Estimating parameters in spatio-temporal Quermass-interaction process

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Outline

1. Quermass-interaction process and its extension
2. Simulation
3. Spatio-temporal Quermass-interaction process
4. Maximum likelihood method using MCMC
5. Particle filtering
6. Particle MCMC

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Notation

- $x = b(u, r)$ ... a disc with centre in $u \in \mathbb{R}^2$ and radius $r \in (0, \infty)$
- $\mathbf{x} = \{x_1, \ldots, x_n\}$ ... finite configuration of n discs
- $U_{\mathbf{x}}$ ... the union of discs from the configuration $\mathbf{x}$.
- $\mathbf{Y}$ ... random disc Boolean model (i.e. union of discs without any interactions) with an intensity function of discs centers $\rho(u)$ and probability distribution of the discs radii Q
- $\mathbf{X}$ ... random disc process which is absolutely continuous with respect to the process $\mathbf{Y}$

Back
Close

Assumptions

- The intensity function $\rho(u) = 1$ on a bounded set S and $\rho(u) = 0$ otherwise, i.e. the centers of the reference Boolean model form unit Poisson process on S.

- For any finite configuration of discs $\mathbf{x} = \{x_1, \ldots, x_n\}$, the probability measure of $\mathbf{X}$ with respect to the probability measure of $\mathbf{Y}$ is given by a density

$$f_\theta(\mathbf{x}) = \frac{\exp\{\theta \cdot T(U_\mathbf{x})\}}{c_\theta},$$

where

  - c_θ is the normalizing constant,
  - θ is d-dimensional vector of parameters,
  - $T = T(U_\mathbf{x})$ is a d-dimensional vector of geometrical characteristics of the union $U_\mathbf{x}$ of the discs from the configuration $\mathbf{x}$.

Quermass-interaction process

The density is of the form

$$f_\theta(\mathbf{x}) = \frac{1}{c_\theta} \exp\{\theta_1 A(U_\mathbf{x}) + \theta_2 L(U_\mathbf{x}) + \theta_3 \chi(U_\mathbf{x})\},$$

where

- $A = A(U_\mathbf{x})$ is the area,
- $L = L(U_\mathbf{x})$ is the perimeter,
- $\chi = \chi(U_\mathbf{x})$ is the Euler-Poincaré characteristic (the number of connected components minus the number of holes, i.e. $\chi(U_\mathbf{x}) = N_{\mathrm{cc}}(U_\mathbf{x}) - N_{\mathrm{h}}(U_\mathbf{x})$)

of the union $U_\mathbf{x}$.

Extended Quermass-interaction process

- Møller, Helisová (2008):
  - In the density

$$f_\theta(\mathbf{x}) = \frac{\exp\{\theta \cdot T(U_\mathbf{x})\}}{c_\theta},$$

we have $T = (A, L, \chi, N_h, N_{bv}, N_{id})$, where

$N_{bv} = N_{bv}(U_\mathbf{x})$ is the number of boundary vertices,

$N_{id} = N_{id}(U_\mathbf{x})$ is the number of isolated discs,

of the union $U_\mathbf{x}$.

  - Theory and simulations studied.
- Møller, Helisová (2010):
  - $T = (A, L, N_{cc}, N_h)$.
  - Statistical analysis.

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Back
Close

Papangelou conditional intensity

Definition For a finite $\mathbf{x} \subset S \times (0, \infty)$ and $y \in S \times (0, \infty) \setminus \mathbf{x}$, *Papangelou conditional intensity* is defined as

$$\lambda_\theta(\mathbf{x}, y) = f_\theta(\mathbf{x} \cup \{y\}) / f_\theta(\mathbf{x}).$$

Denoting

$$\begin{aligned} A(\mathbf{x}, y) =& A(U_{\mathbf{x} \cup y}) - A(U_{\mathbf{x}}), \\ L(\mathbf{x}, y) =& L(U_{\mathbf{x} \cup y}) - L(U_{\mathbf{x}}), \\ \chi(\mathbf{x}, y) =& \chi(U_{\mathbf{x} \cup y}) - \chi(U_{\mathbf{x}}), \end{aligned}$$

we get

$$\lambda_\theta(\mathbf{x}, y) = \exp\left(\theta_1 A(\mathbf{x}, y) + \theta_2 L(\mathbf{x}, y) + \theta_3 \chi(\mathbf{x}, y)\right).$$

