Approximate Bayesian Computation (ABC): model choice and empirical likelihood

Christian P. Robert

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Université Paris-Dauphine, IuF, & CREST Joint works with J.-M. Cornuet, J.-M. Marin, K.L. Mengersen, N. Pillai, P. Pudlo and J. Rousseau

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MCMSki IV to be held in Chamonix M^t Blanc, France, from Monday, Jan. 6 to Wed., Jan. 8, 2014 All aspects of MCMC⁺⁺ theory and methodology Parallel (invited and contributed) sessions: call for proposals on website http://www.pages.drexel.edu/ mwl25/mcmski/



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Outline

Introduction

ABC

ABC as an inference machine

ABC for model choice

Model choice consistency

 $\mathsf{ABC}_{\mathsf{el}}$



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Case of a well-defined statistical model where the likelihood function

$$\ell(\boldsymbol{\theta}|\mathbf{y}) = f(y_1, \dots, y_n|\boldsymbol{\theta})$$

- is (really!) not available in closed form
- can (easily!) be neither completed nor demarginalised
- cannot be estimated by an unbiased estimator

© Prohibits direct implementation of a generic MCMC algorithm like Metropolis–Hastings

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What is the (most) fundamental issue?

- a mere computational issue (that will eventually end up being solved by more powerful computers, &tc, even if too costly in the short term)
- an inferential issue (opening opportunities for new inference machine, with different legitimity than classical B approach)
- a Bayesian conundrum (while inferential methods available, how closely related to the B approach?)

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Econom'ections

Similar exploration of simulation-based and approximation techniques in Econometrics

- Simulated method of moments
- Method of simulated moments
- Simulated pseudo-maximum-likelihood
- Indirect inference

[Gouriéroux & Monfort, 1996]

even though motivation is partly-defined models rather than complex likelihoods

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Minimise [in θ] a distance between estimators $\hat{\beta}$ based on a pseudo-model for genuine observations and for observations simulated under the true model and the parameter θ .

[Gouriéroux, Monfort, & Renault, 1993; Smith, 1993; Gallant & Tauchen, 1996]

Indirect inference (PML vs. PSE)

Example of the pseudo-maximum-likelihood (PML)

$$\hat{\beta}(\mathbf{y}) = \arg \max_{\beta} \sum_{t} \log f^{\star}(y_t | \beta, y_{1:(t-1)})$$

leading to

$$\arg\min_{\boldsymbol{\theta}} \| \hat{\boldsymbol{\beta}}(\boldsymbol{y}^{o}) - \hat{\boldsymbol{\beta}}(\boldsymbol{y}_{1}(\boldsymbol{\theta}), \dots, \boldsymbol{y}_{\mathcal{S}}(\boldsymbol{\theta})) \|^{2}$$

when

$$\mathbf{y}_{s}(\mathbf{\theta}) \sim f(\mathbf{y}|\mathbf{\theta}) \qquad s = 1, \dots, S$$

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Indirect inference (PML vs. PSE)

Example of the pseudo-score-estimator (PSE)

$$\hat{\beta}(\mathbf{y}) = \arg\min_{\beta} \left\{ \sum_{t} \frac{\partial \log f^{\star}}{\partial \beta} (y_t | \beta, y_{1:(t-1)}) \right\}^2$$

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"...in order to get a unique solution the dimension of the auxiliary parameter β must be larger than or equal to the dimension of the initial parameter θ . If the problem is just identified the different methods become easier..."

Consistency depending on the criterion and on the asymptotic identifiability of $\boldsymbol{\theta}$

[Gouriéroux & Monfort, 1996, p. 66]

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[Gouriéroux & Monfort, 1996, p. 66]

Arbitrariness of pseudo-model Pick model such that

- 1. $\hat{\beta}(\theta)$ not flat (i.e. sensitive to changes in θ)
- 2. $\hat{\beta}(\theta)$ not dispersed (i.e. robust agains changes in $y^{s}(\theta)$)

[Frigessi & Heggland, 2004]

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Approximate Bayesian computation

Introduction

ABC

Genesis of ABC ABC basics Advances and interpretations ABC as knn

ABC as an inference machine

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ABCe

▶ skip genetics

ABC is a recent computational technique that only requires being able to sample from the likelihood $f(\cdot|\theta)$

This technique stemmed from population genetics models, about 15 years ago, and population geneticists still contribute significantly to methodological developments of ABC.

