

# Approximate Bayesian Computation

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# Objective & Motivation

The objective of this presentation is to give an overview of the Approximate Bayesian Computation (ABC) algorithm through the replication of the paper **Approximate Bayesian computational methods** by Marin et al. (2012).

The paper talks about different variants of ABC by estimating the posterior of Moving Average models.

ABC methods are known as likelihood-free techniques, thus are a useful approach in problems that the likelihood is intractable, e.g., likelihood not available in closed form, or likelihood too expensive to calculate.

- Coalescent models in population genetics (Tavaré et al., 1997);
- Species dynamics (Jabot and Lohier, 2016);
- Real-world model of HIV transmission (McKinley et al., 2018).

# Objective & Motivation

In some settings where we have latent variables, the likelihood is expressed as:

$$\ell(\boldsymbol{\theta} \mid \mathbf{y}) = \int \ell^*(\boldsymbol{\theta} \mid \mathbf{y}, \mathbf{u}) d\mathbf{u}$$

Hence,  $\mathbf{y}$  is observed and  $\mathbf{u}$  is latent and  $\boldsymbol{\theta}$  is the parameter of interest.

# Original ABC Algorithm

Rubin (1984) described the ABC algorithm as a thought experiment to explain how to sample from a posterior distribution. Tavaré et al. (1997) is usually considered the paper responsible for the proposing ABC for inferring the posterior distribution.

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## Algorithm 1: Original ABC method

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```
for  $i=1$  to  $N$  do  
  repeat  
    Sample  $\theta' \sim \pi(\cdot)$   
    Generate  $\mathbf{z} \sim p(\cdot \mid \theta')$   
  until  $\mathbf{y} = \mathbf{z};$   
end
```

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# Original ABC Algorithm

Below we have an schematic drawing with an example of the ABC method for Beta/Binomial model.

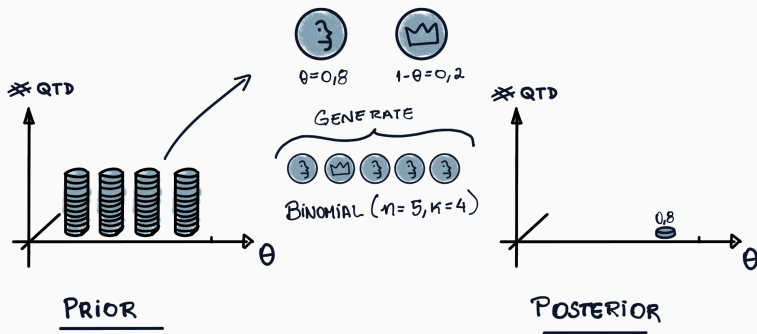


Figure 1: Schematic drawing of ABC method for Beta/Binomial model

# Original ABC Algorithm

The proof that the algorithm indeed results in an iid sample from the posterior is shown below. Let  $\mathbf{y}$  be the observed,  $\boldsymbol{\theta}$  the parameter of interest and  $\mathbf{z}$  the generated samples.

$$f(\boldsymbol{\theta}_i) \propto \sum_{\mathbf{z} \in \mathbb{D}} \pi(\boldsymbol{\theta}_i) p(\mathbf{z} \mid \boldsymbol{\theta}_i) \mathbb{I}_{\mathbf{y}}(\mathbf{z}) = \pi(\boldsymbol{\theta}_i) p(\mathbf{y} \mid \boldsymbol{\theta}_i) \propto \pi(\boldsymbol{\theta}_i \mid \mathbf{y})$$



# Original ABC Algorithm

Pritchard et al. (1999) extended the original algorithm to the case of continuous sample spaces.

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**Algorithm 2:** ABC method for discrete and continuous distributions

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```
for  $i=1$  to  $N$  do  
  repeat  
    Sample  $\theta' \sim \pi(\cdot)$   
    Generate  $\mathbf{z} \sim p(\cdot \mid \theta')$   
  until  $\rho[\eta(\mathbf{y}), \eta(\mathbf{z})] \leq \epsilon$ ;  
end
```

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- $\eta$ : function defining a statistic (e.g. the mean),
- $\rho$ : a distance function,
- $\epsilon$ : acceptance tolerance.