MCMC algorithm

1. Suppose that in iteration t, we have a configuration $\mathbf{x_t} = \{x_1, \ldots, x_n\}$
2. Proposal in iteration $t+1$:
   (a) with probability 1/2, the proposal is $\mathbf{x_t} \cup \{x_{n+1}\}$
      i. we accept the proposal with probability $min\{1; H(\mathbf{x_t}, x_{n+1})\}$ and set $\mathbf{x_{t+1}} = \mathbf{x_t} \cup \{x_{n+1}\}$
      ii. else we set $\mathbf{x_{t+1}} = \mathbf{x_t}$
   (b) else, the proposal is $\mathbf{x_t} \backslash \{x_i\}$
      i. we accept the proposal with probability $min\{1; 1/H(\mathbf{x_t}\backslash\{x_i\}, x_i)\}$ and set $\mathbf{x_{t+1}} = \mathbf{x_t}\backslash\{x_i\}$
      ii. else $\mathbf{x_{t+1}} = \mathbf{x_t}$

where $H(\mathbf{x_t}, x_{n+1}) = \lambda_\theta(\mathbf{x_t}, x_{n+1})\frac{|S|}{n+1}$
and $H(\mathbf{x_t}\backslash\{x_i\}, x_i) = \lambda_\theta(\mathbf{x_t}\backslash\{x_i\}, x_i)\frac{|S|}{n}$

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Spatio-temporal Quermass-interaction process

Zikmundová, Staňková Helisová, Beneš (2012):

$$f_{\theta^{(k)}}(\mathbf{x}) = \frac{\exp\{\theta^{(k)} \cdot T(U_{\mathbf{x}})\}}{c_{\theta^{(k)}}},$$

where

$$\theta^{(k)} = \theta^{(k-1)} + \eta^{(k)},\ k = 1, 2 \ldots, T,$$

where $\theta^{(0)}$ fixed is given and $\eta^{(k)}$ are iid random vectors with Gaussian distribution $\mathcal{N}(a, \sigma^2 I)$, where $a \in \mathbf{R}^d$ ($d = 3$ for basic Quermass-interactio process and $d = 4, 5, 6$ for extended versions), $\sigma^2 > 0$ and I is the unit matrix.

Temporal dependence

is given within its simulation algorithm:

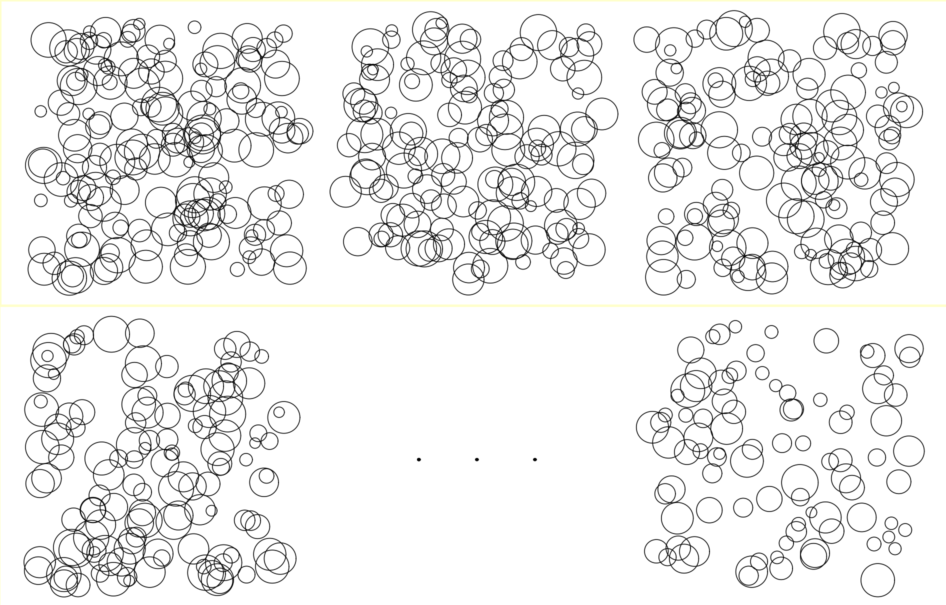
1. Choose a fixed $\theta^{(0)}$
2. Simulate parameter vectors $\theta^{(k)}, k = 1, 2, \ldots, T$.
3. Simulate a realization $\mathbf{x}_0$ (using M-H algorithm described above).
4. Simulate realizations $\mathbf{x}_k$, $k = 1, 2 \ldots, T$ (M-H alg.) with the proposal distribution $Prop_k$ of newly added disc at time k given by

$$Prop_k = (1 - \beta) \cdot Prop^{(RP)} + \beta \cdot Prop_{k-1}^{(emp)}, \quad \beta \in (0, 1),$$

where $Prop^{(RP)}$ is a distribution of the reference process, $Prop_{k-1}^{(emp)}$ is the empirical distribution obtained from the configuration $\mathbf{x}_{k-1}$ and β is a chosen constant.