[Griffith & al., 1997; Tavaré & al., 1999]

Each model is characterized by a set of parameters θ that cover historical (time divergence, admixture time ...), demographics (population sizes, admixture rates, migration rates, ...) and genetic (mutation rate, ...) factors

The goal is to estimate these parameters from a dataset of polymorphism (DNA sample) \boldsymbol{y} observed at the present time

Problem:

most of the time, we cannot calculate the likelihood of the polymorphism data $f(y|\theta)...$

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Sample of 8 genes

Mutations according to the Simple stepwise Mutation Model (SMM)

 \bullet date of the mutations \sim Poisson process with intensity $\theta/2$ over the branches

- MRCA = 100
- independent mutations:



Kingman's genealogy When time axis is normalized, $T(k) \sim \text{Exp}(k(k-1)/2)$

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= n<0</p>



Observations: leafs of the tree $\hat{\theta} = ?$

Kingman's genealogy

When time axis is normalized, $T(k) \sim \mathrm{Exp}(k(k-1)/2)$

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Much more interesting models...

several independent locus

Independent gene genealogies and mutations

different populations

linked by an evolutionary scenario made of divergences, admixtures, migrations between populations, etc.

larger sample size

usually between 50 and 100 genes



A typical evolutionary scenario:

Missing (too missing!) data structure:

$$f(\mathbf{y}|\mathbf{\theta}) = \int_{G} f(\mathbf{y}|G, \mathbf{\theta}) f(G|\mathbf{\theta}) \mathrm{d}G$$

cannot be computed in a manageable way ...

The genealogies are considered as nuisance parameters

This modelling clearly differs from the phylogenetic perspective where the tree is the parameter of interest.

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a dubious ancestry...



You went to school to learn, girl (...) Why 2 plus 2 makes four Now, now, now, I'm gonna teach you (...)

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All you gotta do is repeat after me! A, B, C! It's easy as 1, 2, 3! Or simple as Do, Re, Mi! (...)

A?B?C?

- A stands for approximate [wrong likelihood / picture]
- ► B stands for Bayesian
- C stands for computation [producing a parameter sample]



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Could we turn the resolution into a Bayesian answer?

- ▶ ideally so (not meaningfull: requires ∞-ly powerful computer
- asymptotically so (when sample size goes to ∞ : meaningfull?)
- approximation error unknown (w/o costly simulation)
- true Bayes for wrong model (formal and artificial)
- true Bayes for estimated likelihood (back to econometrics?)

Untractable likelihood

Back to stage zero: what can we do when a likelihood function $f(\mathbf{y}|\theta)$ is well-defined but impossible / too costly to compute...?

- MCMC cannot be implemented!
- shall we give up Bayesian inference altogether?!
- or settle for an almost Bayesian inference/picture...?

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ABC methodology

Bayesian setting: target is $\pi(\theta)f(x|\theta)$

When likelihood $f(x|\theta)$ not in closed form, likelihood-free rejection technique:

Foundation

For an observation $\mathbf{y} \sim f(\mathbf{y}|\mathbf{\theta})$, under the prior $\pi(\mathbf{\theta})$, if one keeps *jointly* simulating

$$\mathbf{ heta}' \sim \pi(\mathbf{ heta}) \,, oldsymbol{z} \sim oldsymbol{f}(oldsymbol{z}|\mathbf{ heta}') \,,$$

until the auxiliary variable z is equal to the observed value, z = y, then the selected

$$\theta' \sim \pi(\theta|\mathbf{y})$$

[Rubin, 1984; Diggle & Gratton, 1984; Tavaré et al., 1997]

ABC methodology

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$$\theta' \sim \pi(\theta), \boldsymbol{z} \sim f(\boldsymbol{z}|\theta'),$$

