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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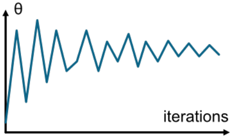
A complex problem



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Unbiased Markov chain Monte Carlo methods with couplings

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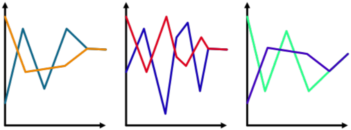
Approximate Bayesian Computation



Unbiased Markov chain Monte Carlo methods with couplings

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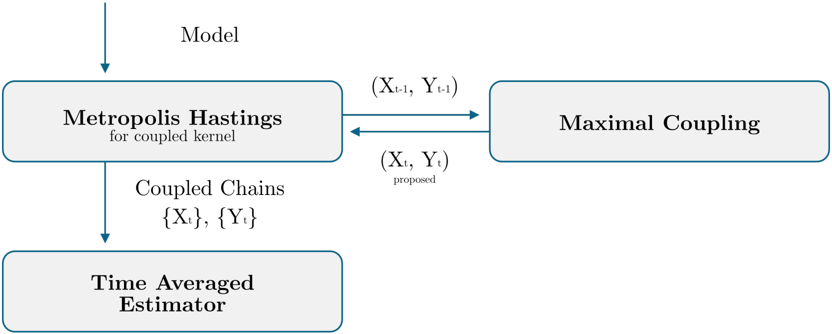
Structure of the method



Time-averaged estimator

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:

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

Metropolis–Hasting algorithm for a coupled kernel

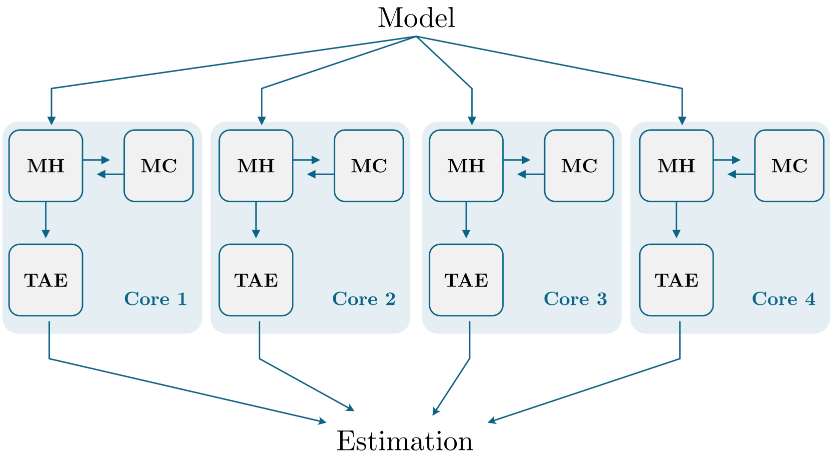
1. sample $(X^\star, Y^\star)|(X_t, Y_{t-1})$ from a maximal coupling of $q(X_t, \cdot)$ and $q(Y_{t-1}, \cdot)$;
2. sample $U \sim \mathcal{U}([0,1])$;
3. if
$$U \leq \min\left\{1, \frac{\pi(X^\star)q(X^\star, X_t)}{\pi(X_t)q(X_t, X^\star)}\right\}$$
then $X_{t+1} = X^\star$; otherwise $X_t = X_{t-1}$;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

Maximal coupling

Set $p = \mathcal{N}(X_{t-1}, 1)$ and $q = \mathcal{N}(Y_{t-1}, 1)$, then:

1. sample $X_t \sim p$;
2. sample $W|X_t \sim \mathcal{U}\{[0, p(X_t)]\}$;
3. if $W \leq q(X_t)$ then output (X_t, X_t), otherwise:
   1. sample $Y_t \sim q$;
   2. sample $W^\star|Y_t \sim \mathcal{U}\{[0, q(Y_t)]\}$ until $W^\star > p(Y_t)$ and output (X_t, Y_t).