Remark: Idea is that β describs the power of time dependence so that $(\beta \times 100)\%$ of the added discs are taken from the previous configuration and the remaining discs are simulated randomly, so the dependence is stronger when β is bigger.

Example



A realization of the (A, L, N_{cc}, N_h)-interaction process in $S = [0, 10] \times [0, 10]$ with Q the uniform distribution on the interval $[0.2, 0.7]$, $\theta^{(0)} = (0.5, -0.25, -0.5, 0.5)$, $a = (-0.1, 0.05, 0.1, -0.1)$, $\sigma^2 = 0.001$ and $\beta = 0.5$ in times $k = 0, 1, 2$ (upper row) and $k = 3, ..., 10$ (lower row).

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Maximum likelihood method using MCMC simulations (MCMC MLE)

- Denote $f_{\theta^{(k)}}(\mathbf{x}) = h_{\theta^{(k)}}(\mathbf{x})/c_{\theta^{(k)}}$ (i.e. $h_{\theta^{(k)}}(\mathbf{x}) = \exp\{\theta^{(k)} \cdot T(U_{\mathbf{x}})\}$ is the unnormalized density).

- For an observation $\mathbf{x}$, the log likelihood function is given by

$$l(\theta^{(k)}) = \log h_{\theta^{(k)}}(\mathbf{x}) - \log c_{\theta^{(k)}} = \theta^{(k)} \cdot T(U_{\mathbf{x}}) - \log c_{\theta^{(k)}}.$$

Problem: $c_{\theta^{(k)}}$ has no explicit expression.

Solution: We maximize the likelihood ratio $f_{\theta^{(k)}}/f_{\theta_0^{(k)}}$ for a fixed vector $\theta_0^{(k)}$ instead.

MCMC MLE

- For the fixed $\theta_0^{(k)}$, the log likelihood ratio

$$l(\theta^{(k)}) - l(\theta_0^{(k)}) = \log(h_{\theta^{(k)}}(\mathbf{x})/h_{\theta_0^{(k)}}(\mathbf{x})) - \log(c_{\theta^{(k)}}/c_{\theta_0^{(k)}})$$

  can be approximated by

$$l(\theta^{(k)}) - l(\theta_0^{(k)}) = \log(h_{\theta}(\mathbf{x})/h_{\theta_0^{(k)}}(\mathbf{x})) - \log \frac{1}{n} \sum_{i=1}^{n} h_{\theta^{(k)}}(\mathbf{z}_j)/h_{\theta_0^{(k)}}(\mathbf{z}_j),$$

  where $\mathbf{z}_j$ are realizations from $f_{\theta_0^{(k)}}(\mathbf{x})$ obtained by MCMC simulations.

- This is applied to the observations in each time k.