# Original ABC Algorithm

For this ABC algorithm, instead of the actual posterior, we get

$$\pi_{\epsilon}(\boldsymbol{\theta}, \mathbf{z} \mid \mathbf{y}) = \frac{\pi(\boldsymbol{\theta})p(\mathbf{z} \mid \boldsymbol{\theta})\mathbb{I}_{A_{\epsilon, \mathbf{y}}}(\mathbf{z})}{\int_{A_{\epsilon, \mathbf{y}} \times \boldsymbol{\theta}} \pi(\boldsymbol{\theta})p(\mathbf{z} \mid \boldsymbol{\theta})d\mathbf{z}d\boldsymbol{\theta}}$$

Where,  $A_{\epsilon, \mathbf{y}} = \{\mathbf{z} \in \mathcal{D} \mid \rho[\eta(\mathbf{z}), \eta(\mathbf{y})] \leq \epsilon\}.$

Hence, for a tolerance ( $\epsilon$ ) "small enough", we expect a good approximation.

$$\pi_{\epsilon}(\boldsymbol{\theta} \mid \mathbf{y}) = \int \pi_{\epsilon}(\boldsymbol{\theta}, \mathbf{z} \mid \mathbf{y})d\mathbf{z} \approx \pi(\boldsymbol{\theta} \mid \mathbf{y})$$

# Moving Average

We will use the Moving Average model, also denoted as  $MA(q)$ , for assessing the performance of the ABC methods. The  $MA(q)$  process is a stochastic process defined by:

$$y_k = u_k + \sum_{i=1}^q \theta_i u_{k-i}$$

Where  $(u_k)_{k \in \mathbb{Z}} \stackrel{iid}{\sim} N(0, 1)$ . For a  $q = 2$ , imposing the standard identifiability condition we obtain the following conditions:

$$-2 < \theta_1 < 2, \quad \theta_1 + \theta_2 > -1, \quad \theta_1 - \theta_2 < 1.$$

Hence, we use an uniform distribution over this triangular region as prior for  $\theta$ . The likelihood of  $\mathbf{y} \mid \theta$  is more complex because of the need to integrate  $\mathbf{u}$ .

# Moving Average

We generate a synthetic sample of length 100 using  $(\theta_1, \theta_2) = (0.6, 0.2)$ . For  $q = 2$  we can also numerically calculate the real posterior and the marginal distributions.

$$\pi(\boldsymbol{\theta} \mid \mathbf{y}) \propto \pi(\boldsymbol{\theta})p(\mathbf{y} \mid \boldsymbol{\theta}), \quad \mathbf{y} \mid \boldsymbol{\theta} \sim \text{MVN}(0, \Sigma)$$

$$\Sigma = \begin{bmatrix} 1 + \theta_1^2 + \theta_2^2 & \theta_1 + \theta_2\theta_1 & \theta_2 & 0 & 0 & 0 & \dots & 0 \\ \theta_1 + \theta_2\theta_1 & 1 + \theta_1^2 + \theta_2^2 & \theta_1 + \theta_2\theta_1 & \theta_2 & 0 & 0 & \dots & 0 \\ \theta_2 & \theta_1 + \theta_2\theta_1 & 1 + \theta_1^2 + \theta_2^2 & \theta_1 + \theta_2\theta_1 & \theta_2 & 0 & \dots & 0 \\ 0 & \theta_2 & \theta_1 + \theta_2\theta_1 & 1 + \theta_1^2 + \theta_2^2 & \theta_1 + \theta_2\theta_1 & \theta_2 & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & 0 & \theta_2 & \theta_1 + \theta_1\theta_2 & 1 + \theta_1^2 + \theta_2^2 \end{bmatrix}$$

# Moving Average

For this model, the ABC algorithm consists of:

- Sample  $\theta^*$  from the uniform triangular prior using rejection sampling;
- For each  $k \in \{-1, 0, 1, \dots, 100\}$ , sample  $u_k \stackrel{iid}{\sim} N(0, 1)$ .
- For each  $k \in \{1, 2, \dots, 100\}$ , calculate  $z_k = u_k + \sum_{i=1}^2 \theta_i^* u_{k-i}$ .

