + \sum_{T \in N} h(t - T) \]

| Spontaneous | Self-interaction |
The Hawkes process interaction with itself + an additional interaction

\[ \lambda(t) = \nu + \sum_{T \in N} h(t - T) + \sum_{X \in N_2} h_2(t - X) \]

Spontaneous  Self-interaction  Interaction with other type
The Hawkes process interaction with itself $+$ an additional interaction

$$\lambda(t) = \left( \nu + \sum_{T \in N_1} h(t - T) + \sum_{X \in N_2} h_2(t - X) \right)^+$$

- **Spontaneous**
- **Self-interaction**
- **Interaction with other type**

If $h$ is null and if $N_2$ is fixed (no reciprocal interaction), then $N$ is a Poisson process given $N_2$. 
The multivariate Hawkes process

One observes $N^{(1)}, ..., N^{(r)}, ..., N^{(M)}$ processes such that
The multivariate Hawkes process

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\[
\lambda^{(1)}(t) = \\
\lambda^{(2)}(t) = \\
\lambda^{(r)}(t) = \\
\]
The multivariate Hawkes process

One observes \( N^{(1)}, \ldots, N^{(r)}, \ldots, N^{(M)} \) processes such that

\[
\begin{align*}
\lambda^{(1)}(t) &= \nu_1 \\
\lambda^{(2)}(t) &= \\
\lambda^{(r)}(t) &=
\end{align*}
\]
The multivariate Hawkes process

One observes $N^{(1)}, \ldots, N^{(r)}, \ldots, N^{(M)}$ processes such that

$$\lambda^{(1)}(t) = \nu_1 + \sum_{T \in N^{(1)}} h_1^{(1)}(t - T)$$

$$\lambda^{(2)}(t) =$$

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The multivariate Hawkes process

One observes \(N^{(1)}, \ldots, N^{(r)}, \ldots, N^{(M)}\) processes such that

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One observes $N^{(1)}, \ldots, N^{(r)}, \ldots, N^{(M)}$ processes such that

$$\lambda^{(1)}(t) = \nu_1 + \sum_{T \in N^{(1)}} h^{(1)}_1(t - T)$$

$$\lambda^{(2)}(t) = \lambda^{(r)}(t) = \frac{t}{9/32}$$
The multivariate Hawkes process

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$$\lambda^{(2)}(t) =$$

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Biological motivation

The probabilistic model(s)

Parametric estimation

Adaptive estimation

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$$\lambda^{(1)}(t) = \nu_1 + \sum_{T \in N^{(1)}} h^{(1)}_1(t - T) + \sum_{\ell \neq 1} \sum_{T \in N^{(\ell)}} h^{(1)}_\ell(t - T)$$

$$\lambda^{(2)}(t) = \nu_2$$

$$\lambda^{(r)}(t) = \frac{t}{32}$$
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$$
\lambda^{(2)}(t) = \nu_2
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\lambda^{(r)}(t) = \nu_2
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$$\lambda^{(2)}(t) = \nu_2 + \sum_{T \in N^{(2)}} h_2^{(2)}(t - T)$$

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The multivariate Hawkes process

One observes $N^{(1)}, \ldots, N^{(r)}, \ldots, N^{(M)}$ processes such that

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\]

\[
\lambda^{(2)}(t) = \nu_2 + \sum_{T \in N^{(2)}} h^{(2)}_2(t - T) + \sum_{\ell \neq 2} \sum_{T \in N^{(\ell)}} h^{(2)}_\ell(t - T)
\]

\[
\lambda^{(r)}(t) = \ldots
\]
The multivariate Hawkes process (2)

Link with graphical model of local independence (see Didelez (2008))
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Link with graphical model of local independence (see Didelez (2008))
The multivariate Hawkes process (3)

- Only excitation (all the $h^{(r)}_{\ell}$ are positive): for all $r$,

$$
\lambda^{(r)}(t) = \nu_r + \sum_{\ell=1}^{M} \int_{-\infty}^{t-} h^{(r)}_{\ell}(t - u) dN^{(\ell)}_u.
$$

Branching / Cluster representation, stationary process if the spectral radius of $\left( \int h^{(r)}_{\ell}(t) dt \right)$ is $< 1$. 
The multivariate Hawkes process (3)