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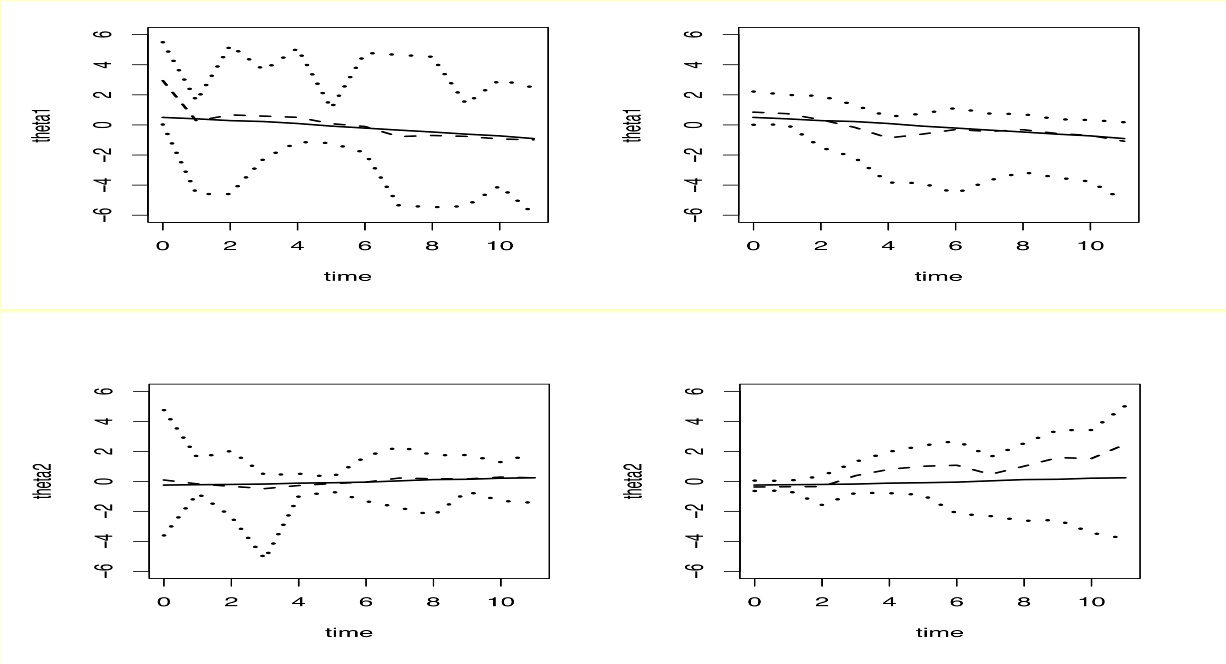
Particle filter estimate (PFE)

1. In time $k = 0$, sample particles $\theta^{(0,i)}$, $i = 1, \ldots, m$, independently from a proposal density $p(\theta^{(0)})$.
2. For times $k = 1, ..., T$
   (a) for $i = 1, \ldots, m$, sample $\tilde{\theta}^{(k,i)}$ from $q(\theta^{(k)}|\theta^{(k-1,i)})$ and denote $\tilde{\theta}^{(0:k,i)} = (\theta^{(0:k-1,i)}, \tilde{\theta}^{(k,i)})$,
   (b) for $i = 1, \ldots, m$, set $w_k^i = f_{\tilde{\theta}^{(k,i)}}(\mathbf{x}_k)$ and normalize them,
   (c) for $i = 1, \ldots, m$, sample with replacement $\theta^{(0:k,i)}$ from $\tilde{\theta}^{(0:k,i)}$ with normalized weights from (b).
3. Filtered estimate is $\hat{\theta}^{(0:T)} = \frac{1}{m} \sum_{i=1}^{m} \theta^{(0:T,i)}$.

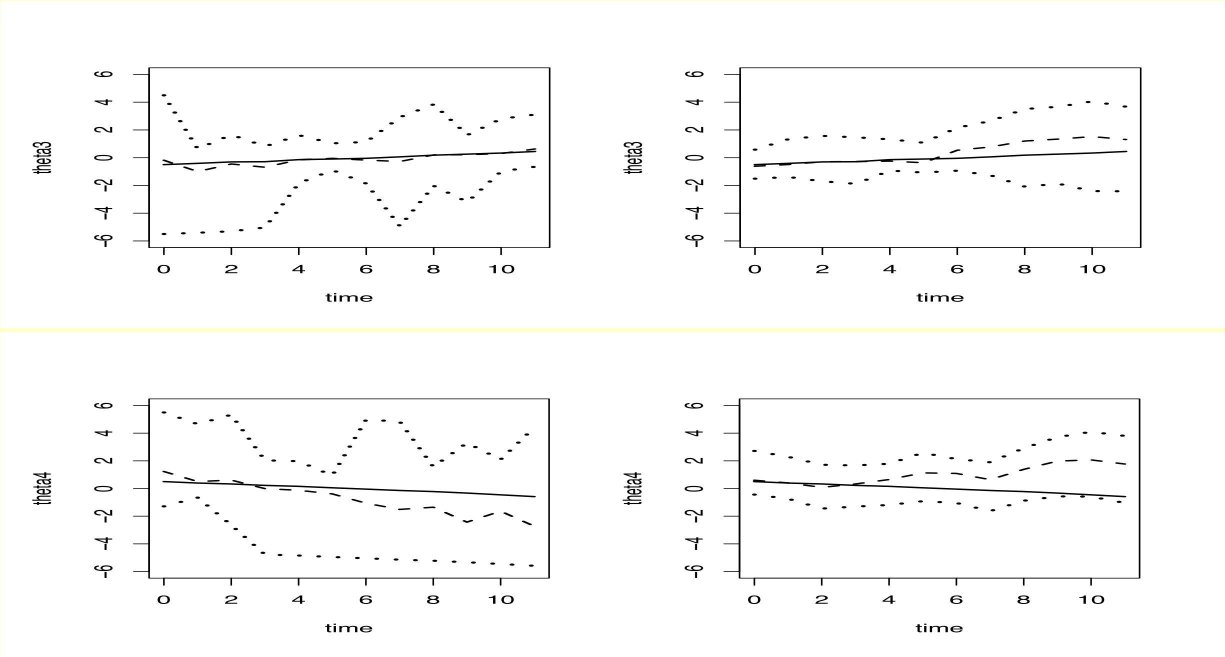
Remark: Here, denoting $\hat{\theta}_{mle}$ the MLE estimate of θ, we set $p(\theta^{(0)}) \sim U(0, 2\hat{\theta}_{mle}^{(0)})$ for $\hat{\theta}_{mle}^{(0)}$ positive or $p(\theta^{(0)}) \sim U(2\hat{\theta}_{mle}^{(0)}, 0)$ for $\hat{\theta}_{mle}^{(0)}$ negative, and $q(\theta^{(k)}|\theta^{(k-1,i)}) \sim N(\hat{\theta}_{mle}^{(k-1,i)} + \hat{a}, \hat{\sigma}^2)$, where $\hat{a}, \hat{\sigma}^2$ are obtained by standard linear regression methods from MLE estimates.

