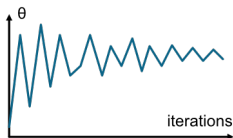# Coupled Markov chains with applications to Approximate Bayesian Computation for model based clustering

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

10 January 2022

Approximate Bayesian Computation

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

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 $K_h(\| s^{(0)} - s_{obs} \|) > 0$.

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- a kernel function $K_h(u)$ and a scale parameter $h > 0$:

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

$$\Downarrow$$

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

Where K is a standard smoothing kernel function and:

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

Inputs:

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- a low dimensional vector of summary statistics $s = S(y)$:

$$K_h(\| y - y_{obs} \|)$$
$$\Downarrow$$
$$K_h(\| S(y) - S(y_{obs}) \|)$$

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 $g(\theta, \theta')=g(\theta'|\theta)$;
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- a low dimensional vector of summary statistics $s = S(y)$.

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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 $K_h(\| s^{(0)} - s_{obs} \|) > 0$.

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 $\pi_{ABC}(\theta|S_{obs})$.

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Summary statistic:

Sample mean, vector of 9 quantiles

Distance:

2-norm of the difference

Kernel:

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

Model

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

$$\mu \sim \mathcal{N}(\mu_0, \sigma_0^2)$$
$$\mu_0 = 8, \quad \sigma_0^2 = 4$$

Dataset

100 samples generated from a Gaussian distribution:

$$Y_{obs} \sim \mathcal{N}(\mu_{obs}, \sigma_{obs}^2)$$
$$\mu_{obs} = 10, \quad \sigma_{obs}^2 = 3$$

Posterior distribution:
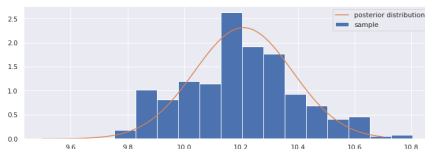
$$\mathcal{N}(\mu_n, \sigma_n^2),$$

$$\mu_n = \frac{1}{\frac{1}{\sigma_0^2} + \frac{n}{\sigma_{obs}^2}} \cdot \left(\frac{\mu_0}{\sigma_0^2} + \frac{\sum y_{obs}}{\sigma_{obs}^2} \right) \simeq 10.151,$$

$$\sigma_n^2 = \frac{1}{\frac{1}{\sigma_0^2} + \frac{n}{\sigma_{obs}^2}} \simeq 0.0298$$
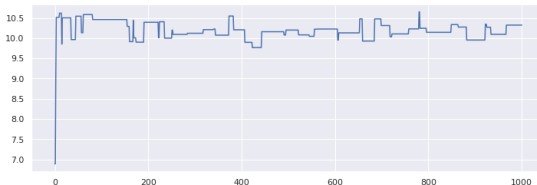
Sampling
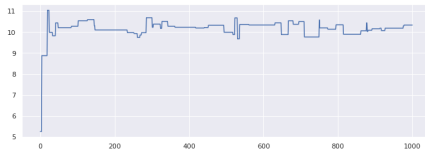
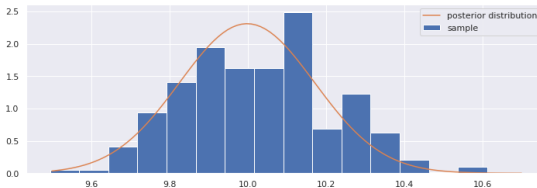**Sampling histogram with real distribution**

The same model using as summary statistic a vector of 9 quantiles:

Sampling
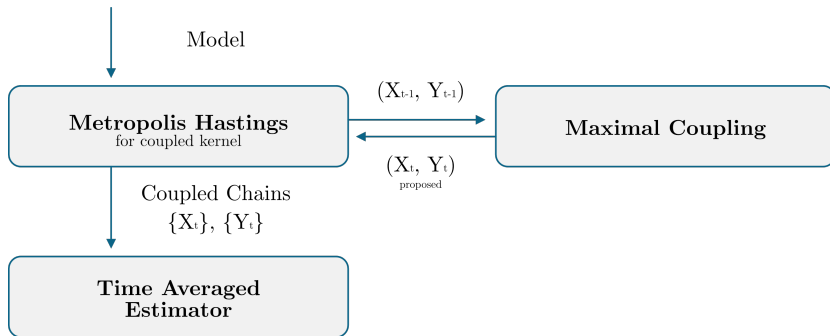

Sampling histogram with real distribution

Unbiased Markov chain Monte Carlo methods with couplings

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

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
$$U \le \min \left\{ 1, \frac{\pi(X^\star)q(X^\star, X_t)}{\pi(X_t)q(X_t, X^\star)} \right\}$$

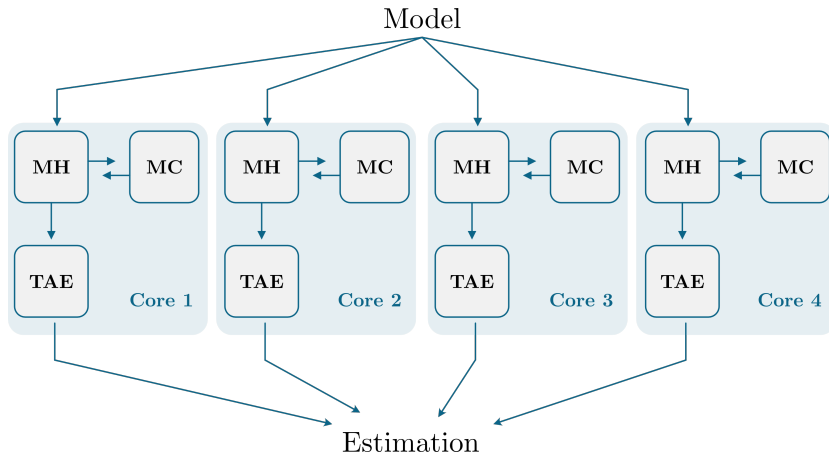   then $X_{t+1} = X^\star$; otherwise $X_t = X_{t-1}$;

4. if
$$U \le \min \left\{ 1, \frac{\pi(Y^\star)q(Y^\star, Y_t)}{\pi(Y_t)q(Y_t, Y^\star)} \right\}$$

   then $Y_{t+1} = Y^\star$; otherwise $Y_t = Y_{t-1}$.