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When y is a continuous random variable, strict equality z = y is replaced with a tolerance zone

 $\rho(\mathbf{y}, \mathbf{z}) \leqslant \epsilon$

where ρ is a distance

Output distributed from

 $\pi(\theta) \, P_{\theta}\{\rho(\mathbf{y}, z) < \varepsilon\} \stackrel{\mathsf{def}}{\propto} \pi(\theta|\rho(\mathbf{y}, z) < \varepsilon)$

[Pritchard et al., 1999]

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[Pritchard et al., 1999]

ABC algorithm

In most implementations, further degree of A...pproximation:

```
Algorithm 1 Likelihood-free rejection samplerfor i = 1 to N dorepeatgenerate \theta' from the prior distribution \pi(\cdot)generate z from the likelihood f(\cdot|\theta')until \rho\{\eta(z), \eta(y)\} \leq \epsilonset \theta_i = \theta'end for
```

where $\eta(\boldsymbol{y})$ defines a (not necessarily sufficient) statistic

The likelihood-free algorithm samples from the marginal in z of:

$$\pi_{\epsilon}(\boldsymbol{\theta}, \boldsymbol{z} | \boldsymbol{y}) = \frac{\pi(\boldsymbol{\theta}) f(\boldsymbol{z} | \boldsymbol{\theta}) \mathbb{I}_{\mathcal{A}_{\epsilon, \boldsymbol{y}}}(\boldsymbol{z})}{\int_{\mathcal{A}_{\epsilon, \boldsymbol{y}} \times \boldsymbol{\Theta}} \pi(\boldsymbol{\theta}) f(\boldsymbol{z} | \boldsymbol{\theta}) \mathrm{d} \boldsymbol{z} \mathrm{d} \boldsymbol{\theta}} \,,$$

where $A_{\varepsilon, \mathbf{y}} = \{ z \in \mathcal{D} | \rho(\eta(z), \eta(\mathbf{y})) < \varepsilon \}.$

The idea behind ABC is that the summary statistics coupled with a small tolerance should provide a good approximation of the posterior distribution:

$$\pi_{\epsilon}(\mathbf{ heta}|\mathbf{y}) = \int \pi_{\epsilon}(\mathbf{ heta}, z|\mathbf{y}) \mathrm{d} z pprox \pi(\mathbf{ heta}|\mathbf{y}) \,.$$

...does it?!

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The likelihood-free algorithm samples from the marginal in z of:

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where $A_{\varepsilon, \mathbf{y}} = \{ z \in \mathcal{D} | \rho(\eta(z), \eta(\mathbf{y})) < \varepsilon \}.$

The idea behind ABC is that the summary statistics coupled with a small tolerance should provide a good approximation of the restricted posterior distribution:

$$\pi_{\varepsilon}(\boldsymbol{\theta}|\mathbf{y}) = \int \pi_{\varepsilon}(\boldsymbol{\theta}, \boldsymbol{z}|\mathbf{y}) \mathsf{d} \boldsymbol{z} pprox \pi(\boldsymbol{\theta}|\boldsymbol{\eta}(\mathbf{y})) \,.$$

Not so good ..!

skip convergence details!

Convergence of ABC

What happens when $\epsilon \rightarrow 0$?

For $B \subset \Theta$, we have



which indicates convergence for a continuous $\pi(B|z)$.

Convergence of ABC

What happens when $\epsilon \rightarrow 0$?