Comparing MCMC MLE and PFE



Comparing the real parameters (solid line) with envelopes (dotted lines) and averages (dashed lines) of estimates obtained from 39 realizations of the process by MCMC MLE (left) and PFE (right).

Comparing MCMC MLE and PFE



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Comparing MCMC MLE and PFE

- MCMC MLE seems to be better in average in later times
- PFE has smaller variance

$\downarrow$

Possible reason: small number of components and number of holes in earlier and later times, respectively.

$\downarrow$

Next steps:

- Application to Quermass-interaction process
- Consider longer time sequence
- Try also particle MCMC

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Particle MCMC

- Idea: Particle filter running in more iterations.
- Algorithm:
  1. Iteration 0:
     (a) Set $(\theta^{(0)}(0), a(0), \sigma^2(0))$ arbitrarily (e.g. ML estimates).
     (b) Using steps 2 and 3 from PFE algorithm, obtain $\theta^{(0:T)}(0)$.
  2. Iteration $t+1$:
     (a) Given $(\theta^{(0)}(t), a(t), \sigma^2(t))$, propose $(\theta^{(0)*}, a^*, \sigma^{2*})$ (e.g. random walk).
     (b) Using steps 2 and 3 from PFE algorithm, obtain $\theta^{(0:T)*}$.
     (c) Accept this proposal (i.e. set $(\theta^{(0)}(t+1), a(t+1), \sigma^2(t+1)) = (\theta^{(0)*}, a^*, \sigma^{2*})$) with probability $min(1; MH)$, where MH is Metropolis-Hastings ratio.

Metropolis-Hastings ratio in particle MCMC

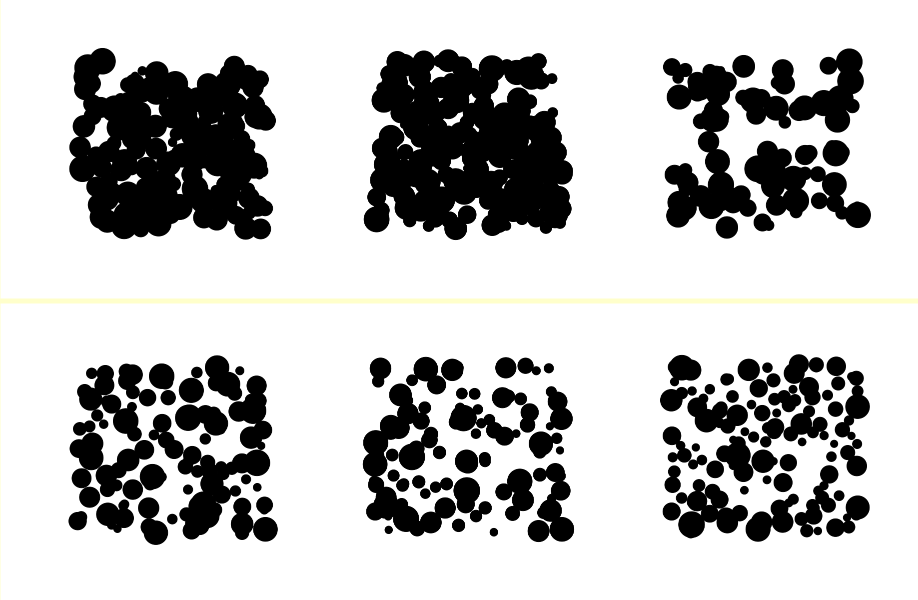
$$MH = \frac{p_1(\theta^{(0)*}, a^*, \sigma^{2*})}{p_1(\theta^{(0)}(t-1), a(t-1), \sigma^2(t-1))}$$

