Coupled Markov chains with applications to Approximate Bayesian Computation for model based clustering

E. Bertoni, M. Caldarini, F. Di Filippo, G. Gabrielli, E. Musiari

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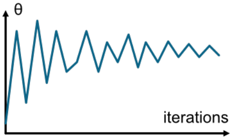
A complex problem



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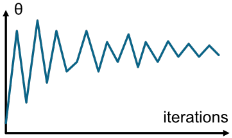
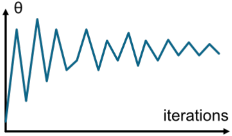


likelihood

A complex problem



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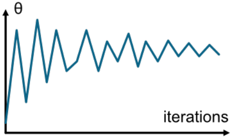
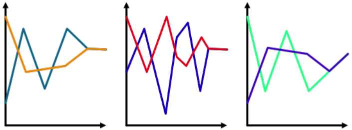


$\Downarrow$

Unbiased Markov chain Monte Carlo methods with couplings



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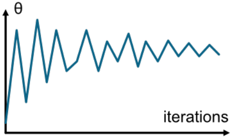

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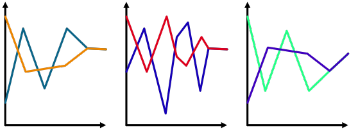

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Approximate Bayesian Computation

Unbiased Markov chain Monte Carlo methods with couplings

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The road to parallelization: coupling of Markov chains

Faster MCMC $\implies$ Parallelization

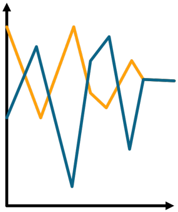
The road to parallelization: coupling of Markov chains

Faster MCMC $\implies$ Parallelization $\iff$ **Unbiased estimator**

The road to parallelization: coupling of Markov chains

Faster MCMC $\Longrightarrow$ Parallelization $\Longleftrightarrow$ **Unbiased estimator**

Exact estimations algorithms using **coupling of Markov chain**.



Rhee–Glynn estimator I

The goal is to estimate

$$\mathbb{E}_\pi[h(X)] = \int h(x)\pi(\mathrm{d}x).$$

The estimator we are going to construct is based on a coupled pair of Markov chains, $(X_t)_{t\geq 0}$ and $(Y_t)_{t\geq}$, which marginally start from π_0 and evolve accordingly to P.

Rhee–Glynn estimator II

We consider some assumptions:

1. as $t \to \infty$,
$$\mathbb{E}[h(X_t)] \to \mathbb{E}_\pi[h(X)];$$
and there exists $\eta > 0$ and $D < \infty$ such that $\mathbb{E}[|h(X_t)|^{2+\eta}] \leq D$ for all $t \geq 0$;

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2. the chains are such that the meeting time
$$\tau = \inf\{t \geq 1 : X_t = Y_{t-1}\}$$
satisfies $\mathbb{P}(\tau > t) \leq C\delta^t$ for all $t \geq 0$, for some constants $C < \infty$ and $\delta \in (0, 1)$;

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3. the chains stay together after meeting:
$$X_t = Y_{t-1} \text{ for all } t \geq \tau.$$

Rhee–Glynn estimator III

Thanks to the previous assumptions we can prove that:

$$\mathbb{E}_\pi[h(X)] = \mathbb{E}\Big[h(X_k) + \sum_{t=k+1}^{\tau-1} \{h(X_t) - h(Y_{t-1})\}\Big];$$

Rhee–Glynn estimator III

Thanks to the previous assumptions we can prove that:

$$\mathbb{E}_\pi[h(X)] = \mathbb{E}[h(X_k) + \sum_{t=k+1}^{\tau-1} \{h(X_t) - h(Y_{t-1})\}];$$

and we define the Rhee–Glynn estimator as:

$$H_k(X, Y) = h(X_k) + \sum_{t=k+1}^{\tau-1} \{h(X_t) - h(Y_{t-1})\}$$

which is **unbiased** by construction.