Two distance metrics are used. The raw distance between the series

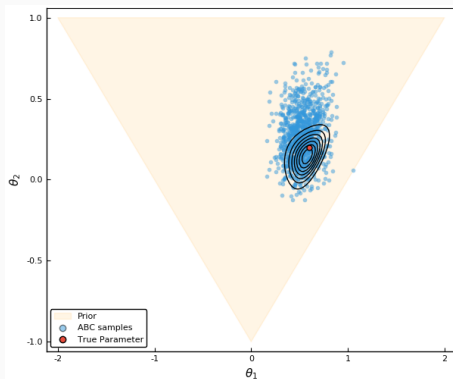
$$\rho^2\{\mathbf{z}, \mathbf{y}\} = \sum_{k=1}^{n=100} (y_k - z_k)^2$$

And the sum of the quadratic distances between the first  $q = 2$  autocovariances

$$\tau_j(\mathbf{x}) = \sum_{k=j+1}^{n=100} x_k x_{k-j}, \quad \rho^2 = \sum_{j=0}^{q=2} (\tau_j(\mathbf{y}) - \tau_j(\mathbf{z}))^2$$

# Moving Average

Below we present the results of running ABC for the MA(2) process.



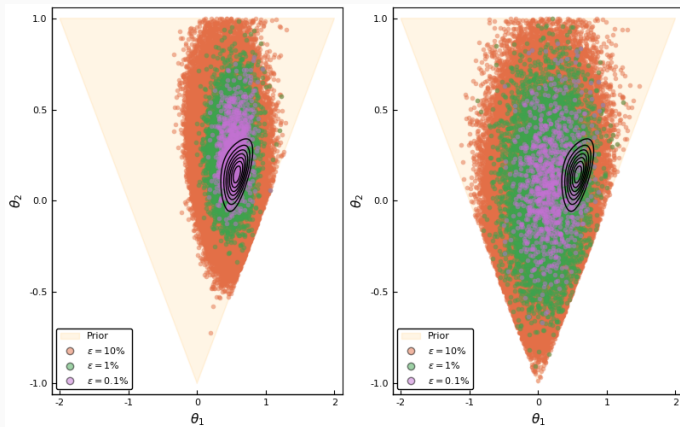
**Figure 2:** Comparison between the true posterior (*line in black*), with the samples produced using the ABC . The number of simulations is  $N = 10^6$ , and the threshold  $\epsilon$  corresponds to the quantile of accepting 0.1%. The  $\rho$  used was the distance of the autocovariances.

**Summary Statistics( $\eta$ ).** As the number of observations grow, using the raw distance between each observation becomes too prohibitive. The alternative is to try using summary statistics, if possible, sufficient statistics.

Fearnhead and Prangle (2010) created a way of constructing appropriate summary statistics for ABC in a semi-automatic manner.

