

A Nonparametric Analysis of ABC

Arnaud Guyader

Journées MAS de la SMAI
27-29 août 2014, Toulouse

Framework and Objective [Marin et al. (2012)]

- **Parameter:** $\theta \in \mathbb{R}^p$ generated from the prior $\pi(\theta)$.
- **Observations:** $y \in \mathbb{R}^m$ generated from the likelihood $f(y|\theta)$.
- **Goal:** given a **fixed** observation y_0 , estimate the posterior

$$\pi(\theta|y_0) = \frac{f(y_0|\theta)\pi(\theta)}{f(y_0)} \propto f(y_0|\theta)\pi(\theta).$$

- **Classical Tool:** MCMC methods (e.g. Metropolis algorithm), but sometimes computationally intractable...

⇒ **Another Strategy:** Approximate Bayesian Computation (ABC), a family of likelihood-free computational techniques.

The Original ABC Algorithm [Rubin (1984), Tavaré et al. (1997)]

Require: An integer N

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

 Generate θ_i from the prior $\pi(\theta)$

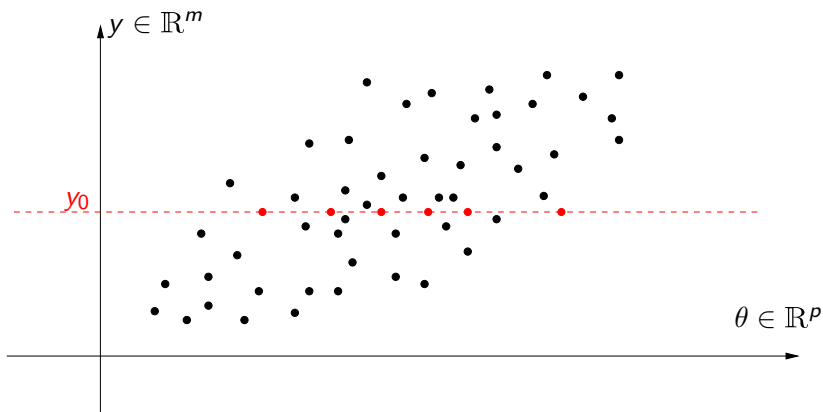
 Generate y_i from the likelihood $f(\cdot|\theta_i)$

end for

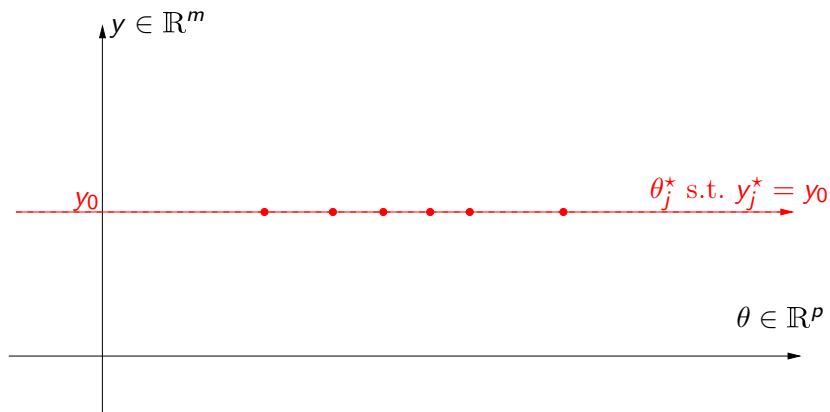
return The values θ_j^* such that $y_j^* = y_0$.

- **Conclusion:** the θ_j^* 's are i.i.d. with law $\pi(\theta|Y = y_0)$.
- **Drawback:** unrealistic unless the support of Y is countable.