Time-averaged estimator I

$$H_{k:m}(X,Y) = \frac{1}{m-k+1}\sum_{l=k}^{m} h(X_l) + \sum_{l=k+1}^{\tau-1} \min\left(1, \frac{l-k}{m-k+1}\right)\{h(X_l) - h(Y_{l-1})\}$$

Time-averaged estimator I

$$H_{k:m}(X,Y) = \underbrace{\frac{1}{m-k+1}\sum_{l=k}^{m} h(X_l)}_{MCMC_{k:m}} + \sum_{l=k+1}^{\tau-1} \min\left(1, \frac{l-k}{m-k+1}\right)\{h(X_l) - h(Y_{l-1})\}$$

- $MCMC_{k:m}$ is the standard MCMC average;

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- $MCMC_{k:m}$ is the standard MCMC average;
- $BC_{k:m}$ is the bias correction;

Time-averaged estimator II

1. draw X_0 and Y_0 from an initial distribution π_0 and draw $X_1 \sim P(X_0, \cdot)$;
2. set $t = 1$: while $t < \max\{m, \tau\}$ and:
   a. draw $(X_{t+1}, Y_t) \sim \bar{P}\{(X_t, Y_{t-1}), \cdot\}$;
   b. set $t \leftarrow t + 1$;
3. compute the time-averaged estimator:

$$H_{k:m}(X, Y) = \frac{1}{m-k+1} \sum_{l=k}^{m} h(X_l) + \sum_{l=k+1}^{\tau-1} \min(1, \frac{l-k}{m-k+1}) \{h(X_l) - h(Y_{l-1})\}.$$

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$\bar{P}$ must be evaluated before!

$$H_{k:m}(X, Y) = \frac{1}{m-k+1} \sum_{l=k}^{m} h(X_l) + \sum_{l=k+1}^{\tau-1} \min(1, \frac{l-k}{m-k+1})\{h(X_l) - h(Y_{l-1})\}.$$

Time-averaged estimator III

Metropolis–Hasting algorithm allow us to calculate the coupled kernel $\bar{P}\{(X_t, Y_{t-1}), \cdot\}$:

1. sample $(X^\star, Y^\star)|(X_t, Y_{t-1})$ from a maximal coupling of $q(X_t, \cdot)$ and $q(Y_{t-1}, \cdot)$;
2. sample $U \sim \mathcal{U}([0,1])$;
3. if
$$U \leq \min\left\{1, \frac{\pi(X^\star)q(X^\star, X_t)}{\pi(X_t)q(X_t, X^\star)}\right\}$$
then $X_{t+1} = X^\star$; otherwise $X_t = X_{t-1}$;
4. if
$$U \leq \min\left\{1, \frac{\pi(Y^\star)q(Y^\star, Y_t)}{\pi(Y_t)q(Y_t, Y^\star)}\right\}$$
then $Y_{t+1} = Y^\star$; otherwise $Y_t = Y_{t-1}$.

Time-averaged estimator III

Metropolis–Hasting algorithm allow us to calculate the coupled kernel $\bar{P}\{(X_t, Y_{t-1}), \cdot\}$:

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Approximate Bayesian Computation

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Likelihood-free rejection sampling algorithm I

Inputs:

- a target posterior density $\pi(\theta|y_{obs}) \propto p(y_{obs}|\theta)\pi(\theta)$, consisting of a prior distribution $\pi(\theta)$ and a procedure of generating data under the model $p(y_{obs}|\theta)$;
- a proposal density $g(\theta)$, with $g(\theta) > 0$ if $\pi(\theta|y_{obs}) > 0$;
- an integer $N > 0$.

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Sampling for $i = 1, ..., N$:

1. generate $\theta^{(i)} \sim g(\theta)$ from sampling density g;
2. generate $y \sim p(y|\theta^{(i)})$ from the likelihood;
3. if $y = y_{obs}$, then accept $\theta^{(i)}$ with probability $\frac{\pi(\theta^{(i)})}{Kg(\theta^{(i)})}$, where $K \geq \max_\theta \frac{\pi(\theta)}{g(\theta)}$; else go to 1.

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Output:

- a set of parameter vectors $\theta^{(1)}, ..., \theta^{(N)}$ which are samples from $\pi(\theta|y_{obs})$.

Likelihood-free rejection sampling algorithm II

Is this an efficient method for complex analysis?

Likelihood-free rejection sampling algorithm II

Is this an efficient method for complex analysis?