**Tolerance threshold.** The standard practice is to use  $\epsilon$  as a quantile of the simulated distances.

# Calibration of ABC

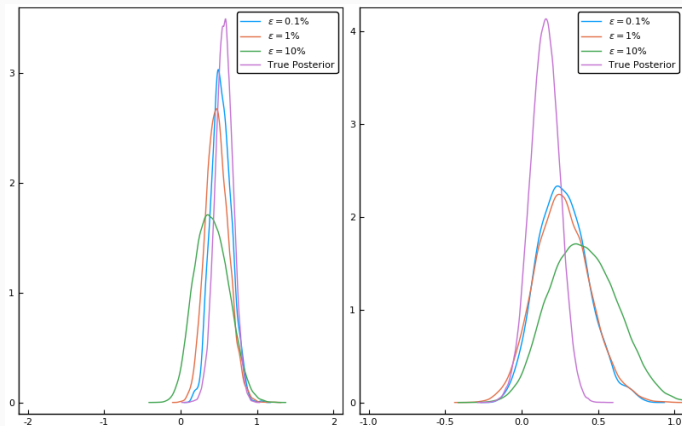


**Figure 3:** Comparison of ABC method when using autocovariance distance <sup>1</sup> (*left*) versus raw distance (*right*). The number of simulations is  $N = 10^6$  and different thresholds  $\epsilon$  are used.

<sup>1</sup>in the rest of the slides we will only use the autocovariance distances



# Calibration of ABC



**Figure 4:** Comparison of ABC samples with the true posterior marginal distribution for  $\theta_1$  (left) and  $\theta_2$  (right).

# ABC Variations

Using non-informative priors is usually very inefficient, because it leads to lots of rejections. To tackle this problem, Marjoram et al. (2003) came up with MCMC-ABC.

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## Algorithm 3: MCMC-ABC

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Use Algorithm 2 to get  $(\theta^{(0)}, z^{(0)})$  from the target  $\pi_{\epsilon}(\theta, z \mid y)$ .

for  $i=1$  to  $N$  do

    repeat

        Sample  $\theta'$  from the Markov kernel  $q(\cdot \mid \theta^{(i-1)})$

        Generate  $z \sim p(\cdot \mid \theta')$

        Sample  $u \sim U[0, 1]$

        if  $u \leq \frac{\pi(\theta')q(\theta^{(i-1)} \mid \cdot)}{\pi(\theta^{(i-1)})q(\theta' \mid \cdot)}$  and  $\rho\{\eta(z'), \eta(y)\} \leq \epsilon$  then

            Set  $(\theta^{(i)}, z^{(i)}) = (\theta', z')$

        end

        else

            Set  $(\theta^{(i)}, z^{(i)}) = (\theta^{(i-1)}, z^{(i-1)})$

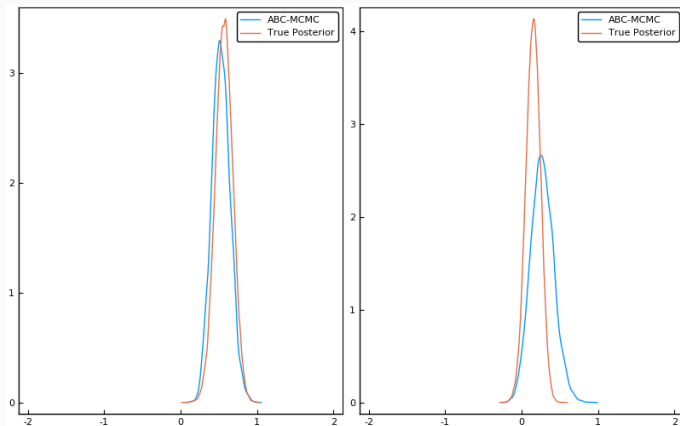
        end

    until  $\rho[\eta(y), \eta(z)] \leq \epsilon$ ;

end

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# ABC Variations



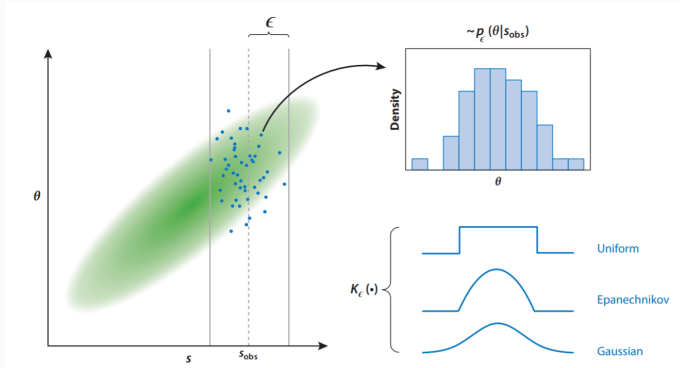
**Figure 5:** Comparison of ABC-MCMC samples with the true posterior marginal distribution for  $\theta_1$  (*left*) and  $\theta_2$  (*right*) using  $\epsilon = 0.1\%$ .