Illustration



Illustration

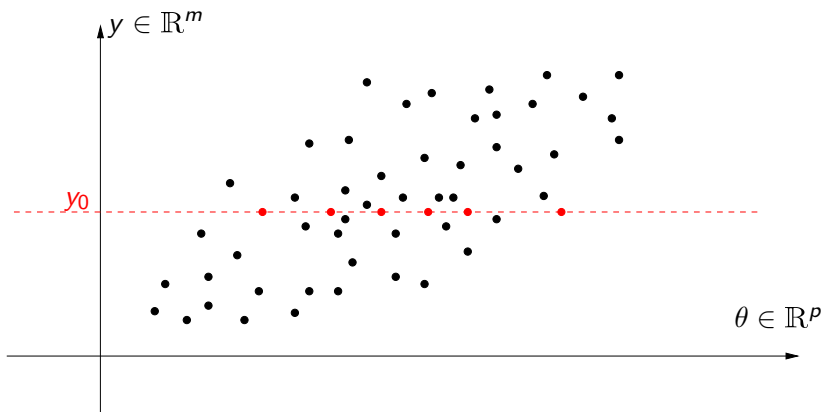


Extension of ABC [Pritchard et al. (1999)]

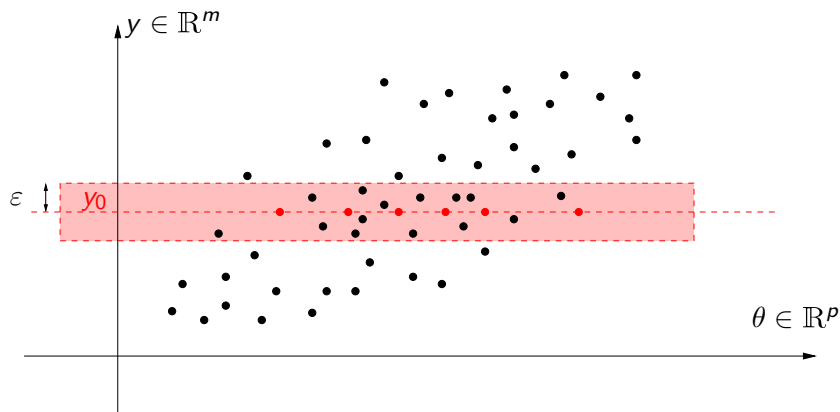
Require: An integer N , a tolerance level ε , a distance d on \mathbb{R}^m
for $i = 1$ to N **do**
 Generate θ_i from the prior $\pi(\theta)$
 Generate y_i from the likelihood $f(\cdot|\theta_i)$
end for
return The couples (θ_j^*, y_j^*) such that $d(y_j^*, y_0) \leq \varepsilon$.

- **Practical Issue:** use a low-dimensional summary statistic $s(y)$ and a distance $\rho(s(y), s(y_0))$ instead of $d(y, y_0)$.
- **Question:** how to tune ε ?