$$\cdot \frac{p_2((\theta^{(0)}(t), a(t), \sigma^2(t)) | (\theta^{(0)*}, a^*, \sigma^{2*}))}{p_2((\theta^{(0)*}, a^*, \sigma^{2*}) | (\theta^{(0)}(t), a(t), \sigma^2(t)))}$$

$$\cdot \frac{\prod_k \bar{w}_k^*}{\prod_k \bar{w}_k},$$

where $\bar{w}_k = \frac{1}{m} \sum_{i=1}^m f_{\theta^{(k,i)}}(\mathbf{x}_k)$ and analogously $\bar{w}_k^* = \frac{1}{m} \sum_{i=1}^m f_{\theta^{(k,i)*}}(\mathbf{x}_k)$

Application



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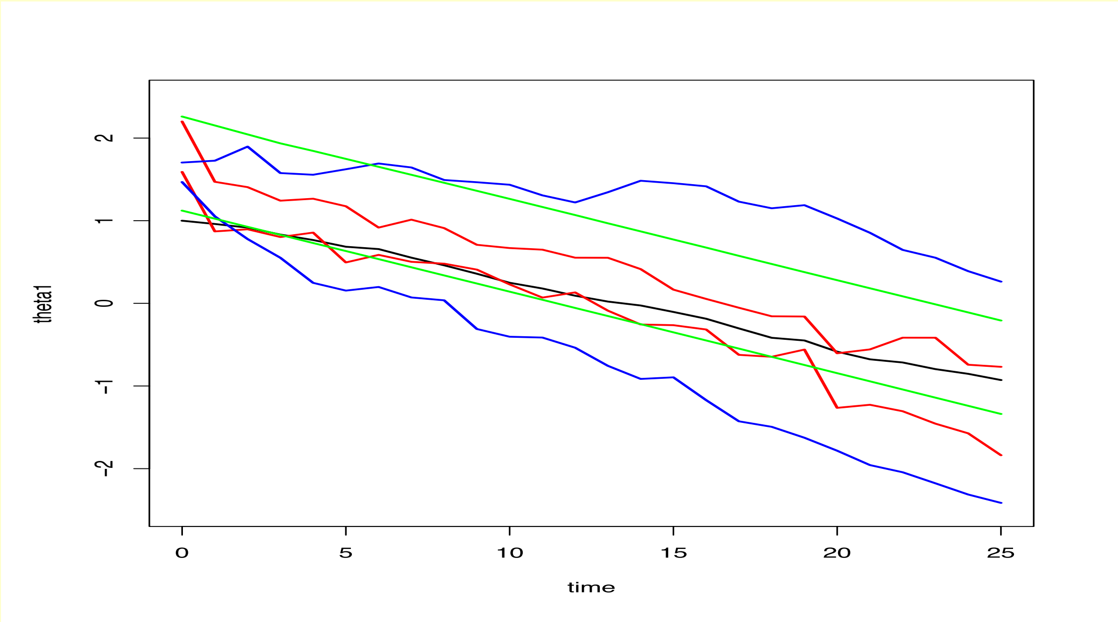
Comparing all three methods



Comparing the real parameters (black line) with envelopes obtained from 19 realizations of the process by MCMC MLE (red lines) and PFE (blue lines) and PMCMC (green lines).