For $B \subset \Theta$, we have

$$\begin{split} \int_{B} & \frac{\int_{A_{\epsilon,\mathbf{y}}} f(\boldsymbol{z}|\boldsymbol{\theta}) d\boldsymbol{z}}{\int_{A_{\epsilon,\mathbf{y}}\times\Theta} \pi(\boldsymbol{\theta}) f(\boldsymbol{z}|\boldsymbol{\theta}) d\boldsymbol{z} d\boldsymbol{\theta}} \pi(\boldsymbol{\theta}) d\boldsymbol{\theta} = \int_{A_{\epsilon,\mathbf{y}}} \frac{\int_{B} f(\boldsymbol{z}|\boldsymbol{\theta}) \pi(\boldsymbol{\theta}) d\boldsymbol{\theta}}{\int_{A_{\epsilon,\mathbf{y}}\times\Theta} \pi(\boldsymbol{\theta}) f(\boldsymbol{z}|\boldsymbol{\theta}) d\boldsymbol{z} d\boldsymbol{\theta}} d\boldsymbol{z} \\ &= \int_{A_{\epsilon,\mathbf{y}}} \frac{\int_{B} f(\boldsymbol{z}|\boldsymbol{\theta}) \pi(\boldsymbol{\theta}) d\boldsymbol{\theta}}{m(\boldsymbol{z})} \frac{m(\boldsymbol{z})}{\int_{A_{\epsilon,\mathbf{y}}\times\Theta} \pi(\boldsymbol{\theta}) f(\boldsymbol{z}|\boldsymbol{\theta}) d\boldsymbol{z} d\boldsymbol{\theta}} d\boldsymbol{z} \\ &= \int_{A_{\epsilon,\mathbf{y}}} \pi(B|\boldsymbol{z}) \frac{m(\boldsymbol{z})}{\int_{A_{\epsilon,\mathbf{y}}\times\Theta} \pi(\boldsymbol{\theta}) f(\boldsymbol{z}|\boldsymbol{\theta}) d\boldsymbol{z} d\boldsymbol{\theta}} d\boldsymbol{z} \end{split}$$

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which indicates convergence for a continuous $\pi(B|z)$.

If $\eta(\boldsymbol{y})$ is not a sufficient statistics, the best one can hope for is

 $\pi(\theta|\eta(\mathbf{y})), \text{ not } \pi(\theta|\mathbf{y})$

If $\eta(y)$ is an ancillary statistic, the whole information contained in y is lost!, the "best" one can "hope" for is

 $\pi(\boldsymbol{\theta}|\boldsymbol{\eta}(\boldsymbol{y})) = \pi(\boldsymbol{\theta})$

Bummer!!!

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MA example

Inference on the parameters of a MA(q) model

$$x_t = \epsilon_t + \sum_{i=1}^q \vartheta_i \epsilon_{t-i}$$
 ϵ_{t-i} i.i.d.w.n.

bypass MA illustration

Simple prior: uniform over the inverse [real and complex] roots in

$$\mathfrak{Q}(u) = 1 - \sum_{i=1}^{q} \vartheta_{i} u^{i}$$

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under the identifiability conditions

Inference on the parameters of a MA(q) model

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bypass MA illustration

Simple prior: uniform prior over the identifiability zone in the parameter space, i.e. triangle for MA(2)

MA example (2)

ABC algorithm thus made of

- 1. picking a new value $(\vartheta_1, \vartheta_2)$ in the triangle
- 2. generating an iid sequence $(\epsilon_t)_{-q < t \leqslant T}$
- 3. producing a simulated series $(x'_t)_{1 \leq t \leq T}$

Distance: basic distance between the series

$$\rho((\mathbf{x}_t')_{1 \leqslant t \leqslant T}, (\mathbf{x}_t)_{1 \leqslant t \leqslant T}) = \sum_{t=1}^T (\mathbf{x}_t - \mathbf{x}_t')^2$$

or distance between summary statistics like the q = 2autocorrelations

$$\tau_j = \sum_{t=j+1}^{l} x_t x_{t-j}$$

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- 3. producing a simulated series $(x'_t)_{1 \leq t \leq T}$

Distance: basic distance between the series

$$\rho((x_t')_{1 \leqslant t \leqslant T}, (x_t)_{1 \leqslant t \leqslant T}) = \sum_{t=1}^T (x_t - x_t')^2$$

or distance between summary statistics like the q = 2 autocorrelations

$$\tau_j = \sum_{t=j+1}^{l} x_t x_{t-j}$$

Comparison of distance impact



Impact of tolerance on ABC sample against either distance ($\varepsilon=100\%, 10\%, 1\%, 0.1\%)$ for an MA(2) model

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Comparison of distance impact



Impact of tolerance on ABC sample against either distance ($\varepsilon=100\%, 10\%, 1\%, 0.1\%)$ for an MA(2) model

- ▶ Role of distance paramount (because $\epsilon \neq 0$)
- Scaling of components of $\eta(y)$ is also determinant
- ε matters little if "small enough"
- representative of "curse of dimensionality"
- small is beautiful!
- the data as a whole may be paradoxically weakly informative for ABC

how approximative is ABC?

