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

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

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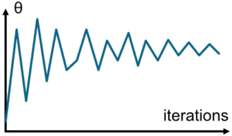
# A complex problem







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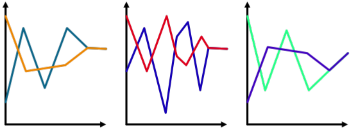
**Unbiased Markov chain Monte Carlo methods with couplings**



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**Approximate Bayesian Computation**

# Approximate Bayesian Computation

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*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**:

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

Same as previous: - DA RIVEDERE

### Model

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

$$\mu \sim \mathcal{N}(\mu_0, \sigma^2_0)$$
$$\mu_0 = 38, \quad \sigma^2_0 = 4$$

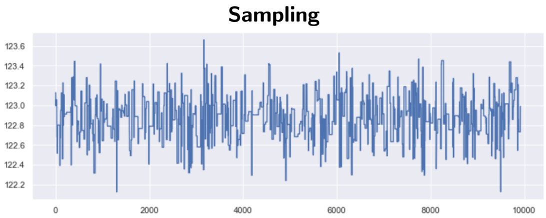
### Dataset

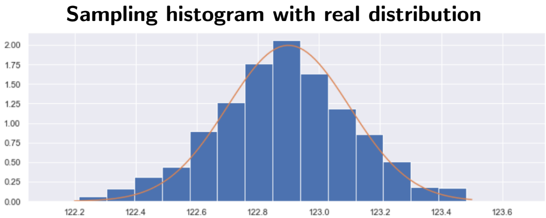
1000 samples generated from a Gaussian distribution:

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

# Results




Sampling
123.6
123.4
123.2
123.0
122.8
122.6
122.4
122.2
0
2000
4000
6000
8000
10000


Sampling histogram with real distribution
2.00
1.75
1.50
1.25
1.00
0.75
0.50
0.25
0.00
122.2
122.4
122.6
122.8
123.0
123.2
123.4
123.6

# Unbiased Markov chain Monte Carlo methods with couplings

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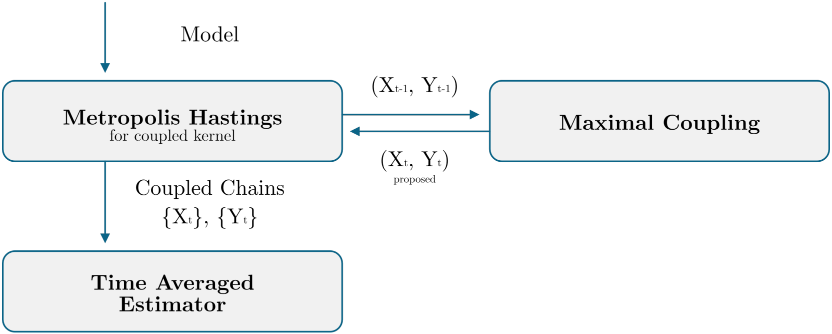
# Structure of the method





## Time-averaged estimator



1. draw $X_0$ and $Y_0$ from an initial distribution $\pi_0$ 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:

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

## 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

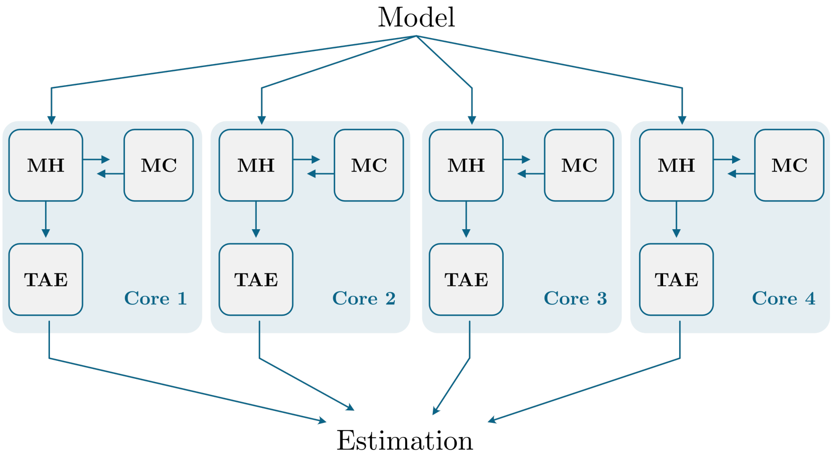


Set $p = \mathcal{N}(X_{t-1}, 1)$ and $q = \mathcal{N}(Y_{t-1}, 1)$, then:

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

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

$$\mu \sim \mathcal{N}(\mu_0, \sigma^2_0)$$
$$\mu_0 = 38, \quad \sigma^2_0 = 4$$

## Dataset

1000 samples generated from a Gaussian distribution:

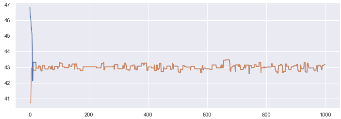
$$Y_{obs} \sim \mathcal{N}(\mu_{obs}, \sigma^2_{obs})$$
$$\mu_{obs} = 43, \quad \sigma^2_{obs} = 5$$

# Results

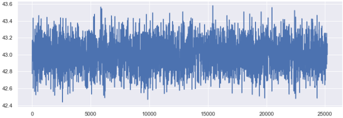


$$\mathcal{N}(\mu_n, \sigma_n^2), \quad \mu_n = \frac{1}{\frac{1}{\sigma_0^2} + \frac{n}{\sigma_{obs}^2}} \cdot \left( \frac{\mu_0}{\sigma_0^2} + \frac{\sum y_{obs}}{\sigma_{obs}^2} \right) \simeq 42.99, \quad \sigma_n^2 = \frac{1}{\frac{1}{\sigma_0^2} + \frac{n}{\sigma_{obs}^2}} \simeq 0.025$$

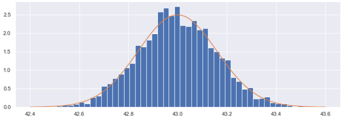
**Coupled chains**




**Complete sampling**




**Sampling histogram**

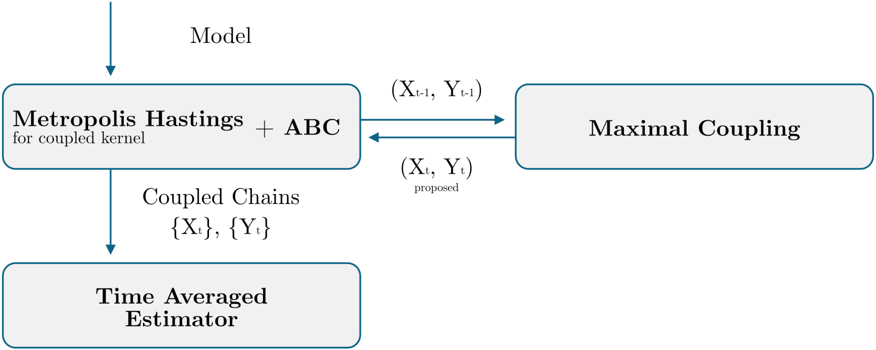



**Time Averaged Estimators mean:**

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

# 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. until $Kh(||s_x^{(0)} - s_{obs}||) > 0$:
   - 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. until $Kh(||s_y^{(0)} - s_{obs}||) > 0$:
   - 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:

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

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

**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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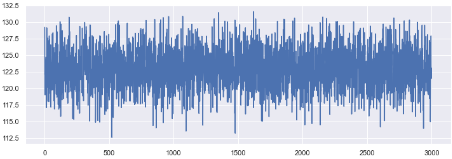
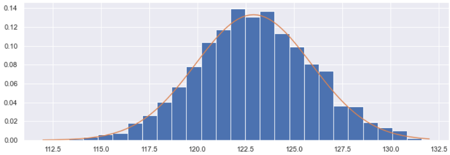



**Sampling histogram with real distribution**



# 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.

# Bibliography




Pierre Jacob, John O'Leary, and Yves Atchadé.
Unbiased markov chain monte carlo with couplings.
*Journal of the Royal Statistical Society: Series B (Statistical Methodology)*, 82, 08 2017.

Peter W. Glynn and Chang han Rhee.
Exact estimation for markov chain equilibrium expectations, 2014.

Jeffrey S. Rosenthal.
Faithful couplings of markov chains: Now equals forever.
*Advances in Applied Mathematics*, 18(3):372–381, 1997.

Dylan Cordaro.
Markov chain and coupling from the past.
2017.

Jinming Zhang.
Markov chains, mixing times and coupling methods with an application in social learning.
2020.

S. A. Sisson, Y. Fan, and M. A. Beaumont.
Overview of approximate bayesian computation, 2018.

Y. Fan and S. A. Sisson.
Abc samplers, 2018.

Dennis Prangle.
Summary statistics in approximate bayesian computation, 2015.