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- Interaction, for instance

$$\lambda^{(r)}(t) = \left( \nu_r + \sum_{\ell=1}^{M} \int_{-\infty}^{t-} h^{(r)}_\ell(t-u) dN^{(\ell)}_u \right)^+.$$
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- Interaction, for instance

$$\lambda^{(r)}(t) = \nu_r + \sum_{\ell=1}^{M} \int_{-\infty}^{t-} h^{(r)}_{\ell}(t-u) dN_{u}^{(\ell)} + \nu_r + \sum_{\ell=1}^{M} \int_{-\infty}^{t-} h^{(r)}_{\ell}(t-u) dN_{u}^{(\ell)}.$$ 

- Exponential

$$\lambda^{(r)}(t) = \exp \left( \nu_r + \sum_{\ell=1}^{M} \int_{-\infty}^{t-} h^{(r)}_{\ell}(t-u) dN_{u}^{(\ell)} \right).$$ 

Multiplicative shape but no guarantee of a stationary version.
Biological motivation

The probabilistic model(s)

Parametric estimation

Adaptive estimation

Maximum likelihood estimation

• Only the shape of the intensity is necessary.
Maximum likelihood estimation

- Only the shape of the intensity is necessary.
- Given the "past" before 0, for one process observed until time $T$,

$$L_T(\theta) = \int_0^T \ln(\lambda_\theta(t))dN_t - \int_0^T \lambda_\theta(t)dt.$$
Maximum likelihood estimation

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- Maximizing gives $\hat{\theta}$. 
Maximum likelihood estimation

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  \]
  - maximizing gives \( \hat{\theta} \).
- If several processes or \( n \) sample → sum
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- If several processes or $n$ sample $\rightarrow$ sum
- Not necessary to have a stationary version, it depends on the considered asymptotics.
Maximum likelihood estimation

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- Maximizing gives $\hat{\theta}$.
- If several processes or $n$ sample → sum
- Not necessary to have a stationary version, it depends on the considered asymptotics.
- Consistence, asymptotic normality under smooth conditions, see Ogata and Akaike (1982), Ozaki (1979) or Andersen et al (1993).
Maximum likelihood estimation

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- maximizing gives $\hat{\theta}$.
- If several processes or $n$ sample $\rightarrow$ sum
- not necessary to have a stationary version, it depends on the considered asymptotics.
- Consistence, asymptotic normality under smooth conditions, see Ogata and Akaike (1982), Ozaki (1979) or Andersen et al (1993).
- Even tests of the nullity of $h^{(r)}_\ell$ and access to a graphical model (see Carstensen et al (2010)).
Model choice

![Graph showing model choice with parameters T=2000 and μ=0.1]
Model choice

- Biological motivation
- The probabilistic model(s)
- Parametric estimation
- Adaptive estimation

![Graphs showing model choice](image-url)
Model choice

The biggest model is not the correct one, it overfits but ...
The biggest model is not the correct one, it overfits but ...
AIC criterion

If several parametric models $m$ with different dimensions $D_m$,

- for each model one has an MLE $\hat{\theta}_m$
AIC criterion

If several parametric models $m$ with different dimensions $D_m$,
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- one can always select one model by minimizing

$$-L_T(\hat{\theta}_m) + D_m$$
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- If the family of models is fixed and if there is a true model, it should select the correct one asymptotically (see for instance Vere-Jones and Ozaki (1982), Gusto and Schbath (2005)).
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- What if no true model? What if family too big with respect to $T$?
- Gusto PhD thesis numerical study shows that AIC does not select a sparse model if spline with not equally spaced knots.
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- Gusto PhD thesis numerical study shows that AIC does not select a sparse model if spline with not equally spaced knots.
- Gusto and Schbath program, FADO, only works for equally spaced knots.
- Hence no clear access to favoured or avoided distance
Aim

- We want to perform an adaptive estimation of the functions $h!$
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- ie select a model $m \rightarrow \hat{h}$ sparse and picky: one can read on the selected estimate favored or avoided distances if any.
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- ie select a model $m \rightarrow \hat{h}$ sparse and picky: one can read on the selected estimate favored or avoided distances if any.
- More likely that no true model and that the family of models grows with $T$. 
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- ie select a model $m \rightarrow \hat{h}$ sparse and picky: one can read on the selected estimate favored or avoided distances if any.
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- $\rightarrow$ penalized model selection (Birgé and Massart, see Massart course in St Flour (2007))
Aim