▶ ABC as knn

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Simulating from the prior is often poor in efficiency

Either modify the proposal distribution on θ to increase the density of x's within the vicinity of y...

[Marjoram et al, 2003; Bortot et al., 2007, Sisson et al., 2007]

...or by viewing the problem as a conditional density estimation and by developing techniques to allow for larger ϵ [Beaumont et al., 2002]

....or even by including ε in the inferential framework $[ABC_{\mu}]$ [Ratmann et al., 2009]

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ABC-NP

Better usage of [prior] simulations by adjustement: instead of throwing away θ' such that $\rho(\eta(z), \eta(y)) > \epsilon$, replace θ 's with locally regressed transforms

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



[Csilléry et al., TEE, 2010]

where $\hat{\beta}$ is obtained by [NP] weighted least square regression on $(\eta(z)-\eta(y))$ with weights

 $\mathit{K}_{\delta}\{\rho(\eta(\boldsymbol{z}),\eta(\boldsymbol{y}))\}$

[Beaumont et al., 2002, Genetics]

Also found in the subsequent literature, e.g. in Fearnhead-Prangle (2012): weight directly simulation by

 $K_{\delta}\{\rho(\eta(\boldsymbol{z}(\boldsymbol{\theta})), \eta(\boldsymbol{y}))\}$

or

$$\frac{1}{S}\sum_{s=1}^{S} \mathcal{K}_{\delta}\{\rho(\eta(\boldsymbol{z}^{s}(\boldsymbol{\theta})),\eta(\boldsymbol{y}))\}$$

[consistent estimate of $f(\eta|\theta)$]

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Use of the kernel weights

 $\textit{K}_{\delta}\{\rho(\eta(\textbf{\textit{z}}(\theta)),\eta(\textbf{\textit{y}}))\}$

leads to the NP estimate of the posterior expectation

 $\frac{\sum_{i} \theta_{i} K_{\delta} \{ \rho(\eta(\boldsymbol{z}(\theta_{i})), \eta(\boldsymbol{y})) \}}{\sum_{i} K_{\delta} \{ \rho(\eta(\boldsymbol{z}(\theta_{i})), \eta(\boldsymbol{y})) \}}$

[Blum, JASA, 2010]

Use of the kernel weights

 $\textit{K}_{\delta}\{\rho(\eta(\boldsymbol{z}(\boldsymbol{\theta})),\eta(\boldsymbol{y}))\}$

leads to the NP estimate of the posterior conditional density

$$\frac{\sum_{i} \tilde{K}_{b}(\theta_{i} - \theta) K_{\delta} \{\rho(\eta(\boldsymbol{z}(\theta_{i})), \eta(\boldsymbol{y}))\}}{\sum_{i} K_{\delta} \{\rho(\eta(\boldsymbol{z}(\theta_{i})), \eta(\boldsymbol{y}))\}}$$

[Blum, JASA, 2010]

Other versions incorporating regression adjustments

$$\frac{\sum_{i} \tilde{K}_{b}(\theta_{i}^{*} - \theta) K_{\delta} \{ \rho(\eta(\boldsymbol{z}(\theta_{i})), \eta(\boldsymbol{y})) \}}{\sum_{i} K_{\delta} \{ \rho(\eta(\boldsymbol{z}(\theta_{i})), \eta(\boldsymbol{y})) \}}$$

In all cases, error

$$\mathbb{E}[\hat{g}(\theta|\mathbf{y})] - g(\theta|\mathbf{y}) = cb^2 + c\delta^2 + O_P(b^2 + \delta^2) + O_P(1/n\delta^d)$$
$$\operatorname{var}(\hat{g}(\theta|\mathbf{y})) = \frac{c}{nb\delta^d}(1 + o_P(1))$$

