

# 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.

- Coalecent 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.

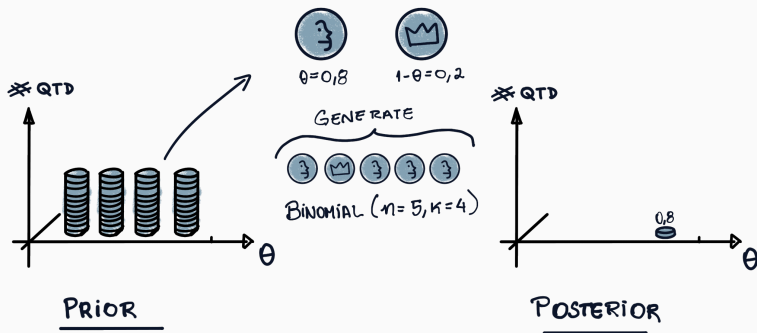


Figure 1: Schematic drawing of ABC method for Beta/Binomial model

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.

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



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

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

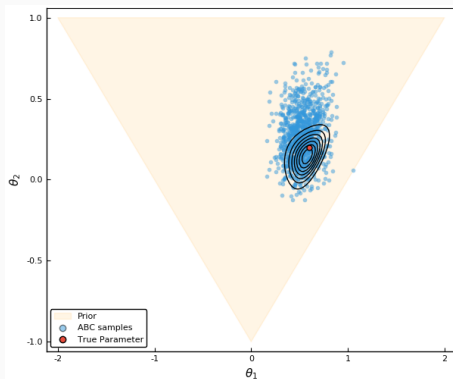
$$\rho^2\{\mathbf{z}, \mathbf{y}\} = \sum_{k=1}^{n=100} (y_k - z_k)^2$$

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.



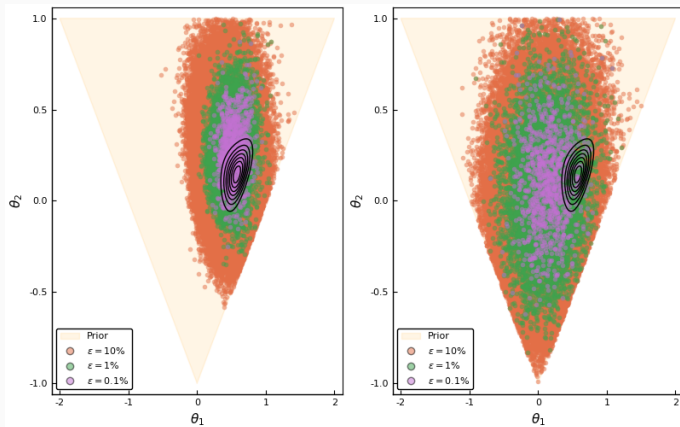
**Figure 2:** Comparison between the true posterior (*line in black*), with the samples produced using the ABC . The number of simulations is  $N = 10^6$ , and the threshold  $\epsilon$  corresponds to the quantile of accepting 0.1%. The  $\rho$  used was the distance of the autocovariances.

**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

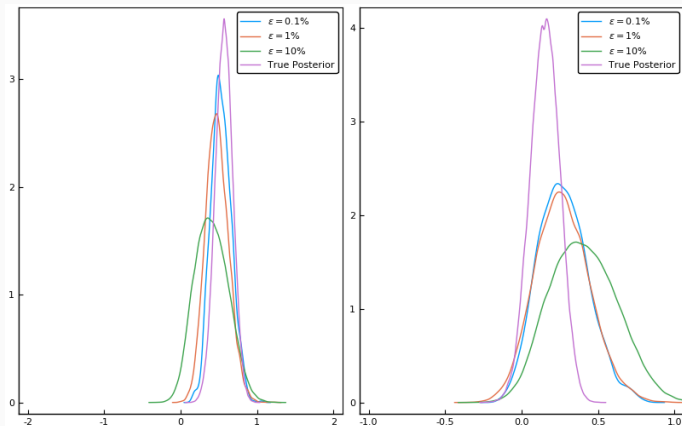


**Figure 3:** Comparison of ABC method when using autocovariance distance <sup>1</sup> (*left*) versus raw distance (*right*). The number of simulations is  $N = 10^6$  and different thresholds  $\epsilon$  are used.