- We want to perform an adaptive estimation of the functions $h$!
- ie select a model $m \rightarrow \hat{h}$ sparse and picky: one can read on the selected estimate favored or avoided distances if any.
- More likely that no true model and that the family of models grows with $T$.
- → penalized model selection (Birgé and Massart, see Massart course in St Flour (2007))
- but also, thresholding or Lasso methods.
Least-square contrast for one process

- The meaningful quantity is $\lambda(t)$. 
Least-square contrast for one process

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- It may depend on the process itself.
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- It is the "mean" version of the point measure $\delta_{T=t}$. 
Least-square contrast for one process

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Least-square contrast for one process

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- It may depend on the process itself.
- It is the "mean" version of $dN_t$.
- A good estimate of the parameters should correspond to an intensity candidate close to the true one.
Least-square contrast for one process

- It is the "mean" version of $dN_t$.
- A good estimate of the parameters should correspond to an intensity candidate close to the true one.
- Let $\eta$ be an intensity candidate.

**Least-square contrast**

$$\gamma_T(\eta) = -\frac{2}{T} \int_0^T \eta(t) dN_t + \frac{1}{T} \int_0^T \eta(t)^2 dt$$
Least-square contrast for one process

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- A good estimate of the parameters should correspond to an intensity candidate close to the true one.
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### Least-square contrast

$$\gamma_T(\eta) = -\frac{2}{T} \int_0^T \eta(t) dN_t + \frac{1}{T} \int_0^T \eta(t)^2 dt$$

- $\eta$ is better if $\gamma_T(\eta)$ is small.
Least-square contrast for one process

- It is the "mean" version of $dN_t$.
- A good estimate of the parameters should correspond to an intensity candidate close to the true one.
- Let $\eta$ be an intensity candidate.

**Least-square contrast**

$$
\gamma_T(\eta) = -\frac{2}{T} \int_0^T \eta(t) dN_t + \frac{1}{T} \int_0^T \eta(t)^2 dt
$$

- $\eta$ is better if $\gamma_T(\eta)$ is small.

$$
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- We will minimize $\gamma_T$ for precise shape of intensity candidates.
Least-square contrast on a toy model

Let $[a, b]$ an interval of $\mathbb{R}^+$. 
Least-square contrast on a toy model

Let \([a, b]\) an interval of \(\mathbb{R}^+\).

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\eta(t) = \sum_{T \in \mathbb{N}} \alpha \mathbf{1}_{a \leq t - T \leq b} = \alpha N_{[t-b, t-a]}
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For the simple Hawkes process

\[ \mathbb{L}_2 = \left\{ f = (\mu, g) : \text{Supp}(g) = [0, A], \| f \|^2 = \mu^2 + \int_0^A g^2(x) dx < +\infty \right\} \]

s = (\nu, h) to estimate
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\]

\[\hat{s}_m = \arg \min_{f \in S_m} \gamma_T(f).\text{ no close formula in general.}\]
Risk study

Only for simple Hawkes process

Risk

The risk of $\hat{s}$ is $\mathbb{E}(\|s - \hat{s}\|^2)$. 
Risk study

Only for simple Hawkes process

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The risk of \( \hat{s} \) is \( \mathbb{E}(\|s - \hat{s}\|^2) \).

One can show, under technical assumptions,

\[
\mathbb{E}(\|\hat{s}_m - s\|^2) \leq \square \left[ d(s, S_m)^2 + D_m \frac{\log T}{T} \right]
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- The bigger is $S_m$ the smaller is the bias, $d(s, S_m)^2$ but $D_m$ is big.
Biological motivation

The probabilistic model(s)

Parametric estimation

Adaptive estimation

Risk study

Only for simple Hawkes process

**Risk**

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- The bigger is \( S_m \) the smaller is the **bias**, \( d(s, S_m)^2 \) but \( D_m \) is big.
- \( \rightarrow \) compromise: the best (or oracle) in a family is the one that minimizes the sum.
Model selection with dimension-based penalty

Joint work with S. Schbath (2010). Only for simple Hawkes process
Model selection with dimension-based penalty