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[standard NP calculations]

ABC-NCH

Incorporating non-linearities and heterocedasticities:

$$\theta^* = \hat{m}(\eta(\mathbf{y})) + \left[\theta - \hat{m}(\eta(\mathbf{z}))\right] \frac{\hat{\sigma}(\eta(\mathbf{y}))}{\hat{\sigma}(\eta(\mathbf{z}))}$$

where

• $\hat{m}(\eta)$ estimated by non-linear regression (e.g., neural network)

• $\hat{\sigma}(\eta)$ estimated by non-linear regression on residuals

$$\log\{\theta_i - \hat{m}(\eta_i)\}^2 = \log \sigma^2(\eta_i) + \xi_i$$

[Blum & François, 2009]

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[Blum & François, 2009]
[Biau et al., 2012, arxiv:1207.6461]

Practice of ABC: determine tolerance ε as a quantile on observed distances, say 10% or 1% quantile,

$$\epsilon = \epsilon_N = q_{\alpha}(d_1, \ldots, d_N)$$

 Interpretation of ε as nonparametric bandwidth only approximation of the actual practice
[Blum & François, 2]

► ABC is a k-nearest neighbour (knn) method with $k_N = N \epsilon_N$ [Loftsgaarden & Quesenberry, 1965]

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ABC consistency

Provided

$k_N/\log \log N \longrightarrow \infty$ and $k_N/N \longrightarrow 0$

as $N \to \infty$, for almost all s_0 (with respect to the distribution of S), with probability 1,

$$\frac{1}{k_N}\sum_{j=1}^{k_N} \varphi(\theta_j) \longrightarrow \mathbb{E}[\varphi(\theta_j)|S = s_0]$$

[Devroye, 1982]

Biau et al. (2012) also recall pointwise and integrated mean square error consistency results on the corresponding kernel estimate of the conditional posterior distribution, under constraints

 $k_N \to \infty, \quad k_N/N \to 0, \quad h_N \to 0 \quad \text{and} \quad h_N^p k_N \to \infty,$

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Rates of convergence

Further assumptions (on target and kernel) allow for precise (integrated mean square) convergence rates (as a power of the sample size N), derived from classical k-nearest neighbour regression, like

• when
$$m = 1, 2, 3$$
, $k_N \approx N^{(p+4)/(p+8)}$ and rate $N^{-\frac{4}{p+8}}$

• when
$$m = 4$$
, $k_N \approx N^{(p+4)/(p+8)}$ and rate $N^{-\frac{4}{p+8}} \log N$

• when
$$m > 4$$
, $k_N \approx N^{(p+4)/(m+p+4)}$ and rate $N^{-\frac{4}{m+p+4}}$

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Only applies to sufficient summary statistics

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Only applies to sufficient summary statistics

ABC inference machine

Introduction

ABC

ABC as an inference machine Error inc. Exact BC and approximate targets summary statistic

ABC for model choice

Model choice consistency



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ABC_e

- maybe a convergent method of inference (meaningful? sufficient? foreign?)
- approximation error unknown (w/o simulation)
- pragmatic Bayes (there is no other solution!)
- many calibration issues (tolerance, distance, statistics)

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...should Bayesians care?!

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yes they should!!!

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Idea Infer about the error as well as about the parameter: Use of a joint density

$f(\theta, \varepsilon | \mathbf{y}) \propto \xi(\varepsilon | \mathbf{y}, \theta) \times \pi_{\theta}(\theta) \times \pi_{\varepsilon}(\varepsilon)$

where \mathbf{y} is the data, and $\xi(\epsilon|\mathbf{y}, \theta)$ is the prior predictive density of $\rho(\eta(\boldsymbol{z}), \eta(\mathbf{y}))$ given θ and \mathbf{y} when $\boldsymbol{z} \sim f(\boldsymbol{z}|\theta)$ Warning! Replacement of $\xi(\epsilon|\mathbf{y}, \theta)$ with a non-parametric kernel approximation.