Another variation of ABC is called **Noisy ABC**, that was proposed by Wilkinson (2013). The original ABC algorithm can be thought as a rejection algorithm using a uniform kernel ( $\mathbb{I}_{A_{\epsilon, y}}(z)$ ). The *Noisy* version generalizes this, allowing the use of different kernels, hence:

$$\pi_{\epsilon}(\theta, \mathbf{z} \mid \mathbf{y}) = \frac{\pi(\theta)p(\mathbf{z} \mid \theta)K_{\epsilon}(\mathbf{y} - \mathbf{z})}{\int \pi(\theta)p(\mathbf{z} \mid \theta)K_{\epsilon}(\mathbf{y} - \mathbf{z})d\mathbf{z}d\theta}$$

Now, instead of accepting if  $\rho\{\eta(\mathbf{y}), \eta(\mathbf{z})\} \leq \epsilon$ , we accept with probability  $\frac{K_{\epsilon}(\mathbf{y} - \mathbf{z})}{\max\{K_{\epsilon}(\mathbf{y} - \mathbf{z})\}}$ .

# ABC Variations



**Figure 6:** Illustration of *Noisy* ABC rejection kernels, where  $s$  is the statistic from the ABC sampler and  $s_{obs}$  is the observed value from the data. Figure from Beaumont (2019).

Sequential techniques are also used with ABC to enhance the efficiency of the algorithms. A popular method in this regard is the **ABC-PMC** (ABC population Monte Carlo) by Beaumont et al. (2009). It estimates the scale of the random walk step from the previous simulations and uses a sequence of tolerance thresholds ( $\epsilon_1 \geq \dots \geq \epsilon_T$ ) to approximate the distribution.

A recent work by Simola et al. (2019) proposed a method for adaptively selecting this sequence of tolerances in a way that improves the computational efficiency and defines a stopping rule, thus assisting in automating the termination of the sampling procedure.

The estimation of the posterior using ABC is straightforward.

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## Algorithm 4: ABC-PMC

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At iteration  $t=1$ ,

**for**  $i=1$  to  $N$  **do**

**repeat**

        Sample  $\theta_i^{(1)} \sim \pi(\cdot)$

        Generate  $\mathbf{z} \sim p(\cdot \mid \theta_i^{(1)})$

**until**  $\rho[\eta(\mathbf{y}), \eta(\mathbf{z})] \leq \epsilon$ ;

    Set  $w_i^{(1)} = 1/N$ .

**end**

Set  $\Sigma_1$  as twice the empirical variance of the  $\theta_i^{(1)}$ 's

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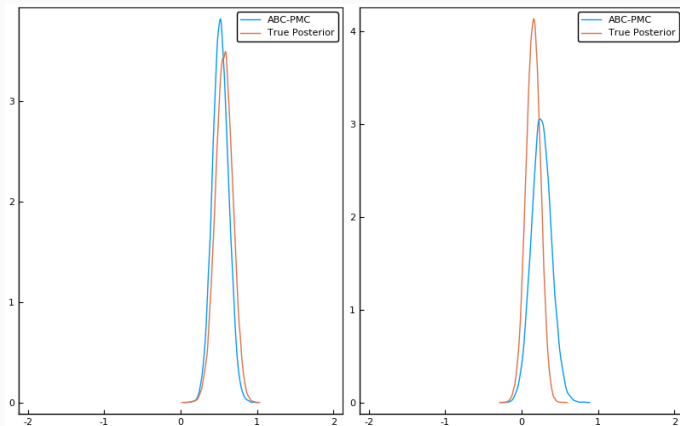
## Algorithm 5: ABC-PMC