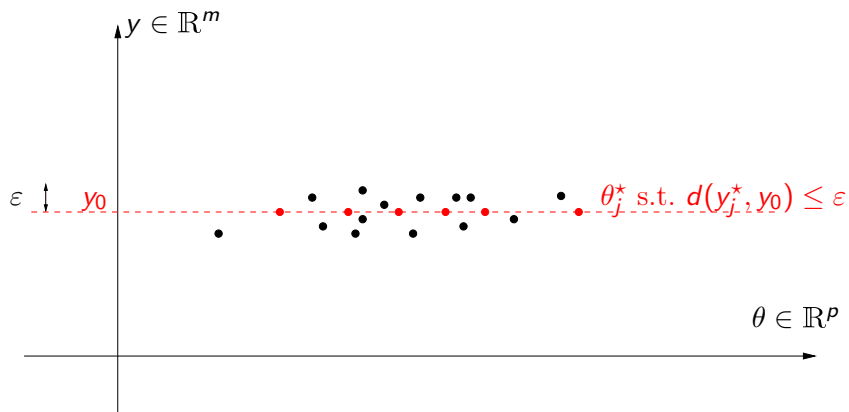
Illustration



Illustration



Illustration



ABC in Practice

Require: Integers N and k , a distance d on \mathbb{R}^m

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

 Generate θ_i from the prior $\pi(\theta)$

 Generate y_i from the likelihood $f(.|\theta_i)$

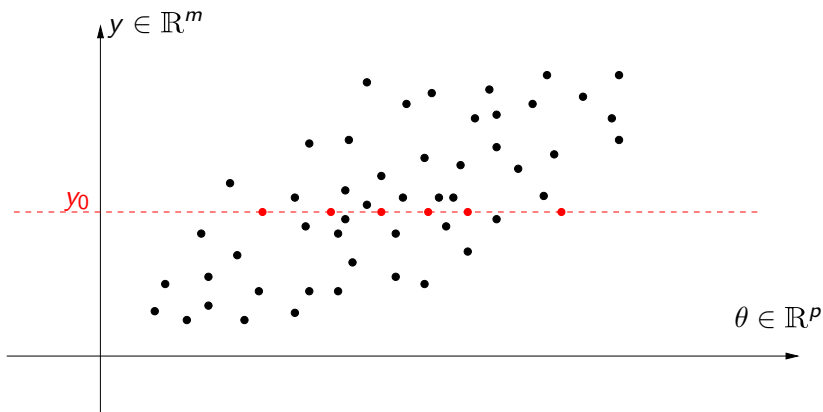
end for

return The k pairs (θ_j^*, y_j^*) such that y_j^* belongs to the k nearest neighbors of y_0 , i.e. such that

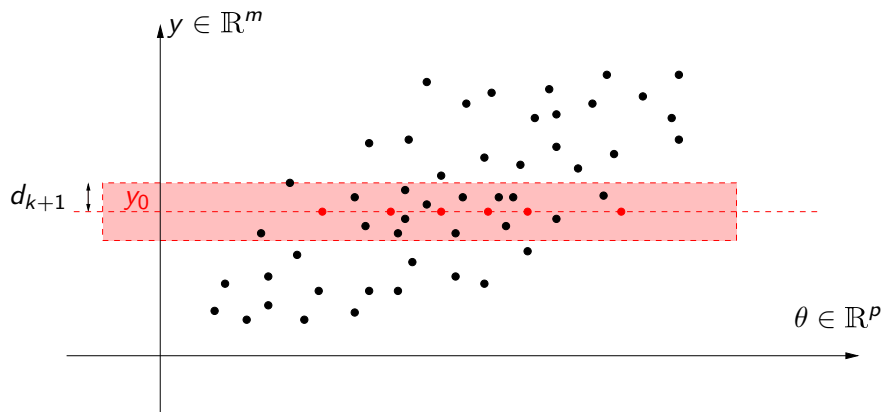
$$d(y_j^*, y_0) < d(y_{(k+1)}, y_0) =: d_{k+1}.$$

Remark: in practice, $k = k_N$ is most commonly expressed as a percentile of N , e.g. $N = 10^6$ and $k_N/N = 0.1\%$.

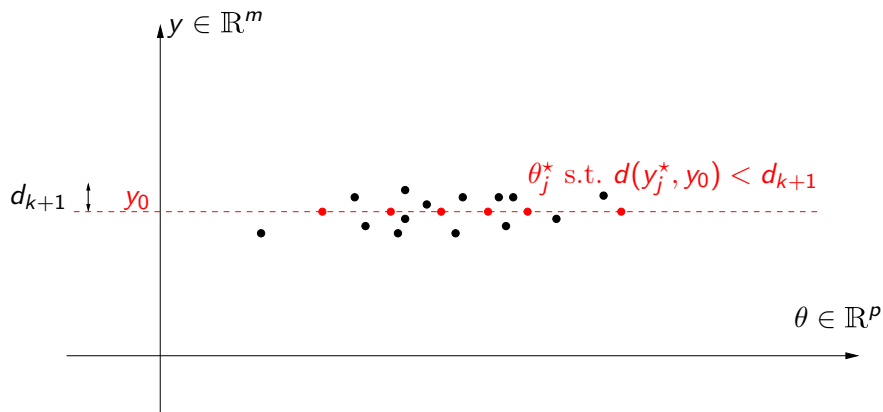
Illustration



Illustration



Illustration



Why Does It Work?