Joint work with S. Schbath (2010). Only for simple Hawkes process

Models

\[ S_m = \{ f = (\mu, g), \text{ } g \text{ } \text{piecewise constant on } m \} \text{ where } m \text{ set of disjoint intervals in } [0, A] \]
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Models

\[ S_m = \{ f = (\mu, g), g \text{ piecewise constant on } m \} \text{ where } m \text{ set of disjoint intervals in } [0, A] = \text{model} \]

- NESTED Regular dyadic partitions constructed on \( \Gamma \).
- REGULAR Regular partitions until a certain prescribed bandwidth
- IRREGULAR All irregular partitions constructed on \( \Gamma \).
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Joint work with S. Schbath (2010). Only for simple Hawkes process

Models

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\begin{align*}
\text{Gamma} & \\
\text{ISLANDS} & 
\end{align*}
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  - [ ] [ ] [ ] [ ] [ ] [ ] [ ]
  - [ ] [ ]
  - [ ] [ ]
  - [ ] [ ] [ ]

- **ISLANDS**
  - [ ] [ ] [ ] [ ]
  - [ ]
  - [ ]

All models included in $\Gamma$. The most adapted to the biological question.
Model selection with dimension-based penalty (2)

Only for simple Hawkes process
Let \( \mathcal{M}_T \) be a family of models \( (m \in \mathcal{M}_T) \).

\( M_T \)
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**Penalized Criterion**

$$\hat{m} = \arg\min_{m \in \mathcal{M}_T} [\gamma_T(\hat{s}_m) + \text{pen}(m)].$$
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Selected estimator

$$\check{s} = (\check{\nu}, \check{h}) = \hat{s}_{\hat{m}}.$$
Model selection with dimension-based penalty (3)

Only for simple POSITIVE Hawkes process

Under technical assumptions, if

\[ \text{pen}(m) = \kappa Q(|m| + 1) \frac{\log(T)^2}{T}, \]

with \( \kappa \) depending on unobserved parameters
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Under technical assumptions, if

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$$\mathbb{E}(\|\tilde{s} - s\|^2) \leq \square \inf_{m \in \mathcal{M}_T} \left[ d(s, S_m)^2 + (|m| + 1) \frac{\log(T)^2}{T} \right] + \square \frac{\# \{\mathcal{M}_T\}}{T^Q}. $$
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- family grows with \( T \) at a moderate rate, especially for Islands
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- It is an oracle inequality!
- family grows with \( T \) at a moderate rate, especially for Islands
- also adaptive minimax results for Hölder functions.
**Model selection with dimension-based penalty (4)**

**Only for simple Hawkes process**

- In practice, one can use least-square estimators even for possibly negative $h$. 
Model selection with dimension-based penalty (4)

Only for simple Hawkes process

- In practice, one can use least-square estimators even for possibly negative $h$.
- Theoretical penalty not observed, Slope heuristics does not work especially for Islands
Model selection with dimension-based penalty(4)

Only for simple Hawkes process

- In practice, one can use least-square estimators even for possibly negative $h$.
- Theoretical penalty not observed, Slope heuristics does not work especially for Islands
- An angle is perfectly clear on the simulations at the correct dimension:

$$-\bar{k} = \frac{\gamma_T(\hat{s}_\Gamma) - \gamma_T(\hat{s}_1)}{|\Gamma| - 1}$$

and

$$\hat{m} = \arg\min_{m \in M_T} \gamma_T(\hat{s}_m) + \bar{k}(|m| + 1).$$
Illustration

Only for simple Hawkes process

<table>
<thead>
<tr>
<th>Contrast</th>
<th>Penalized contrast</th>
</tr>
</thead>
<tbody>
<tr>
<td><img src="image1" alt="Graph" /></td>
<td><img src="image2" alt="Graph" /></td>
</tr>
</tbody>
</table>

Chosen estimator

![Graph](image3)

Selected dimension

![Graph](image4)
On real data

Only for simple Hawkes process

Analysis of the positions of the 4290 genes of E. coli
\((T = 9288442, A = 10000)\) (r-scans)
On real data

Only for simple Hawkes process

Analysis of the positions of the 4290 genes of E. coli
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On real data