3 If $\| y - y_{obs} \| \leq h$, then accept $\theta^{(i)}$ with probability $\frac{\pi(\theta^{(i)})}{Kg(\theta^{(i)})}$, where $K \geq \max_\theta \frac{\pi(\theta)}{g(\theta)}$; else go to 1.

Approximate Bayesian Computation

$$\pi(\theta, y|y_{obs}) \propto \mathbb{1}(\| y - y_{obs} \| \leq h) p(y|\theta)\pi(\theta)$$

$$\Downarrow$$

$$\pi_{ABC}(\theta, y|y_{obs}) \propto K_h(u) p(y|\theta)\pi(\theta)$$

Approximate Bayesian Computation

$$\pi(\theta, y|y_{obs}) \propto \mathbb{I}(\| y - y_{obs} \| \leq h) p(y|\theta)\pi(\theta)$$

$$\Downarrow$$

$$\pi_{ABC}(\theta, y|y_{obs}) \propto K_h(u) p(y|\theta)\pi(\theta)$$

Where we used a **standard smoothing kernel function**:

$$K_h(u) = \frac{1}{h} K\left(\frac{u}{h}\right), \quad \text{with } u = \| y - y_{obs} \|$$

Summary statistics I

Is this feasible in practice?

Summary statistics I

Is this feasible in practice?

No, it's difficult to have $y \approx y_{obs}$: we should use a large h, obtaining a poor posterior approximation!

$\Longrightarrow$ use summary statistics $s = S(y)$

Summary statistics II

Critical decision: choice of summary statistics

Summary statistics II

Critical decision: choice of summary statistics

Dimension of summary statistics:

- large enough to contain as much as information about observed data as possible
- low enough to avoid curse of dimensionality of matching s and s_{obs}

$\Longrightarrow$ choose sufficient statistics, such that:

$$\pi(\theta|s_{obs}) \equiv \pi(\theta|y_{obs})$$

Distance measure

Distance measure: substantial impact on ABC algorithm efficiency

$$\| s - s_{obs} \| = (s - s_{obs})^\top \Sigma^{-1} (s - s_{obs})$$

Distance measure

Distance measure: substantial impact on ABC algorithm efficiency

$$\| s - s_{obs} \| = (s - s_{obs})^\top \Sigma^{-1} (s - s_{obs})$$

- $\Sigma =$ identity matrix $\rightarrow$ Euclidean distance
- $\Sigma =$ diagonal matrix of non-zero weights $\rightarrow$ Weighted Euclidean distance
- $\Sigma =$ full covariance matrix of s $\rightarrow$ Mahalanobis distance

ABC rejection sampling algorithm

Inputs:

- a target posterior density $\pi(\theta|y_{obs}) \propto p(y_{obs}|\theta)\pi(\theta)$, consisting of a prior distribution $\pi(\theta)$ and a procedure of generating data under the model $p(y_{obs}|\theta)$;
- a proposal density $g(\theta)$, with $g(\theta) > 0$ if $\pi(\theta|y_{obs}) > 0$;
- an integer $N > 0$;
- a kernel function $K_h(u)$ and a scale parameter $h > 0$;
- a low dimensional vector of summary statistics $s = S(y)$.

ABC rejection sampling algorithm

Sampling for $i = 1, ..., N$:

1. generate $\theta^{(i)} \sim g(\theta)$ from sampling density g;
2. generate $y \sim p(y|\theta^{(i)})$ from the likelihood;
3. compute summary statistic $s = S(y)$;
4. accept $\theta^{(i)}$ with probability $\frac{K_h(\|s - s_{obs}\|)\pi(\theta^{(i)})}{Kg(\theta^{(i)})}$, where $K \geq K_h(0) \max_\theta \frac{\pi(\theta)}{g(\theta)}$; else go to 1.

Output:

- a set of parameter vectors $\theta^{(1)}, ..., \theta^{(N)} \sim \pi_{ABC}(\theta|S_{obs})$.

Conclusions

Next steps

Our focus till now was to understand the fundamental concepts and collect the missing information.

The next step will be a **simple and separate implementation** of both solution to be tested on simulated data.

Further steps will consider the **integration** of both solution into a single implementation and the testing on more complex data.

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