Proposition (Conditional Distribution)

Given d_{k+1} , the $(\Theta_j^*, Y_j^*)_{1 \leq j \leq k}$ are i.i.d. according to

$$\frac{f(\theta, y) \mathbb{1}_{\mathcal{B}(y_0, d_{k+1})}}{C_{k+1}} = \frac{f(\theta, y) \mathbb{1}_{\mathcal{B}(y_0, d_{k+1})}}{\int_{\mathcal{B}(y_0, d_{k+1})} f(y) dy}$$

that is, the law $\mathcal{L}((\Theta, Y) | d(Y, y_0) < d_{k+1})$.

Corollary (Strong Law of Large Numbers)

Assume that $k_N \rightarrow +\infty$, $k_N/N \rightarrow 0$, and $k_N/\log \log N \rightarrow +\infty$.

Then, for any bounded function φ , one has

$$\frac{1}{k_N} \sum_{j=1}^{k_N} \varphi(\Theta_j^*) \xrightarrow[N \rightarrow +\infty]{a.s.} \mathbb{E}[\varphi(\Theta) | Y = y_0].$$

Kernel Density Estimate

- Density Estimator:

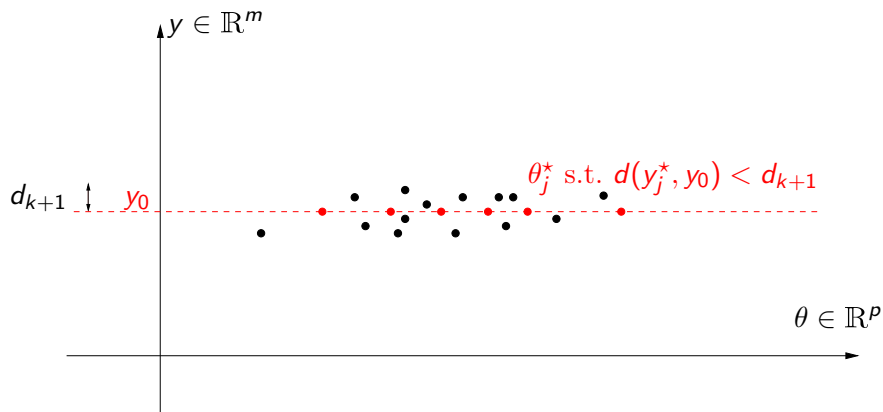
$$\hat{\pi}_N(\theta_0|y_0) = \frac{1}{k_N h_N^p} \sum_{j=1}^{k_N} K\left(\frac{\Theta_j^* - \theta_0}{h_N}\right).$$

- This is a **hybrid** between a k -nearest neighbor and a kernel density estimation procedure.
- **Remark:** an additional degree of smoothing [Blum (2010)]

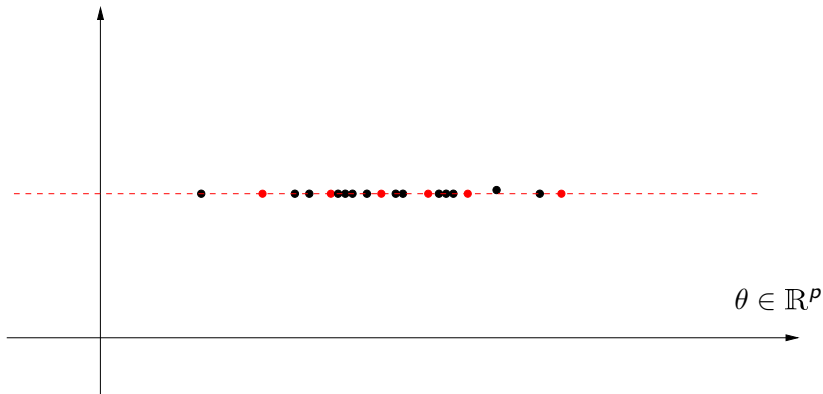
$$\tilde{\pi}_N(\theta_0|y_0) = \frac{\sum_{i=1}^N L\left(\frac{y_i - y_0}{\delta_N}\right) K\left(\frac{\Theta_i - \theta_0}{h_N}\right)}{h_N^p \sum_{i=1}^N L\left(\frac{y_i - y_0}{\delta_N}\right)}.$$