<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  $\pi_{\epsilon}(\theta, z \mid \mathbf{y})$ .

for  $i=1$  to  $N$  do

    repeat

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

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

        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  $\rho\{\eta(\mathbf{z}'), \eta(\mathbf{y})\} \leq \epsilon$  then

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

        end

        else

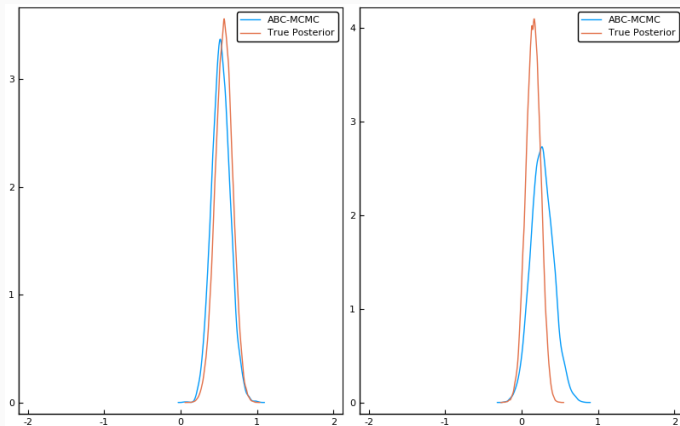
            Set  $(\theta^{(i)}, \mathbf{z}^{(i)}) = (\theta^{(i-1)}, \mathbf{z}^{(i-1)})$

        end

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

end

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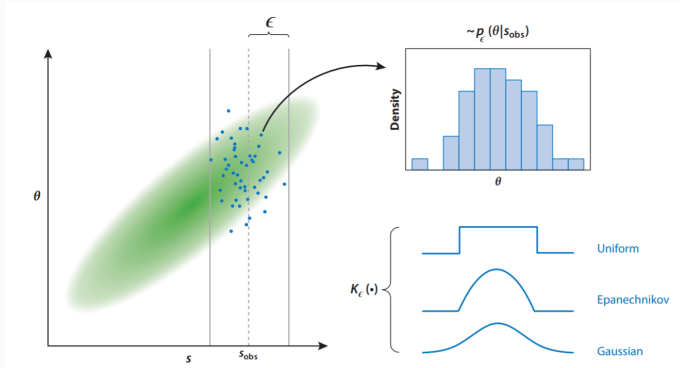
**Figure 5:** Comparison of ABC-MCMC samples with the true posterior marginal distribution for  $\theta_1$  (*left*) and  $\theta_2$  (*right*) using  $\epsilon = 0.1\%$ .

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:

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

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).

- Beaumont, M. A. (2019). Approximate bayesian computation. *Annual Review of Statistics and Its Application*, 6(1):379–403.
- Fearnhead, P. and Prangle, D. (2010). Constructing summary statistics for approximate bayesian computation: Semi-automatic abc.
- Jabot, F. and Lohier, T. (2016). Non-random correlation of species dynamics in tropical tree communities. *Oikos*, 125(12):1733–1742.
- Marin, J.-M., Pudlo, P., Robert, C. P., and Ryder, R. J. (2012). Approximate bayesian computational methods. *Statistics and Computing*, 22(6):1167–1180.
- Marjoram, P., Molitor, J., Plagnol, V., and Tavaré, S. (2003). Markov chain monte carlo without likelihoods. *Proceedings of the National Academy of Sciences*, 100(26):15324–15328.

- McKinley, T. J., Vernon, I., Andrianakis, I., McCreesh, N., Oakley, J. E., Nsubuga, R. N., Goldstein, M., and White, R. G. (2018). Approximate bayesian computation and simulation-based inference for complex stochastic epidemic models. *Statist. Sci.*, 33(1):4–18.
- Pritchard, J. K., Seielstad, M. T., Perez-Lezaun, A., and Feldman, M. W. (1999). Population growth of human Y chromosomes: a study of Y chromosome microsatellites. *Molecular Biology and Evolution*, 16(12):1791–1798.
- Rubin, D. B. (1984). Bayesianly justifiable and relevant frequency calculations for the applied statistician. *Ann. Statist.*, 12(4):1151–1172.
- Tavaré, S., Balding, D. J., Griffiths, R. C., and Donnelly, P. (1997). Inferring coalescence times from dna sequence data. *Genetics*, 145(2):505–518.

Wilkinson, R. D. (2013). Approximate bayesian computation (abc) gives exact results under the assumption of model error. *Statistical Applications in Genetics and Molecular Biology*, 12(2).