Nonasymptotic bounds on the estimation error for regenerative MCMC¹

Wojciech Niemiro

Nicolaus Copernicus University, Toruń and University of Warsaw Poland

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Outline

Introduction

- Computing integrals via MCMC
- Accuracy bounds

Regeneration

- Small set and regeneration
- A sequential-regenerative estimator

3 Accuracy bounds

- Mean Square Error
- Confidence estimation and Median of Averages

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How tight are the bounds?

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Computing integrals via MCMC

We are to compute

$$\theta = \int_{\mathcal{X}} f(x) \pi(x) \mathrm{d}x =: \pi(f),$$

where

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- π probability distribution on \mathcal{X} ,

Markov chain

 $X_0, X_1, \ldots, X_t, \ldots$ $\mathbb{P}(X_t \in \cdot) \to \pi(\cdot), \quad (t \to \infty).$

MCMC estimator

$$\hat{\theta}_T = rac{1}{T} \sum_{i=0}^{T-1} f(X_i) \to heta \qquad (T \to \infty).$$

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Computing integrals via MCMC

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where

- \mathcal{X} state space,
- π probability distribution on \mathcal{X} ,

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Accuracy bounds

Mean square error:

$$\mathsf{MSE} \ = \ \mathbb{E} \, (\hat{\theta}_{\mathcal{T}} - \theta)^2 \leq ?$$

Confidence bounds:

$$\mathbb{P}(|\hat{ heta}_{ au} - heta| > arepsilon) \leq ?$$

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How tight are the bounds?

Small set and regeneration

$$P(x,A) = \mathbb{P}(X_n \in A | X_{n-1} = x).$$

ASSUMPTION (Small set)

There exist $J \subseteq \mathcal{X}$, a probability measure ν and $\beta > 0$ such that

 $P(x, \cdot) \geq \beta \mathbb{I}(x \in J) \nu(\cdot).$

 $Q(x, \cdot) := P(x, \cdot) - \beta \mathbb{I}(x \in J)\nu(\cdot)$ is the ,,residual' (sub-stochastic) kernel.

- If $X_{n-1} \notin J$ then draw $X_n \sim P(X_{n-1}, \cdot)$, no regeneration;
- If $X_{n-1} \in J$ then
 - with probability 1β draw $X_n \sim Q(X_{n-1}, \cdot)/(1 \beta)$, no regeneration;
 - with probability β draw $X_n \sim \nu(\cdot)$, Regeneration.

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 - with probability β draw $X_n \sim \nu(\cdot)$, Regeneration.

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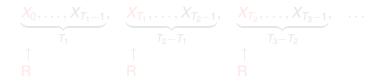
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Regeneration

Remark: Actual sampling from $Q(X_{n-1}, \cdot)/(1 - \beta)$ is **not** necessary (Mykland et al. 1995).

Start with $X_0 \sim \nu(\cdot)$ so that regeneration occurs at $T_0 = 0$. **Times of regeneration** partition a trajectory into **iid blocks**:

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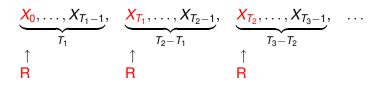
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R = Regeneration

A sequential-regenerative estimator

$$0 = T_0, T_1, \dots, T_r, \dots$$
 – moments of regeneration.
Fix *n*.

$$R(n):=\min\{r:T_r\geq n\}.$$

Estimator:

$$\hat{\theta}_{T_{R(n)}} = \frac{1}{T_{R(n)}} \sum_{i=0}^{T_{R(n)}-1} f(X_i).$$

The estimator uses the part of trajectory written in blue

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Mean Square Error

The integral of interest and its MCMC estimator:

$$heta = \pi(f) = \int_{\mathcal{X}} f(x)\pi(x) \mathrm{d}x, \qquad \hat{ heta}_{T_{R(n)}} = rac{1}{T_{R(n)}} \sum_{i=0}^{T_{R(n)-1}} f(X_i)$$

THEOREM

Under Assumption (Small set),

(*i*)
$$MSE = \mathbb{E} (\hat{\theta}_{T_{R(n)}} - \theta)^2 \leq \frac{\sigma_{as}^2(f)}{n} \left(1 + \frac{\mu_2}{n}\right)$$

(*ii*) $\mathbb{E} T_{R(n)} \leq n + \mu_2$,

where

$$\sigma_{as}^{2}(f) = \frac{1}{\mathbb{E}T_{1}} \mathbb{E}\left[\sum_{i=0}^{T_{1}-1} (f(X_{i}) - \theta)\right]^{2}, \qquad \mu_{2} = \frac{\mathbb{E}T_{1}^{2}}{\mathbb{E}T_{1}} - 1.$$

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Proof

(i) Two identities of Abraham Wald (sequential analysis):

If R is a stopping time then

$$\mathbb{E} \sum_{i=1}^{R} \tau_k = \mathbb{E} R \mathbb{E} \tau_1, \text{ where } \tau_k = T_k - T_{k-1},$$

Var $\sum_{i=1}^{R} d_k = \mathbb{E} R \text{Var} d_1, \text{ where } d_k = \sum_{i=T_{k-1}}^{T_k - 1} (f(X_i) - \theta).$

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(ii) Lorden's theorem (1970, renewal theory).

