On the use of particle Markov chain Monte Carlo in stochastic geometry

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THE MODEL

Denote $\tilde{Y}$ point process of discs with centers in a bounded set $S \in \mathbb{R}^2$ and the density

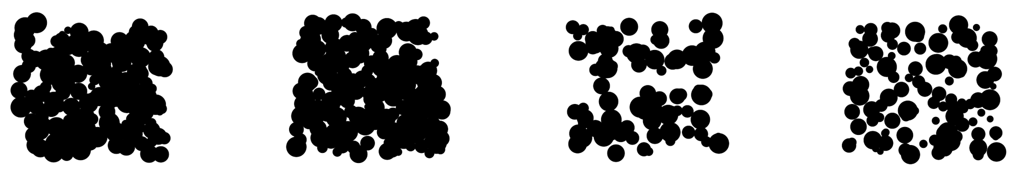
$$p(y|x) = c_x^{-1} \exp(x \cdot T(U_y)), \tag{1}$$

w.r.t. a given reference Poisson point process of discs Ψ on $S \times (0, \infty)$ with intensity measure $\rho(z)dzQ(dr)$. Here c_x^{-1} is a normalising constant and $T(U_y) = (A(U_y), L(U_y), \chi(U_y))$ …three–dimensional vector of geometric characteristics of union U_y for configuration $y \in \tilde{Y}$, where A, L, χ denote area, perimeter and Euler–Poincaré characteristic of U_y respectively.

Further let X_t be a Markov Chain with states in $\mathbb{R}^3$ which developes in time as

$$X_t = X_{t-1} + \eta_t,\ t = 1, 2 \ldots, T, \tag{2}$$

where η is Gaussian $\mathcal{N}(a, \sigma^2 I)$ with $a \in \mathbb{R}^3, \sigma > 0$, so the transition density is $p(x_t|x_{t-1}) = \mathcal{N}(a + x_{t-1}, \sigma^2 I)$.



Sequence of simulated germ-grain model evolution in the time $k = 0, 5, 10, 15, x_0 = (1;, 0.5, -1), a = (-0.07, 0.035, 0.07)$ and $\sigma^2 = 0.001$.

SEQUENTIAL MONTE CARLO

Particle Filter (PF)

is a sequential method used for estimation $p(x_{1:T}|y_{0:T})$ based on Importance sampling. Denote $y_{0:T}$ vector of geometrical characteristics i times $k = 0, \ldots T$ and N the total number of particles.

a) $t = 0,\ i = 1, \ldots, N$, sample x_0^i from $p(x_0)$ independently; $t = 1$,

b) sample $\tilde{x}_t^i$ from $p(x_t|x_{t-1}^i),\ i = 1, \ldots, N$, denote $\tilde{x}_{0:t} = (x_{0:t-1}^i, \tilde{x}_t^i)$.

c) normalize weights $\tilde{w}_t^i \propto p(y_t|\tilde{x}_t^i),\ i = 1, \ldots, N$.

d) sample with replacement $x_{0:t}^i,\ i = 1, \ldots, N$ from $\tilde{x}_{0:t}^i,\ i = 1, \ldots, N$ with normalized weights from c).

e) $t \leftarrow t + 1$, goto b).

Filtered estimate is $\hat{x}_{0:t} = \frac{1}{N}\sum_{i=1}^N x_{0:t}^i$.

Particle Marginal Metropolis Hastings Algorithm

is a combination of Metropolis Hastings algorithm and particle filter ([1]).

Step I - initialization

1 let $\theta = (a, x_0, \sigma^2) \in \mathbb{R}^7$ be a vector of uknown parameters of $x_{1:T}$

2 in iteration $i = 0$ set $\theta(0)$ arbitrarily

3 run PF to estimate $p_{\theta(0)}(.|y_{0:n})$

4 sample $X_{0:n} \sim \hat{p}_{\theta(0)}(.|y_{0:n})$ and denote $\hat{p}_{\theta(0)}(y_{0:n})$ marginal likelihood

Step II

5 now for $i \geq 1$ sample $\theta^* \sim q(.|\theta(i-1))$

6 run PF to estimate $p_{\theta(i-1)}(.|y_{0:n})$

7 sample $X_{0:n} \sim \hat{p}_{\theta^*}(.|y_{0:n})$ and compute $\hat{p}_{\theta^*}(y_{0:n})$

8 with probability

$$1 \wedge \frac{p_{\theta^*}(y_{0:n})p(\theta^*)}{\hat{p}_{\theta(i-1)}(y_{0:n})p(\theta(i-1))}\frac{q(\theta(i-1)|\theta^*)}{q(\theta^*|\theta(i-1))}$$

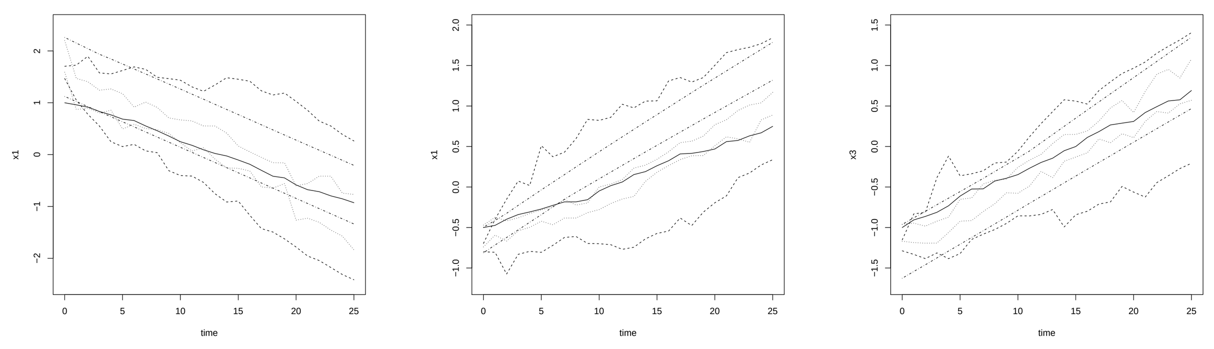
set $\theta(i) = \theta^*$, $X_{0:n}(i) = X_{0:n}^*$, $\hat{p}_{\theta(i)}(y_{0:n}) = \hat{p}_{\theta^*}(y_{0:n})$ and $\theta(i) = \theta(i-1), \ldots$ otherwise

