Explicit error bounds of Markov chain Monte Carlo

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Outline

The problem

Let (D, π) be a probability space. Approximate

$$S(f) = \mathbf{E}_\pi f = \int_D f(x)\pi(dx).$$

We assume that one cannot simulate π directly.

Method:
Simulate π with a suitable Markov chain $X_1, X_2, \ldots$ and compute

$$S_{n,n_0}(f) = \frac{1}{n}\sum_{j=1}^{n} f(X_{j+n_0}).$$

The problem

Under known assumptions (ergodic theorem):

$$S_{n,n_0}(f) = \frac{1}{n}\sum_{j=1}^{n} f(X_{j+n_0}) \underset{n\to\infty}{\longrightarrow} \int_D f(x)\pi(dx) = S(f).$$

Error criterion:

$$e_{\nu,K}(S_{n,n_0}, f) = \left(\mathbf{E}_{\nu,K} \left|S(f) - S_{n,n_0}(f)\right|^2\right)^{1/2}.$$

(Markov chain with transition kernel $K(\cdot,\cdot)$ and initial distribution ν)

- Error bounds?
- How large should the burn-in n_0 be?

Properties of Markov chains

Let $K(\cdot,\cdot)$ be a Markov kernel.

- The distribution π is called **stationary** if

$$\pi(A) = \int_D K(x,A)\pi(dx), \quad A \subset D.$$

- The Markov kernel K is called **reversible** if

$$\int_A K(x,B)\pi(dx) = \int_B K(x,A)\pi(dx), \quad A,B \subset D.$$

- The Markov operator is defined by

$$Pf(x) = \int_D f(y)K(x,dy).$$

It is known: K is reversible $\iff$ P is self-adjoint on $L_2(\pi)$.

Ergodicity

Let $K(\cdot,\cdot)$ be the Markov kernel. For $f \in L_1(\pi)$ recall

$$Pf(x) = \int_D f(y)K(x,dy) \quad \text{and} \quad S(f) = \int_D f(y)\pi(dy).$$

- Let $\alpha \in [0,1)$ and $M < \infty$ then the Markov operator is called L_1**-exponential convergent** with (α, M) if

$$\|P^n - S\|_{L_1 \to L_1} \leq M\alpha^n, \qquad n \in \mathbb{N}.$$

- the Markov chain has an L_2**-spectral gap** if

$$\beta := \|P - S\|_{L_2 \to L_2} < 1.$$

- It is known: L_1-exponential convergent with $(\alpha, M) \underset{\text{rev.}}{\Longrightarrow} \beta \leq \alpha$.

Starting with stationary distribution

Theorem (similar to: Aldous 87, Lovász and Simonovits 93)

Let $X_1, X_2, \ldots$ be a reversible Markov chain with initial and stationary distribution π. Let

$$\Lambda = \sup\{\lambda : \lambda \in \sigma(P - S)\} < 1.$$

Let $f \in L_2(\pi)$ and $S_n(f) = \frac{1}{n}\sum_{j=1}^{n} f(X_j)$. Then

$$\sup_{\|f\|_2 \leq 1} e_{\pi,K}(S_n, f)^2 = \frac{1+\Lambda}{n(1-\Lambda)} - \frac{2\Lambda(1-\Lambda^n)}{n^2(1-\Lambda)^2} \leq \frac{2}{n(1-\Lambda)}.$$

- The initial distribution is the stationary one?
- Note that $\Lambda \leq \beta \leq \alpha$.

Exact error formula

Proposition

Let $X_1, X_2, \ldots$ be a Markov chain with initial distribution ν. Let $f \in L_2(\pi)$ and $g = f - S(f)$. Then

$$e_{\nu,K}(S_{n,n_0}, f)^2 = e_{\pi,K}(S_n, f)^2 + \frac{1}{n^2} \sum_{j=1}^{n} L_{j+n_0}(g^2) + \frac{2}{n^2} \sum_{j=1}^{n-1} \sum_{k=j+1}^{n} L_{j+n_0}(g\, P^{k-j} g),$$

where

$$L_i(h) = \left\langle (P^i - S)h, \left(\frac{d\nu}{d\pi} - 1\right) \right\rangle .$$

- Error presentation where equality holds.

Starting with arbitrary distribution: L_2-result

Proposition

Let $X_1, X_2, \dots$ be a reversible Markov chain which is L_1-exponential convergent with (α, M). The initial distribution ν has a bounded density with respect to π.

