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

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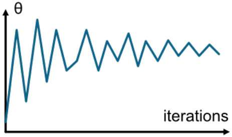
A complex problem



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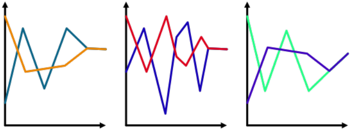
Unbiased Markov chain Monte Carlo methods with couplings



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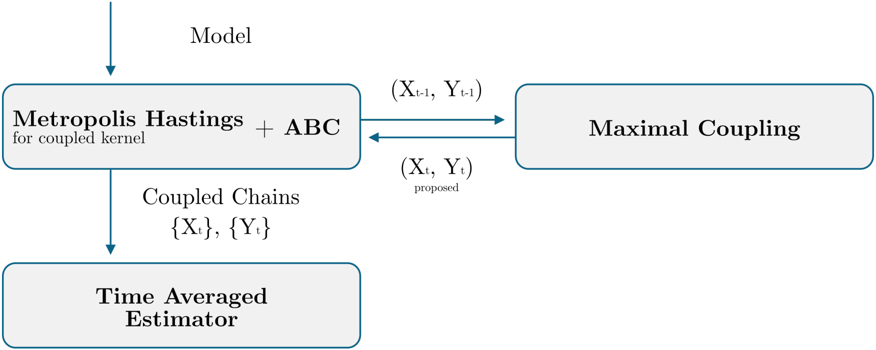
Approximate Bayesian Computation

The complete method: MCMC + Couplings + ABC

Implementation



Maximal coupling

Maximal coupling between two distributions p and q

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

Output

Distribution of a pair of random variables X, Y that maximizes $\mathbb{P}(X = Y)$ subject to the marginal constraints $X \sim p$ and $Y \sim q$

Metropolis Hastings with couplings and ABC

Model

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

$$\mu \sim \mathcal{N}(\mu_0,\sigma_0^2)$$

$$\sigma^2 \sim InvGa(a,b)$$

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

$$a = b = 1$$

Metropolis Hastings with couplings and ABC

Initilization

set $\boldsymbol{\theta} = (\mu, \sigma^2)$
for k=1,2:
until $K_h(||s_k^{(0)} - s_{obs}||) > 0$:

- sample $\boldsymbol{\theta}_k^{(0)} \sim \pi(\boldsymbol{\theta})$
- simulate n_{obs} observations $y_{ki} \sim \mathcal{N}(\mu^{(0)}, \sigma^{2(0)})$ from maximal coupling
- compute $s_k^{(0)} = S(y_k)$;

Metropolis Hastings with couplings and ABC

Iterations

for $i = 1, ..., M$:
given $\boldsymbol{\theta}^{(i-1)} = (\mu^{(i-1)}, \sigma^{2(i-1)})$

- generate $[\boldsymbol{\theta}_1^{(i)}, \boldsymbol{\theta}_2^{(i)}]$ from a maximalcoupling given $[\boldsymbol{\theta}_1^{(i-1)}, \boldsymbol{\theta}_2^{(i-1)}]$;
- for k=1,2:
  1. simulate n_{obs} observations $y_k^{(i)} \sim \mathcal{N}(\mu^{(i)}, \sigma^{2(i)})$ from maximal coupling;
  2. compute $s_k^{(i)} = S(y_k)$;
  3. accept $\boldsymbol{\theta}_k^{(i)}$ with probability

$$\frac{K_h(||s_k^{(i)} - s_{obs}||)\pi(\boldsymbol{\theta}_k^{(i)})}{K_h(||s_k^{(i-1)} - s_{obs}||)\pi(\boldsymbol{\theta}_k^{(i-1)})}$$

Metropolis Hastings with couplings and ABC

Output

for k= 1,2

$$\mu_k^{(1)}, \ldots, \mu_k^{(M)} \sim \pi_{ABC}(\mu | y_{obs});$$

$$\sigma_k^{2(1)}, \ldots, \sigma_k^{2(M)} \sim \pi_{ABC}(\sigma | y_{obs}).$$

Study case

Summary statistics: Sample mean, Sample Variance
Distance: L^2-norm
Kernel: $K(u) = \frac{1}{\sqrt{2\pi}} e^{-\frac{1}{2}u^2}, \quad K_h(u) = \frac{K(\frac{u}{h})}{h}$
Proposal distribution: $\begin{bmatrix} \mu^* \\ \log(\sigma^{2*}) \end{bmatrix} \sim \mathcal{N}\left(\begin{bmatrix} \mu^{(i)} \\ \log(\sigma^{2(i)}) \end{bmatrix}, 0.1^2 \cdot \mathcal{I} \right)$