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```
for  $t=2$  to  $T$  do
  for  $i=1$  to  $N$  do
    repeat
      Sample  $\theta_i^*$  from  $\theta_j^{(t-1)}$ 's with probabilities  $w_j^{(t-1)}$ 
      Generate  $\theta_i^{(t)} \sim N(\theta_i^*, \Sigma_{(t-1)})$  and  $\mathbf{z} \sim p(\cdot \mid \theta_i^{(t)})$ 
    until  $\rho[\eta(\mathbf{y}), \eta(\mathbf{z})] \leq \epsilon$ ;
    Set  $w_i^{(t)} \propto \frac{\pi(\theta_i^{(t)})}{\sum_{j=1}^N w_j^{(t-1)} \phi\{(\Sigma_{t-1})^{-1/2}(\theta_i^{(t)} - \theta_j^{(t-1)})\}}$ 
  end
  Set  $\Sigma_t$  as twice the weighted variance of the  $\theta_i^{(t)}$ 's
end
```

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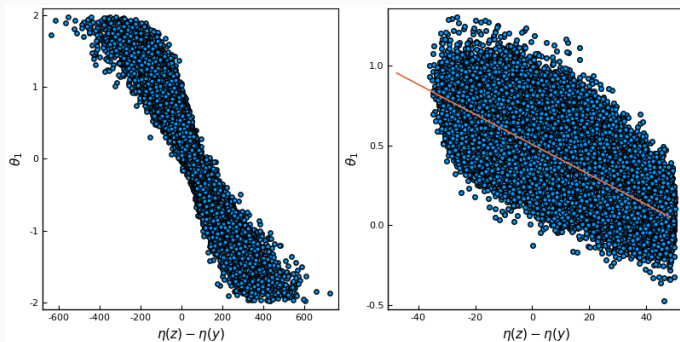


**Figure 7:** Comparison of ABC-PMC samples with the true posterior marginal distribution for  $\theta_1$  (*left*) and  $\theta_2$  (*right*) using  $\epsilon = 0.1\%$ .

*Local linear regression* was proposed by Beaumont et al. (2002) as a way to improve the result of simulations without the need to use restrictively low threshold values. The idea is then to use a weighted least squares regression of  $\theta$  on  $(\eta(\mathbf{y}) - \eta(\mathbf{z}))$ , with weights according to a chosen kernel.

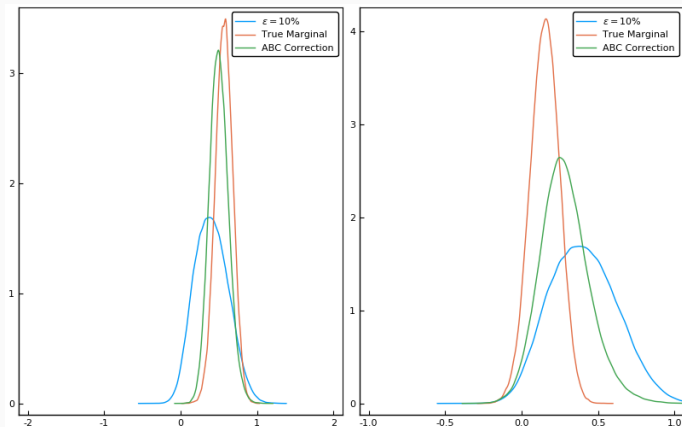
$$\theta^* = \theta - (\eta(\mathbf{y}) - \eta(\mathbf{z}))^T \hat{\beta}$$

# Post-processing of ABC



**Figure 8:** Scatter plots of simulated  $\theta_1$  and  $(\eta(y) - \eta(z))$  for autocovariance with  $lag = 1$ . On the *left* there are all the  $N = 10^6$  simulations, while in the *right* only the accepted samples for  $\epsilon = 10\%$  with the regression line.