[Ratmann, Andrieu, Wiuf and Richardson, 2009, PNAS]

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ABC_{μ} details

Multidimensional distances ρ_k (k = 1, ..., K) and errors $\epsilon_k = \rho_k(\eta_k(z), \eta_k(y))$, with

$$\epsilon_k \sim \xi_k(\epsilon | \mathbf{y}, \theta) \approx \hat{\xi}_k(\epsilon | \mathbf{y}, \theta) = \frac{1}{Bh_k} \sum_b K[\{\epsilon_k - \rho_k(\eta_k(\mathbf{z}_b), \eta_k(\mathbf{y}))\}/h_k]$$

then used in replacing $\xi(\epsilon|\mathbf{y}, \theta)$ with $\min_k \hat{\xi}_k(\epsilon|\mathbf{y}, \theta)$ ABC_µ involves acceptance probability

$$\frac{\pi(\theta',\epsilon')}{\pi(\theta,\epsilon)} \frac{q(\theta',\theta)q(\epsilon',\epsilon)}{q(\theta,\theta')q(\epsilon,\epsilon')} \frac{\min_k \hat{\xi}_k(\epsilon'|\mathbf{y},\theta')}{\min_k \hat{\xi}_k(\epsilon|\mathbf{y},\theta)}$$

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ABC_{μ} multiple errors



[© Ratmann et al., PNAS, 2009]

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ABC_{μ} for model choice



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[© Ratmann et al., PNAS, 2009]

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 $\rho(\epsilon|\mathbf{x}_0, \mathbf{M}_1)$

 $\hat{f}_{\rho}(\epsilon|x_0, M_3)$

Wilkinson's exact BC (not exactly!)

ABC approximation error (i.e. non-zero tolerance) replaced with exact simulation from a controlled approximation to the target, convolution of true posterior with kernel function

$$\pi_{\epsilon}(\theta, \boldsymbol{z}|\boldsymbol{y}) = \frac{\pi(\theta)f(\boldsymbol{z}|\theta)K_{\epsilon}(\boldsymbol{y}-\boldsymbol{z})}{\int \pi(\theta)f(\boldsymbol{z}|\theta)K_{\epsilon}(\boldsymbol{y}-\boldsymbol{z})\mathsf{d}\boldsymbol{z}\mathsf{d}\theta},$$

with K_{ε} kernel parameterised by bandwidth ε .

[Wilkinson, 2008]

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Theorem

The ABC algorithm based on the assumption of a randomised observation $\mathbf{y} = \tilde{\mathbf{y}} + \xi$, $\xi \sim K_{\varepsilon}$, and an acceptance probability of

 $K_{\epsilon}(\mathbf{y}-\mathbf{z})/M$

gives draws from the posterior distribution $\pi(heta|\mathbf{y})$.

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"Using \in to represent measurement error is straightforward, whereas using \in to model the model discrepancy is harder to conceptualize and not as commonly used"

[Richard Wilkinson, 2008]

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How exact a BC?

Pros

- Pseudo-data from *true* model and observed data from *noisy* model
- Interesting perspective in that outcome is completely controlled
- ► Link with ▲ABC_I and assuming y is observed with a measurement error with density K_e
- Relates to the theory of model approximation

[Kennedy & O'Hagan, 2001]

Cons

- Requires K_{ϵ} to be bounded by M
- True approximation error never assessed
- Requires a modification of the standard ABC algorithm

Specific case of a hidden • Markov model

 $\begin{aligned} X_{t+1} &\sim Q_{\theta}(X_t, \cdot) \\ Y_{t+1} &\sim g_{\theta}(\cdot | x_t) \end{aligned}$

where only $y_{1:n}^0$ is observed. [Dean,

[Dean, Singh, Jasra, & Peters, 2011]

Use of specific constraints, adapted to the Markov structure:

$$\{y_1 \in \mathcal{B}(y_1^0, \epsilon)\} \times \cdots \times \{y_n \in \mathcal{B}(y_n^0, \epsilon)\}$$