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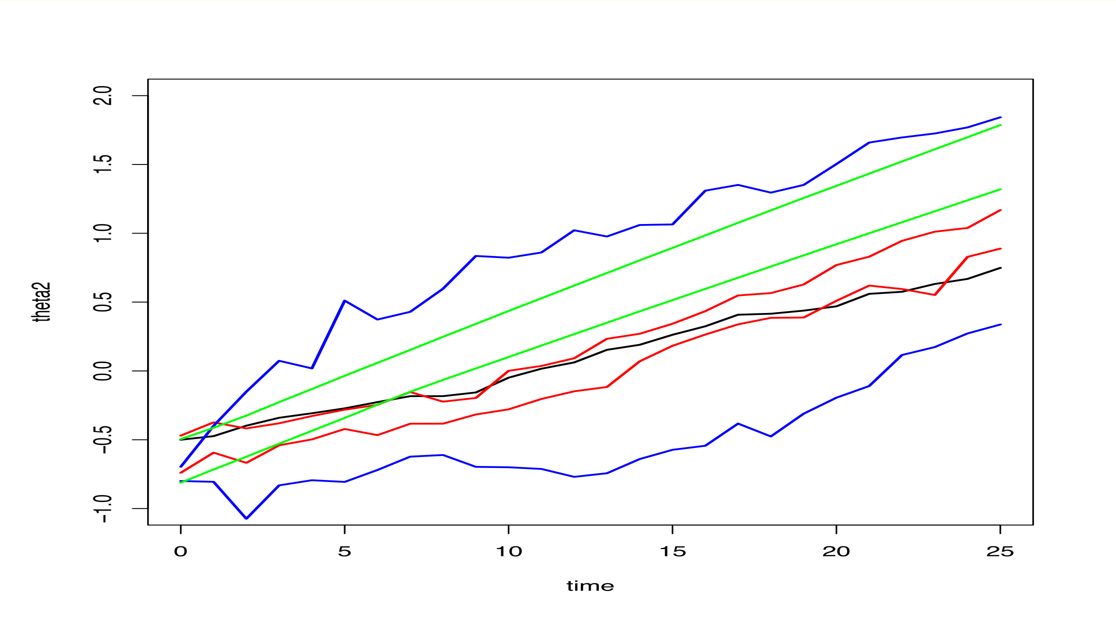

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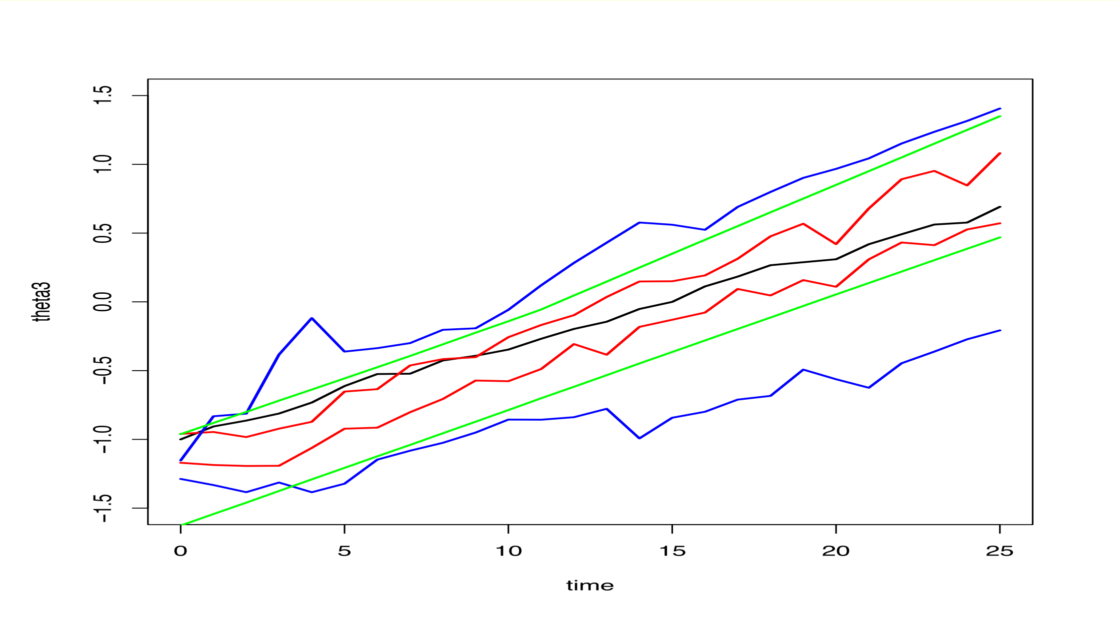

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Thank you for your attention!