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

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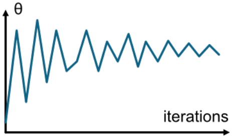
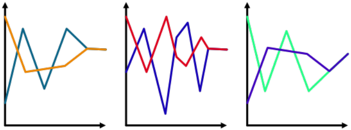
10 January 2022

A complex problem



$\Downarrow$

Unbiased Markov chain Monte Carlo methods with couplings



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Approximate Bayesian Computation

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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

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 $Y_t = Y_{t-1}$.

Maximal coupling

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

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).

Study case

Model

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

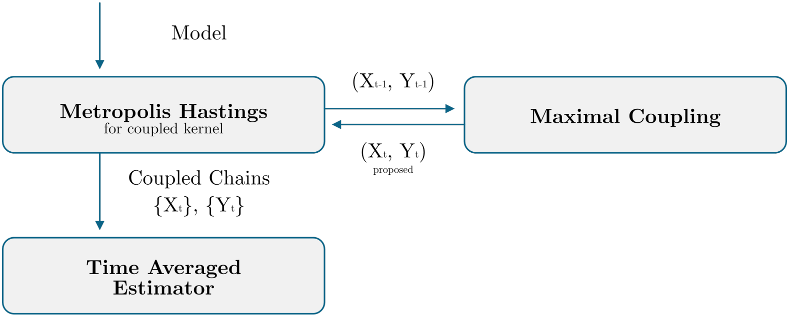
$$\mu \sim \mathcal{N}(\mu_0, \sigma^2_0)$$
$$\mu_0 = 38, \quad \sigma^2_0 = 4$$

Dataset

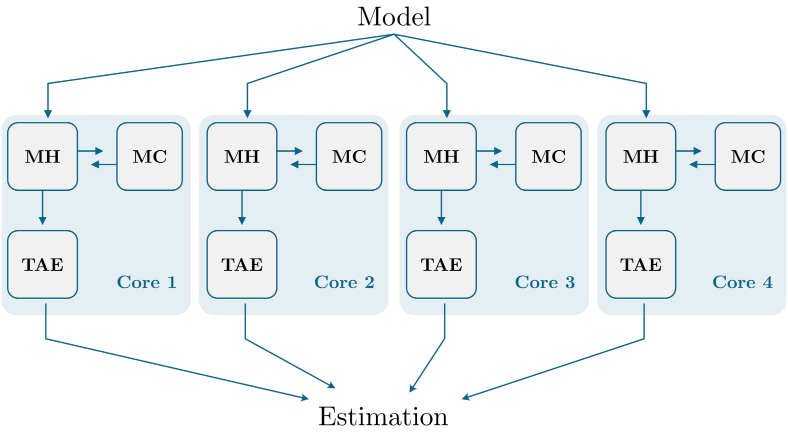
1000 samples generated from a Gaussian distribution:

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

Implementation



Parallelization



Results

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

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

- posterior
- risultato del time averaged
- grafico catene che si incontrano
- istogramma dei samplings (sotto alla posterior)

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 statistics: media distanza: norma (modulo della differenza) (mahalanobis nel caso multivariato) kernel: 1/(np.sqrt(2*math.pi))np.exp(-1/2*u*2)

Study case

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The complete method: Monte Carlo Markov chain method with couplings and approximate bayesian computation

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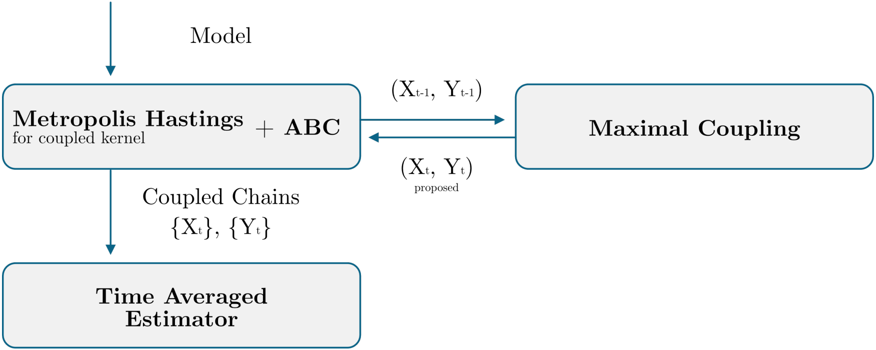
Implementation



Conclusions

Next steps

The next step will be the conclusion of the **separate multivariate implementation** of both solution to be tested on simulated data and the **parallelized multivariate implementation**.

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.