⇒ **Questions:** Consistency? Rates of convergence?

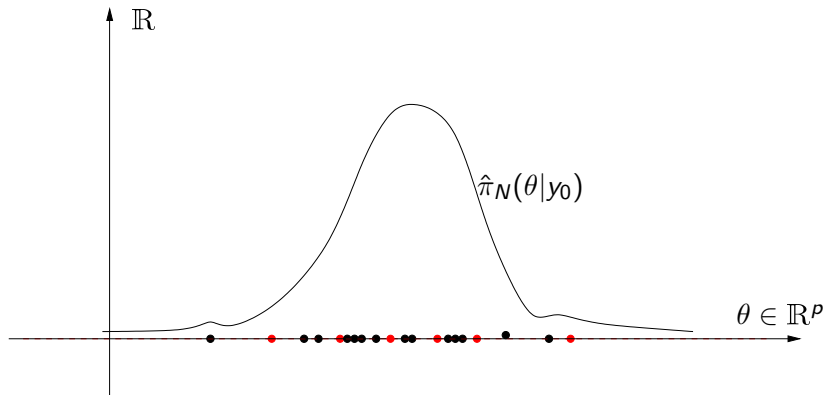
Illustration



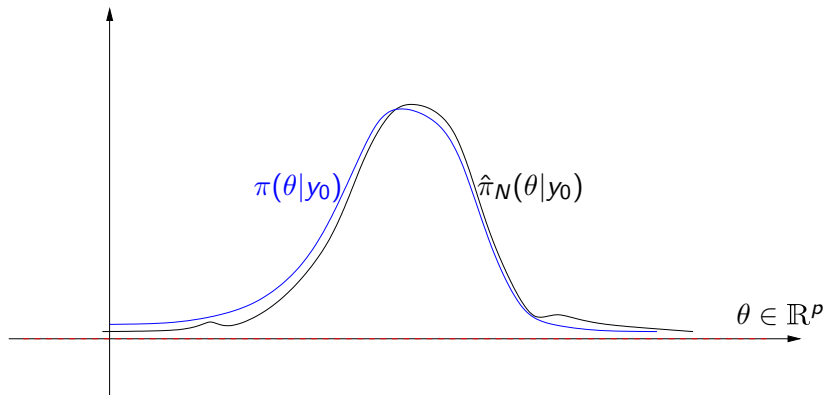
Illustration



Illustration



Illustration



Pointwise Mean Square Error Consistency

Theorem

Assume that the joint probability density f is such that

$$\int_{\mathbb{R}^p} \int_{\mathbb{R}^m} f(\theta, y) \log^+ f(\theta, y) d\theta dy < \infty.$$

If $k_N \rightarrow \infty$, $k_N/N \rightarrow 0$, $h_N \rightarrow 0$ and $k_N h_N^p \rightarrow \infty$, then

$$\mathbb{E} \left[(\hat{\pi}_N(\theta_0|y_0) - \pi(\theta_0|y_0))^2 \right] \xrightarrow[N \rightarrow \infty]{\lambda_p \otimes \lambda_m \text{ a.e.}} 0.$$

Remark: the assumption on f is not very restrictive...