Parallelization



Study case

Model

$$Y_i|\mu \overset{iid}{\sim} \mathcal{N}(\mu, \sigma_{obs}^2)$$

$$\mu \sim \mathcal{N}(\mu_0, \sigma_0^2)$$
$$\mu_0 = 38, \quad \sigma_0^2 = 4$$

Dataset

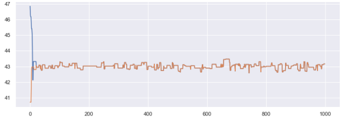
1000 samples generated from a Gaussian distribution:

$$Y_{obs} \sim \mathcal{N}(\mu_{obs}, \sigma_{obs}^2)$$
$$\mu_{obs} = 43, \quad \sigma_{obs}^2 = 5$$

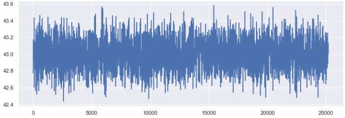
Results

$$\mathcal{N}(\mu_n, \sigma_n^2), \quad \mu_n = \frac{1}{\frac{1}{\sigma_0^2} + \frac{n}{\sigma_{obs}^2}} \cdot \left(\frac{\mu_0}{\sigma_0^2} + \frac{\sum y_{obs}}{\sigma_{obs}^2} \right) \simeq 42.99, \quad \sigma_n^2 = \frac{1}{\frac{1}{\sigma_0^2} + \frac{n}{\sigma_{obs}^2}} \simeq 0.025$$

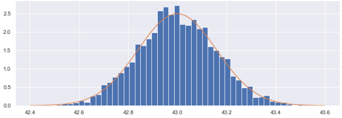
Coupled chains



Complete sampling



Sampling histogram



Time Averaged Estimators mean:

$$\mathbb{E}[H_{k:m}(X, Y)] = 42.9498$$

Approximate Bayesian Computation

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ABC Metropolis Hastings

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 Markov proposal density $g(\theta, \theta')$=$g(\theta'|\theta)$;
- an integer $N > 0$;
- a kernel function $K_h(u)$ and a scale parameter $h > 0$;
- a low dimensional vector of summary statistics $s = S(y)$.

Initialise:

repeat:

1. choose an initial parameter vector $\theta^{(0)}$ from the support of $\pi(\theta)$;
2. generate $y^{(0)} \sim p(y|\theta^{(0)})$ from the model and compute summary statistics $s^{(0)} = S(y^{(0)})$, until $K_h(\| s^{(0)} - s_{obs} \|) > 0$.

ABC Metropolis Hastings

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

1. generate candidate vector $\theta' \sim g(\theta^{(i-1)}, \theta)$ from the proposal density g;
2. generate $y' \sim p(y|\theta')$ from the model and compute summary statistics $s' = S(y')$;
3. with probability

$$\min\{1, \frac{K_h(\| s' - s_{obs} \|)\pi(\theta')g(\theta', \theta^{(i-1)})}{K_h(\| s^{(i-1)} - s_{obs} \|)\pi(\theta^{(i-1)})g(\theta^{(i-1)}, \theta')}\}$$

set $(\theta^{(i)}, s^{(i)}) = (\theta', s')$. Otherwise set $(\theta^{(i)}, s^{(i)}) = (\theta^{(i-1)}, s^{(i-1)})$.

Output:

- a set of correlated parameter vectors $\theta^{(1)}, ..., \theta^{(N)}$ from a Markov chain with stationary distribution $\pi_{ABC}(\theta|S_{obs})$.

Summary statistic:

Sample mean

Distance:

2-norm of the difference.

Kernel:

$$K(u) = \frac{1}{\sqrt{2\pi}} e^{-\frac{1}{2}u^2}, \quad K_h(u) = \frac{K(\frac{u}{h})}{h}.$$

Study case

Same as previous: - DA RIVEDERE

Model

$$Y_i|\mu \overset{iid}{\sim} \mathcal{N}(\mu, \sigma^2_{obs})$$

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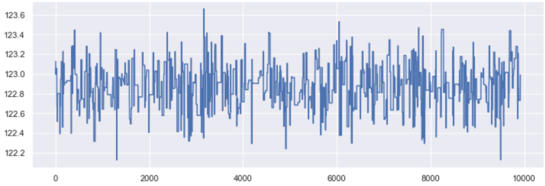
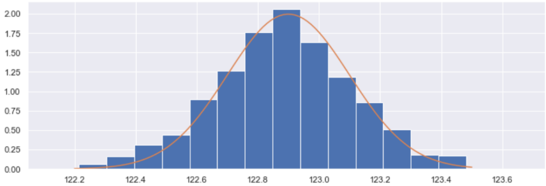
Sampling