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Dataset

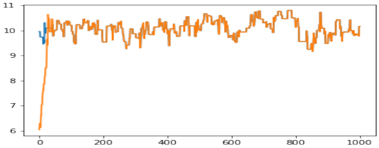
100 samples generated from a Gaussian distribution:

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

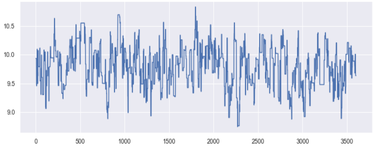
$$\mu_{obs} = 10, \sigma^2_{obs} = 3$$

Results for parameter μ

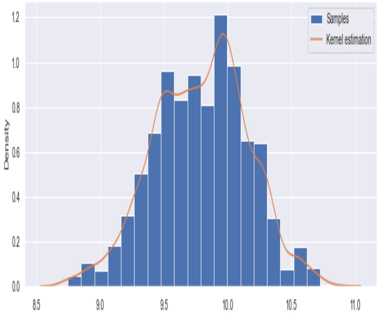
Coupled chains from one processor



Samplings from all accepted chains



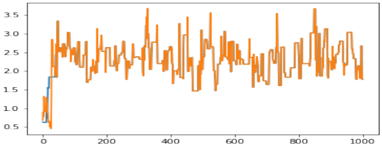
Sampling histogram with estimated distribution



Time Averaged Estimators mean obtained: $\mathbb{E}[H_{k:m}(X_\mu, Y_\mu)] \simeq 9.8$

Results for parameter σ^2

Coupled chains from one processor



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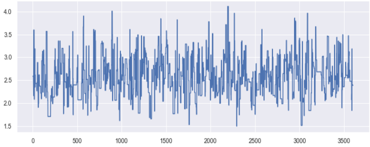
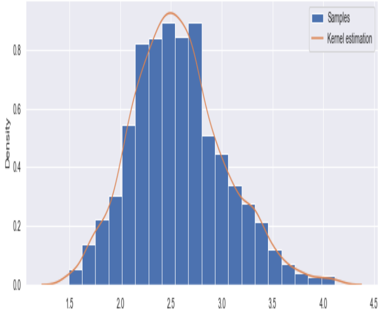


Sampling histogram with estimated distribution



Time Averaged Estimators mean obtained: $\mathbb{E}[H_{k:m}(X_{\sigma^2}, Y_{\sigma^2})] \simeq 2.56$

Numerical experiment: g-and-k distribution

Model

Quantile function

$$r \in (0,1) \longmapsto a + b(1 + 0.8\left(\frac{1 - exp(-g \cdot z(r))}{1 + exp(-g \cdot z(r))}\right)(1 + z(r)^2)^k \cdot z(r)$$

where $z(r)$ is the r-th quantile of the standard Normal distribution.

Prior distributions

$$a \sim \mathcal{U}([0,10])$$

$$b \sim \mathcal{U}([0,10])$$

$$g \sim \mathcal{U}([0,10])$$

$$k \sim \mathcal{U}([0,10])$$

Study case

Summary statistics: 10 quantiles
Distance: $L^2 - norm$
Kernel:

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

Dataset

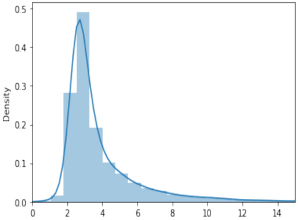
100 samples generated as follows:

$$a_{obs} = 3, b_{obs} = 1, g_{obs} = 2, k_{obs} = 0.5$$

$$y_{obs} \sim quantilefunction(z(r), \theta_{obs})$$

$$z(r) \sim \mathcal{N}(0, 1)$$

Quantile distribution: y_{obs}



Metropolis Hastings with couplings and ABC

Initialization

given $\theta = (a, b, g, k)$
for k=1,2:
Untill $K_h(\|s_k^{(0)} - s_{obs}\|) > 0$:

- Generate $\theta_k^{(0)} \sim \mathcal{U}([0, 10]^4)$ from prior density.
- Generate $z(r) \sim \mathcal{N}(0, 1)$
- Generate a sample of n_{obs} observations such that $y_k \sim quantilefunction(z(r), \theta_k^0)$
- Compute $s_k^{(0)} = S(y_k)$

Metropolis Hastings with couplings and ABC

Iterations

for i in (1,...,M):