Then for $f \in L_2(\pi)$ it holds

$$e_{\nu,K}(S_{n,n_0}, f)^2 \le e_{\pi,K}(S_n, f)^2 + \frac{2M \left\| \frac{d\nu}{d\pi} - 1 \right\|_\infty \alpha^{n_0}}{n^2(1-\alpha)^2} \left\| f \right\|_2^2 .$$

Starting with arbitrary distribution: L_p-result

Proposition

Let $f \in L_p(\pi)$ with $p > 2$. Let $X_1, X_2, \dots$ be a Markov chain with L_2-spectral gap, i.e. $\beta := \|P - S\|_{L_2 \to L_2} < 1$.

- If $p \in (2,4)$ then

$$e_{\nu,K}(S_{n,n_0}, f)^2 \leq e_{\pi,K}(S_n, f)^2 + \frac{16p^2}{(p-2)} \frac{\beta^{\frac{2n_0(p-2)}{p}} \left\| \frac{d\nu}{d\pi} - 1 \right\|_{\frac{p}{(p-2)}}}{n^2(1-\beta)^2} \|f\|_p^2 .$$

- If $p \in [4, \infty]$ then

$$e_{\nu,K}(S_{n,n_0}, f)^2 \leq e_{\pi,K}(S_n, f)^2 + \frac{46\beta^{n_0} \left\| \frac{d\nu}{d\pi} - 1 \right\|_2}{n^2(1-\beta)^2} \|f\|_p^2 .$$

Discussion

- Upper bound has the right asymptotic order for $n \to \infty$.
- If initial distribution $\nu = \pi$ then set burn-in $n_0 = 0$.
- Dependence on p?

Let $p = 2$, then:

$$\sup_{\|f\|_2 \leq 1} e_{\nu,K}(S_{n,n_0}, f)^2 \leq \frac{2}{n(1-\alpha)} + \frac{2M \left\| \frac{d\nu}{d\pi} - 1 \right\|_\infty \alpha^{n_0}}{n^2(1-\alpha)^2}.$$

Burn-in

Theorem:

Suppose that the Markov chain is reversible and L_1-exponential convergent with (α, M). Let the burn-in be given by

$$n_0 := \max\left\{ \left\lceil \frac{\log\left(M \left\| \frac{d\nu}{d\pi} - 1 \right\|_\infty\right)}{\log(\alpha^{-1})} \right\rceil, 0 \right\}.$$

Then

$$\sup_{\|f\|_2 \le 1} e_{\nu,K}(S_{n,n_0}, f)^2 \le \frac{2}{n(1-\alpha)} + \frac{2}{n^2(1-\alpha)^2}.$$

Toy example of Rosenthal 93

Let $D = [-1, 1]$. Markov kernel $K(x, \cdot)$:

- `if` $rand() \geq \frac{1}{2}$ `then return x;`
- `elseif` $x \in [-1, 0)$ `chose` $y \in [0, 1]$ `uniformly;`
  `elseif` $x \in [0, 1]$ `chose` $y \in [-1, 0)$ `uniformly;`
  `return y.`

Properties:

- The Markov kernel is reversible with respect to the uniform distribution.
- The Markov kernel is L_1-exponential convergent with $(\frac{1}{2}, 3)$.
- There exists an L_2-spectral gap: $\beta = \|P - S\|_{L_2 \to L_2} = \frac{1}{2}$.

Let $\nu = K(0, \cdot)$ and $n_0 = 2$. Then the error obeys

$$\sup_{\|f\|_2 \leq 1} e_{\nu,K}(S_{n,n_0}, f)^2 \leq \frac{4}{n} + \frac{8}{n^2}.$$

Summary

- Markov chain L_1-exponential convergent

  $\hookrightarrow$ explicit error bound of S_{n,n_0} for $f \in L_2(\pi)$.

- Markov chain has an L_2-spectral gap

  $\hookrightarrow$ explicit error bounds of S_{n,n_0} for $f \in L_p(\pi)$ with $p > 2$.

- Recipe for the choice of the burn-in n_0.

Thank you for your attention!!

Summary

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  - $\hookrightarrow$ explicit error bound of S_{n,n_0} for $f \in L_2(\pi)$.
- Markov chain has an L_2-spectral gap
  - $\hookrightarrow$ explicit error bounds of S_{n,n_0} for $f \in L_p(\pi)$ with $p > 2$.
- Recipe for the choice of the burn-in n_0.

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