Bias-Variance Decomposition

Conditioning on $d_{k+1} = d_{k_N+1}$ yields

$$\mathbb{E} \left[(\hat{\pi}_N(\theta_0|y_0) - \pi(\theta_0|y_0))^2 \right] = \mathbb{E} [B(d_{k+1})^2] + \mathbb{E} [V(d_{k+1})],$$

where

$$B(d_{k+1}) = \mathbb{E}[\hat{\pi}_N(\theta_0|y_0) | d_{k+1}] - \pi(\theta_0|y_0),$$

and

$$V(d_{k+1}) = \mathbb{E} \left[(\hat{\pi}_N(\theta_0|y_0) - \mathbb{E}[\hat{\pi}_N(\theta_0|y_0) | d_{k+1}])^2 | d_{k+1} \right].$$

The Bias Term

Recall: We have to prove that $\mathbb{E}[B(d_{k+1})^2] \rightarrow 0$, with

$$B(d_{k+1}) = \mathbb{E}[\hat{\pi}_N(\theta_0|y_0)|d_{k+1}] - \pi(\theta_0|y_0),$$

where $\pi(\theta_0|y_0) = f(\theta_0, y_0)/f(y_0)$, and

$$\begin{aligned} \mathbb{E}[\hat{\pi}_N(\theta_0|y_0) | d_{k+1}] &= \left(\frac{1}{V_m d_{k+1}^m} \int_{\mathcal{B}(y_0, d_{k+1})} f(y) dy \right)^{-1} \\ &\times \left(\frac{1}{V_m d_{k+1}^m} \int_{\mathbb{R}^p} \int_{\mathcal{B}(y_0, d_{k+1})} K_h(\theta - \theta_0) f(\theta, y) d\theta dy \right) \end{aligned}$$

\Rightarrow **Tools:** Extensions of Lebesgue's differentiation theorem, and of Jessen-Marcinkiewicz-Zygmund theorem.

The Variance Term

Recall that

$$\mathbb{E}[V(d_{k+1})] = \mathbb{E} \left[\mathbb{E} \left[\left(\hat{\pi}_N(\theta_0|y_0) - \mathbb{E}[\hat{\pi}_N(\theta_0|y_0) \mid d_{k+1}] \right)^2 \mid d_{k+1} \right] \right].$$

Thus, assuming that $\|K\|_\infty = \sup K(\theta) < \infty$, we are led to

$$\mathbb{E}[V(d_{k+1})] \leq \frac{C(\theta_0, y_0) \|K\|_\infty}{k_N h_N^p},$$

and everything is OK, provided that

$$k_N h_N^p \xrightarrow{N \rightarrow \infty} \infty.$$

Rates of Convergence

Theorem (MISE in the case $m > 4$)

Assume that Y has a bounded support. Then, under some regularity assumptions on $f(\theta, y)$ and $f(y)$, we have

$$\begin{aligned} \mathbb{E} \left[\int_{\mathbb{R}^p} [\hat{\pi}_N(\theta_0|y_0) - \pi(\theta_0|y_0)]^2 d\theta_0 \right] &\leq \frac{\int_{\mathbb{R}^p} K^2(\theta) d\theta}{k_N h_N^p} \\ &+ A(y_0) \left(\frac{k_N}{N} \right)^{\frac{4}{m}} + B(y_0) \left(\frac{k_N}{N} \right)^{\frac{2}{m}} h_N^2 + C(y_0) h_N^4 + o \left(\left(\frac{k_N}{N} \right)^{\frac{4}{m}} + h_N^4 \right) \end{aligned}$$

\Rightarrow For $k_N \propto N^{\frac{p+4}{m+p+4}}$ and $h_N \propto N^{\frac{-1}{m+p+4}}$, this leads to

$$\mathbb{E} \left[\int_{\mathbb{R}^p} [\hat{\pi}_N(\theta_0|y_0) - \pi(\theta_0|y_0)]^2 d\theta_0 \right] \leq D(y_0) N^{\frac{-4}{m+p+4}}.$$