- generate $\theta_1^{(i)}, \theta_2^{(i)}$ from maximalcoupling$(\theta_1^{(i-1)}, \theta_2^{(i-1)})$
- simulate n_{obs} observations $y_1^{(i)}$,$y_2^{(i)}$ from maximal coupling
- Compute the summaries $s_k^{(i)} = S(y_k^{(i)})$
- Accept $\theta_k^{(i)}$ with probability

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

otherwise $\theta_k^{(i)} = \theta_k^{(i-1)}$;

Metropolis Hastings with couplings and ABC

Iterations

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Couplings

for j in $(1,\ldots,n_{obs})$:

1. $z^{(i,j)}(r) \sim \mathcal{N}(0,1)$
2. generate:

$$y_1^{(ij)} \sim quantilefunction(z^{(i,j)}(r), \theta_1^{(i-1)})$$

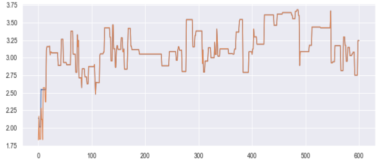
$$y_2^{(ij)} \sim quantilefunction(z^{(i,j)}(r), \theta_2^{(i-1)})$$

$$Kh(\|s_k \quad - s_{obs}\|)\pi(\theta_k \quad)$$

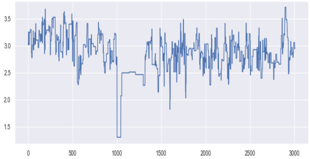
otherwise $\theta_k^{(i)} = \theta_k^{(i-1)}$;

Results for parameter a

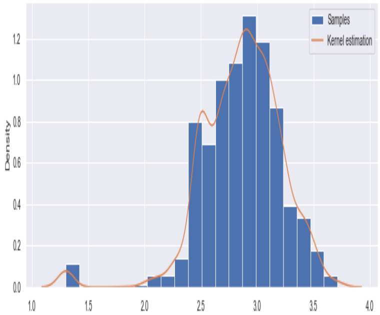
Coupled chains from one core



Samplings from all accepted chains

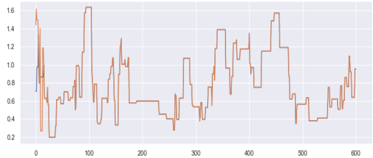


Sampling histogram with estimated distribution

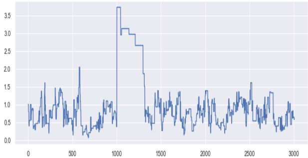


Results for parameter b

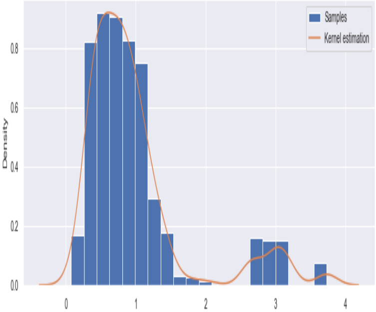
Coupled chains from one core



Samplings from all accepted chains

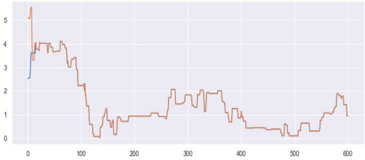


Sampling histogram with estimated distribution



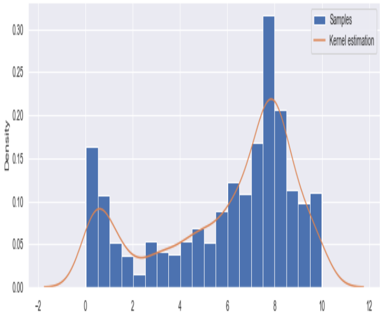
Results for parameter g

Coupled chains from one core



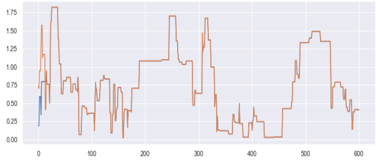
Samplings from all accepted chains

Sampling histogram with estimated distribution

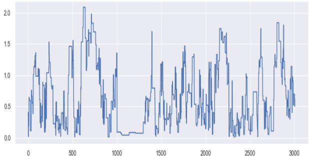


Results for parameter g

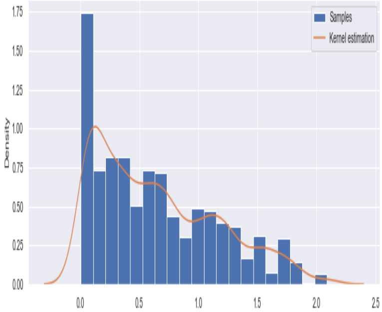
Coupled chains from one core



Samplings from all accepted chains



Sampling histogram with estimated distribution



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.