A geometric drift condition

ASSUMPTION (Drift)

There exist a function $u : \mathcal{X} \to [1, \infty)$, constants $\lambda < 1$ and $c < \infty$ such that

$${\it Qu}(x) \leq egin{cases} \lambda u(x) & ext{for } x
ot\in J, \ c \lambda & ext{for } x \in J, \end{cases}$$

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where $Q(x, \cdot) := P(x, \cdot) - \beta \mathbb{I}(x \in J)\nu(\cdot)$ and $Qu(x) := \int_{\mathcal{X}} Q(x, dy)u(y).$

Explicit bounds under a drift condition

Bounds on $\sigma_{as}^2(f)$ and μ_2 which depend explicitly on the parameters λ , β , *c* and $\pi(u)$:

THEOREM

If Assumptions (Small set), (Drift) hold and $(f - \theta)^2 \le u$ then

$$\begin{split} \sigma_{as}^{2}(f) &\leq \pi(u) \frac{4A_{1}+9}{1-\lambda} + \sqrt{\pi(u)} \frac{A_{2}(1+A_{1})}{(1-\lambda)^{3/2}}, \\ \mu_{2} &\leq 2 \left(\pi(u)+1\right) \frac{1+A_{1}}{1-\lambda}, \\ where A_{1} &= \frac{\log c}{\log(1-\beta)^{-1}}, \\ and A_{2} &= 4 \sqrt{\frac{c}{1-\beta}}. \end{split}$$

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Confidence estimation

Goal:

$$\mathbb{P}(|\hat{\theta} - \theta| \le \varepsilon) \ge 1 - \alpha.$$

(given precision ε at a given level of confidence $1 - \alpha$). We are to choose an estimator and a sufficient number of samples.

Possible approaches:

Chebyshev inequality:

$$\mathbb{P}(|\hat{\theta} - \theta| > \varepsilon) \le \frac{\mathsf{MSE}}{\varepsilon^2}.$$

Problem: appears to be too loose.

Exponential inequalities? Problems with this approach:

- *f* is usually unbounded,
- involve quantities difficult to compute explicitly.

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Median of Averages (MA)

Generate *m* independent copies of the Markov chain and compute estimators (averages):

$$X_0^{(1)}, X_1^{(1)}, \dots, X_t^{(1)}, \dots \longmapsto \hat{\theta}^{(1)},$$

$$\dots$$
$$X_0^{(m)}, X_1^{(m)}, \dots, X_t^{(m)}, \dots \longmapsto \hat{\theta}^{(m)}.$$

Estimator MA:

$$\hat{\theta} = \operatorname{med}\left(\hat{\theta}^{(1)}, \dots, \hat{\theta}^{(m)}\right).$$

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Median of Averages (MA)

$$\hat{ heta} = \mathsf{med}\left(\hat{ heta}^{(1)},\ldots,\hat{ heta}^{(m)}
ight).$$

Idea (Jerrum, Valiant and Vazirani, 1986):

Fix an initial moderate level of confidence $1 - a < 1 - \alpha$ and use Chebyshev inequality to get

$$\mathbb{P}(|\hat{\theta}^{(j)} - \theta| > \varepsilon) \le a$$
 $(j = 1, \dots, m).$

Then boost the level of confidence from 1 - a to $1 - \alpha$ by computing a median:

$$\mathbb{P}(|\hat{ heta} - heta| > \varepsilon) \leq rac{1}{2} \exp\{-m/b\} = lpha.$$

Optimizing the constants: 1 - a = 0.88031, b = 2.3147(Niemiro and Pokarowski, 2009, J. Appl. Probab.)

How tight are the bounds?

Asymptotic level of confidence, based on CLT:

$$\lim_{\varepsilon \to 0} \mathbb{P}(|\hat{\theta} - \theta| > \varepsilon) = \alpha,$$

for the number of samples

$$n \sim \frac{\sigma_{as}^2(f)}{\varepsilon^2} \Big[\Phi^{-1} (1 - \alpha/2) \Big]^2,$$

 $(\hat{\theta} \text{ is a simple average over } n \text{ samples})$

Nonasymptotic level of confidence:

 $\mathbb{P}(|\hat{\theta} - \theta| > \varepsilon) \le \alpha,$

for the expected number of samples

$$m\mathbb{E}T_{R(n)} \sim mn \sim C \cdot rac{\sigma_{as}^2(f)}{arepsilon^2} \log(2lpha)^{-1}$$

($\hat{\theta}$ is MA with sequential/regenerative averages)

Symbol \sim refers to $\alpha, \varepsilon \rightarrow 0$.

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Complexity comparison

Asymptotic:

$$n \sim \frac{\sigma_{as}^2(f)}{\varepsilon^2} \Big[\Phi^{-1} (1 - \alpha/2) \Big]^2,$$

Nonasymptotic:

$$m\mathbb{E}T_{R(n)} \sim mn \sim C \cdot \frac{\sigma_{as}^2(f)}{\varepsilon^2} \log(2\alpha)^{-1},$$

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$$\left[\Phi^{-1}(1-lpha/2)
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 $C pprox 19.34.$

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Problem

How to obtain practically applicable and explicitly computable bounds on $\sigma_{as}^2(f)$?

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