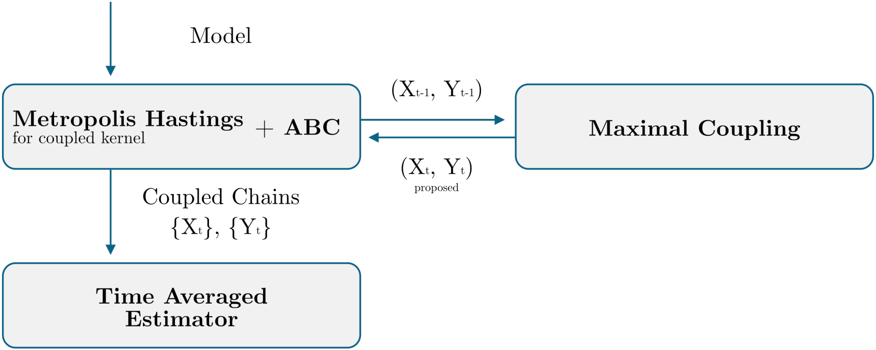


Sampling histogram with real distribution



The complete method: MCMC + Couplings + ABC

Implementation



Metropolis Hastings with couplings and ABC

1. Compute $s_{obs} = S(y_{obs})$;
2. generate $\theta_x^{(0)} \sim \pi(\mu)$ and $\theta_y^{(0)} \sim \pi(\mu)$ from prior density;
3. generate with a maximal coupling two samples of N observations such that $y_{1i} \sim \mathcal{N}(\theta_x^{(0)}, \sigma^2_{obs})$ and $y_{2j} \sim \mathcal{N}(\theta_y^{(0)}, \sigma^2_{obs})$;
4. compute $s_x^{(0)} = S(y_1)$ and $s_y^{(0)} = S(y_2)$;
5. untill $Kh(||s_x^{(0)} - s_{obs}||) > 0$:
    - generate $\theta_x^{(0)} \sim \pi(\mu)$ from prior density;
    - generate a sample of N observations such that $y_{1i} \sim \mathcal{N}(\theta_x^{(0)}, \sigma^2_{obs})$;
    - compute $s_x^{(0)} = S(y_1)$;
6. untill $Kh(||s_y^{(0)} - s_{obs}||) > 0$:
    - generate $\theta_y^{(0)} \sim \pi(\mu)$ from prior density;
    - generate a sample of N observations such that $y_{2j} \sim \mathcal{N}(\theta_y^{(0)}, \sigma^2_{obs})$;
    - compute $s_y^{(0)} = S(y_2)$;

Metropolis Hastings with couplings and ABC

8. for i = 1,...,N:
   - generate $[\theta_x^{(i)}, \theta_y^{(i)}]$ from a maximal coupling given $[\theta_x^{(i-1)}, \theta_y^{(i-1)}]$;
   - generate from a maximal coupling two samples of N observations $y_1 \sim p(y|\theta_x^{(i)})$ and $y_2 \sim p(y|\theta_y^{(i)})$;
   - compute $s_x^{(i)} = S(y_1)$ and $s_y^{(i)} = S(y_2)$;
   - accept $\theta_x^{(i)}$ with probability

$$\frac{Kh(||s_x^{(i)} - s_{obs}||)\pi(\theta_x^{(i)})}{Kh(||s_x^{(i-1)} - s_{obs}||)\pi(\theta_x^{(i-1)})}$$

   and accept $\theta_y^{(i)}$ with probability

$$\frac{Kh(||s_y^{(i)} - s_{obs}||)\pi(\theta_y^{(i)})}{Kh(||s_y^{(i-1)} - s_{obs}||)\pi(\theta_y^{(i-1)})}.$$

Metropolis Hastings with couplings and ABC

As output we get two sets of parameter vectors:

$$\theta_x^{(1)}, ..., \theta_x^{(N)} \sim \pi_{ABC}(\theta | y_{obs});$$

$$\theta_y^{(1)}, ..., \theta_y^{(N)} \sim \pi_{ABC}(\theta | y_{obs}).$$

Study case

Summary statistic:

Sample mean

Distance:

2-norm of the difference.

Kernel:

$$K(u) = \frac{1}{\sqrt{2\pi}} e^{-\frac{1}{2}u^2}, \quad K_h(u) = \frac{K(\frac{u}{h})}{h}.$$

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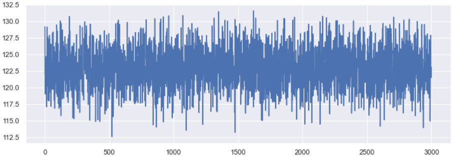
Sampling



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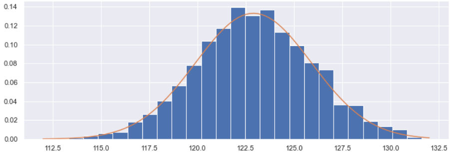

Conclusions

Next steps

The next step will be the conclusion of the **multivariate implementation** the MCMC with couplings and approximate bayesian computation.

Further steps will be testing on more complex data.

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