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).

Model

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

$$\mu \sim \mathcal{N}(\mu_0, \sigma_0^2)$$
$$\mu_0 = 8, \quad \sigma_0^2 = 4$$

Dataset
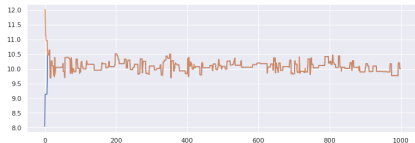
100 samples generated from a Gaussian distribution:

$$Y_{obs} \sim \mathcal{N}(\mu_{obs}, \sigma_{obs}^2)$$
$$\mu_{obs} = 10, \quad \sigma_{obs}^2 = 3$$

Posterior distribution:

$$\mathcal{N}(\mu_n, \sigma_n^2), \quad \mu_n \simeq 10.065, \quad \sigma_n^2 \simeq 0.0298$$
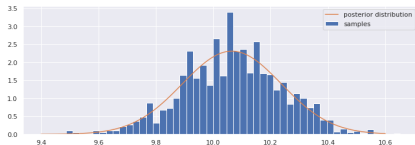
Coupled chains

Complete sampling

Sampling histogram

Time Averaged Estimators mean:
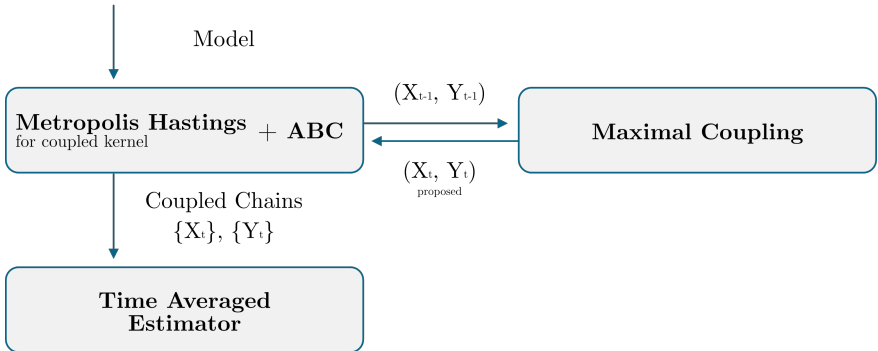$$\mathbb{E}[H_{k:m}(X, Y)] = 10.06$$

The complete method: MCMC + Couplings + ABC

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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 $y_{1i} \sim \mathcal{N}(\theta_x^{(0)}, \sigma_{obs}^2)$ and $y_{2j} \sim \mathcal{N}(\theta_y^{(0)}, \sigma_{obs}^2)$;
4. compute $s_x^{(0)} = S(y_1)$ and $s_y^{(0)} = S(y_2)$;
5. until $K_h(||s_x^{(0)} - s_{obs}||) > 0$:
   - generate $\theta_x^{(0)} \sim \pi(\mu)$ from prior density;
   - generate a sample of N observations such that $y_{1i} \sim \mathcal{N}(\theta_x^{(0)}, \sigma_{obs}^2)$;
   - compute $s_x^{(0)} = S(y_1)$;
6. until $K_h(||s_y^{(0)} - s_{obs}||) > 0$:
   - generate $\theta_y^{(0)} \sim \pi(\mu)$ from prior density;
   - generate a sample of N observations such that $y_{2j} \sim \mathcal{N}(\theta_y^{(0)}, \sigma_{obs}^2)$;
   - compute $s_y^{(0)} = S(y_2)$;

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

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

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

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

As output we get two sets of parameter vectors:

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

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

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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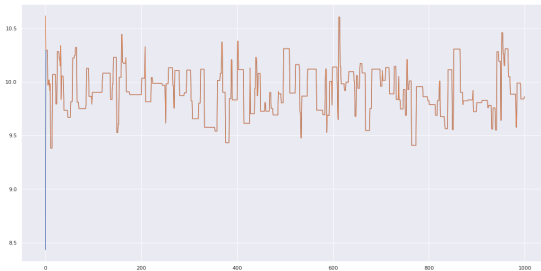$$\mu_0 = 8, \quad \sigma_0^2 = 4$$

Dataset

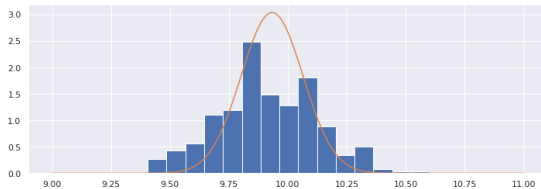100 samples generated from a Gaussian distribution:

$$Y_{obs} \sim \mathcal{N}(\mu_{obs}, \sigma_{obs}^2)$$
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Coupled chains

Sampling histogram with real distribution

Conclusions

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

Further steps will be implementing the version with unknown variance and testing on more complex data.
Finally, making comparisons with a standard MCMC algorithm.

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