An estimate of the marginal likelihood $p_\theta(y_{1:T})$ is given by

$$\hat{p}_\theta(y_{1:T}) = \hat{p}_\theta(y_1)\prod_{t=2}^T \hat{p}_\theta(y_t|y_{1:t-1}),$$

where

$$\hat{p}_\theta(y_j|y_{j-1}) = \frac{1}{N}\sum_{k=1}^N w_j(X_{1:j}^k)$$



The envelopes based on 19 realizations. Full line denotes the true evolution, dotted lines envelopes for MLE, dashed lines for PF and dot–dashed lines for PMMH.

MODEL CONTROL

Contact distribution function

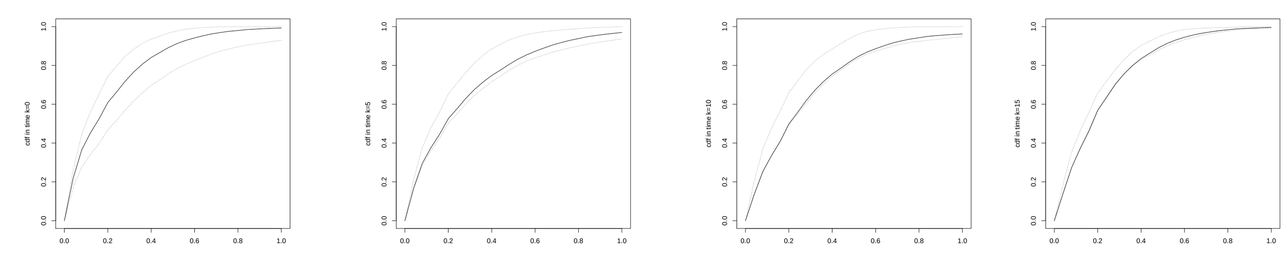
Given a compact convex set $B \subset \mathbb{R}^2$ and random set $\tilde{Y}$ define $D = inf\{r \geq 0 :\ \tilde{Y} \cap rB \neq \emptyset\}$. Assuming $P(D > 0) > 0$ the contact distribution function with structuring element B is

$$H_B(r) = P(D \leq r|D > 0),\ r \geq 0.$$

A non-parametric estimator of H_B for stationary $\tilde{Y}$ including edge-effect correction is

$$\hat{H}_B(r) = \frac{\sum_{u \in L} \mathbf{1}[u \notin \tilde{Y},\ u + rB \subset S,\ (u + rB) \cap \tilde{Y} \neq \emptyset]}{\sum_{u \in L} \mathbf{1}[u \notin \tilde{Y},\ u + rB \subset S]},$$

where L is a regular lattice of test points, B a unit disc.



The envelopes for the contact distribution function at times $t = 0, 5, 10, 15$.

Covariance function

The covariance function of a stationary and isotropic planar random set $\tilde{Z}$ is defined as

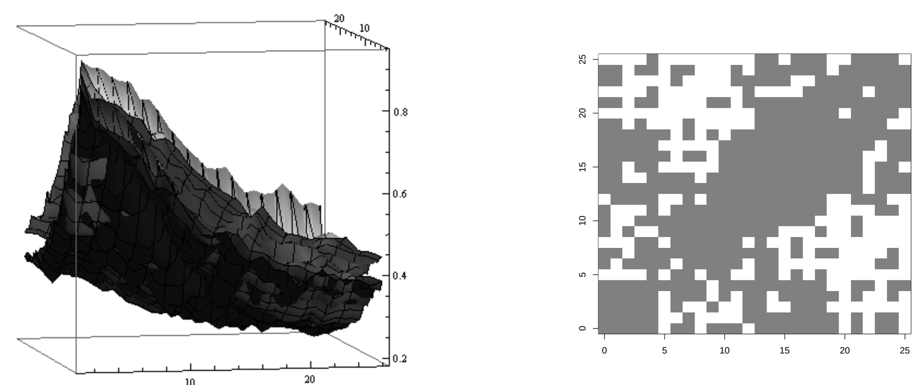
$$C(u, v) = P(u \in \tilde{Z},\ v \in \tilde{Z}),\ u, v \in \mathbb{R}^2.$$

Define the covariance function of two temporal arguments of a space-time random set $Z = \tilde{Z}_{0:T}$ analogously as

$$C(s, t) = P(u \in \tilde{Z}_s,\ u \in \tilde{Z}_t) \quad s, t \in \{0, \ldots, T\}.$$

Assuming planar stationarity of each $\tilde{Z}_t$, $C(s, t)$ does not depend on the choice of $u \in \mathbb{R}^2$. An unbiased and edge-corrected non-parametric estimator of $C(s, t)$ is

$$\hat{C}(s, t) = \frac{\sum_{u \in L} \mathbf{1}[u \in Z_s, u \in Z_t]}{\text{card } L}. \tag{3}$$



The envelopes for covariance function.

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