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Analysis of the positions of the 4290 genes of E. coli
$\left( T = 9288442, \ A = 10000 \right)$ (Islands)
On real data

Only for simple Hawkes process

Analysis of the 1036 occurrences of tataat for E. coli. 
\( T = 9288442, A = 10000 \) (Islands)
Disadvantages of the dimension-based penalty method

- only for simple Hawkes process! (not more than grid with 15 - 26 bins)
Disadvantages of the dimension-based penalty method

- only for simple Hawkes process! (not more than grid with 15 - 26 bins)
- We miss part of the understanding because we do not take external information into account (here interaction tataat - genes).
Poissonian Interaction

Work in progress of Laure Sansonnet.
Poissonian Interaction

Work in progress of Laure Sansonnet. We observe two processes:

1. **Parents**: $U_1, ..., U_n$, $n$ iid uniform random variables on $[0, T]$.
2. **Children**: Poisson process with intensity $\sum_{i=1}^{n} h(t - U_i)$. 
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Pros:

- A pairwise study of two processes is possible (for instance tataat and genes). If $h$ has support in $\mathbb{R}_+ = \text{very special case of multivariate Hawkes process.}$
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- $h$ with support in $[-A, A]$ possible: we look at both direction at the same time.
- unbiased estimator of $\int h(t) \varphi(t) dt$. 
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- Thresholding estimator of $h$ exists. Threshold data-driven!
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- Computation quite fast. Precision $>>$ Islands
Poissonian Interaction

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Cons:

- The presence of Parents will not be explained and is not linked to Children.
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Cons:

- The presence of Parents will not be explained and is not linked to Children.
- Crucial to say who are the parents/ the children (it is not symmetric!).
- For the moment, one cannot explain the Children position, even with an extra spontaneous apparition.
**Poissonian Interaction (2)**

**Interaction tataat - genes.**

Parents = tataat

Parents = Genes
Full Multivariate Hawkes processes and lasso procedure

Joint Work with N.R. Hansen (Copenhagen) and V. Rivoirard (Dauphine), in progress.
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We want to estimate \( s = \left( (\nu_r, (h_r^{(r)})_\ell=1,\ldots,M)_{r=1,\ldots,M} \right) \) in

\[
\mathbb{L}_2 = \left\{ f = \left( (\mu_r, (g^{(r)}_\ell))_{\ell=1,\ldots,M} \right)_{r=1,\ldots,M} \bigg/ g^{(r)}_\ell \text{ with support in } (0, A] \text{ and } \| f \|^2 = \sum_r (\mu_r)^2 + \sum_r \sum_\ell \int_0^A (g^{(r)}_\ell)^2(x) dx < \infty \right\}.
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\]

Intensity candidate per mark

\[
\psi_f^{(r)}(t) = \mu_r + \sum_\ell \int_{-\infty}^t g^{(r)}_\ell(t-u) \, dN_u^{(\ell)}.
\]
Full Multivariate Hawkes processes and lasso procedure (2)

Least-square contrast (full form)

\[ \gamma_T(f) = \sum_r \gamma^{(r)}_T(f) \]  where

\[ \gamma^{(r)}_T(f) = -\frac{2}{T} \int_0^T \psi^{(r)}_f(t) dN_t^{(m)} + \frac{1}{T} \int_0^T \psi^{(r)}_f(t)^2 dt. \]
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If each \( g^{(r)}_{\ell} \)'s in \( f \) are decomposed on a finite orthonormal family of functions with cardinal \( K \), then

- \( f \rightarrow (a_r)_{r \leq M} \) Each \( a_r \) of size \( MK + 1 \).
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- \( f \rightarrow (a_r)_{r \leq M} \) Each \( a_r \) of size \( MK + 1 \).
- \[ \gamma_T^{(r)}(f) = -2a_r^*b_r + a_r^*Ga_r, \]

where

- \( G \) is a random observable matrix, independent of the mark \( r \)
- \( b_r \) is also a random observable vector.
Full Multivariate Hawkes processes and lasso procedure (3)

The Lasso criterion can be expressed independently for each mark.

**Lasso criterion**

\[
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- The vector \(d_r\) is not constant: it is random and depends on the index.
The Lasso criterion can be expressed independently for each mark.

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- Oracle inequality with "high" probability possible....