# Post-processing of ABC



**Figure 9:** Comparison of ABC samples corrected through local linear regression versus the true marginal posterior distribution for  $\theta_1$  (left) and  $\theta_2$  (right) using  $\epsilon = 10\%$ .

# Model Choice

The estimation of the posterior using ABC is straightforward.

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**Algorithm 6:** ABC Model Choice

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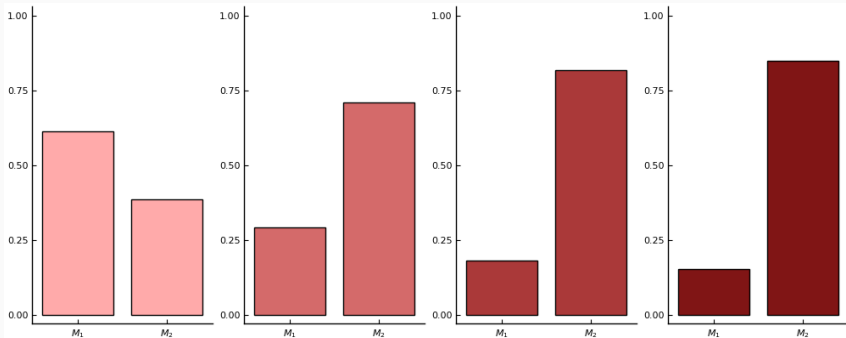
```
for  $i=1$  to  $N$  do  
  repeat  
    Sample  $m \sim \pi(\mathcal{M} = m)$   
    Sample  $\theta_m \sim \pi_m(\theta_m)$   
    Generate  $\mathbf{z} \sim p_m(\cdot \mid \theta_m)$   
  until  $\rho[\eta(\mathbf{y}), \eta(\mathbf{z})] \leq \epsilon$ ;  
  Set  $m^{(i)} = m$  and  $\theta^{(i)} = \theta_m$   
end
```

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The posterior probability  $\pi(\mathcal{M} = m \mid \mathbf{y})$  is the acceptance frequency from model  $m$ ,

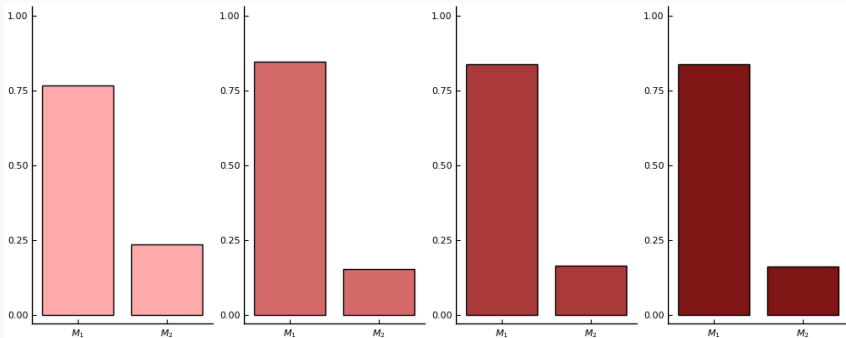
$$\frac{1}{N} \sum_{i=1}^N \mathbb{I}_{m^{(i)}=m}$$

# Model Choice



**Figure 10:** Barplots of evolution of Bayes factor approximations in terms of visits to models MA(1) and MA(2) using ABC using thresholds of 10, 1, 0.1 , 0.01 % on autocovariance distance. The true model is MA(2) and the true Bayes factor is 0.952.

# Model Choice



**Figure 11:** Barplots of evolution of Bayes factor approximations in terms of visits to models MA(1) and MA(2) using ABC using thresholds of 10, 1, 0.1 , 0.01 % on autocovariance distance. The true model is MA(1) and the true Bayes factor is 0.943.

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