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ABC-MLE for HMMs

ABC-MLE defined by

$$\hat{\theta}_n^{\epsilon} = \arg \max_{\theta} \mathbb{P}_{\theta} \left(Y_1 \in \mathcal{B}(y_1^0, \epsilon), \dots, Y_n \in \mathcal{B}(y_n^0, \epsilon) \right)$$

Exact MLE for the likelihood • same basis as Wilkinson!

$$p_{\theta}^{\epsilon}(y_1^0,\ldots,y_n)$$

corresponding to the perturbed process

$$(x_t, y_t + \epsilon z_t)_{1 \leq t \leq n} \quad z_t \sim \mathcal{U}(\mathcal{B}(0, 1))$$

[Dean, Singh, Jasra, & Peters, 2011]

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► ABC-MLE is asymptotically (in *n*) biased with target

$$I^{\epsilon}(\theta) = \mathbb{E}_{\theta^*}[\log p^{\epsilon}_{\theta}(Y_1|Y_{-\infty:0})]$$

but ABC-MLE converges to true value in the sense

 $I^{\epsilon_n}(\theta_n) \to I^{\epsilon}(\theta)$

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for all sequences (θ_n) converging to θ and $\epsilon_n \searrow \epsilon$

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for all sequences (θ_n) converging to θ and $\epsilon_n \searrow \epsilon$

Idea: Modify instead the data from the start

$$(y_1^0 + \epsilon \zeta_1, \ldots, y_n + \epsilon \zeta_n)$$

▶ see Fearnhead-Prangle

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noisy ABC-MLE estimate

$$\arg\max_{\theta} \mathbb{P}_{\theta} \left(Y_1 \in \mathcal{B}(y_1^0 + \varepsilon \zeta_1, \varepsilon), \dots, Y_n \in \mathcal{B}(y_n^0 + \varepsilon \zeta_n, \varepsilon) \right)$$

[Dean, Singh, Jasra, & Peters, 2011]

- Degrading the data improves the estimation performances:
 - Noisy ABC-MLE is asymptotically (in n) consistent
 - under further assumptions, the noisy ABC-MLE is asymptotically normal
 - increase in variance of order ϵ^{-2}
- likely degradation in precision or computing time due to the lack of summary statistic [curse of dimensionality]

Algorithm 2 SMC ABC for HMMs

Given θ

for $k = 1, \ldots, n$ do

generate proposals $(x_k^1, y_k^1), \ldots, (x_k^N, y_k^N)$ from the model weigh each proposal with $\omega'_k = \mathbb{I}_{\mathcal{B}(y_k^0 + \epsilon\zeta_k, \epsilon)}(y'_k)$

renormalise the weights and sample the x_k^l 's accordingly end for

approximate the likelihood by

$$\prod_{k=1}^{n} \left(\sum_{l=1}^{N} \omega_{k}^{l} / N \right)$$

[Jasra, Singh, Martin, & McCoy, 2010]

Which summary?

Fundamental difficulty of the choice of the summary statistic when there is no non-trivial sufficient statistics

Starting from a large collection of summary statistics is available, Joyce and Marjoram (2008) consider the sequential inclusion into the ABC target, with a stopping rule based on a likelihood ratio test

Not taking into account the sequential nature of the tests

- Depends on parameterisation
- Order of inclusion matters
- likelihood ratio test?!

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- likelihood ratio test?!

Depending on the choice of $\eta(\cdot),$ the Bayes factor based on this insufficient statistic,

$$B_{12}^{\eta}(\mathbf{y}) = \frac{\int \pi_1(\theta_1) f_1^{\eta}(\eta(\mathbf{y})|\theta_1) \, \mathrm{d}\theta_1}{\int \pi_2(\theta_2) f_2^{\eta}(\eta(\mathbf{y})|\theta_2) \, \mathrm{d}\theta_2} \,,$$

is consistent or not.

[X, Cornuet, Marin, & Pillai, 2012]

Consistency only depends on the range of $\mathbb{E}_i[\eta(\boldsymbol{y})]$ under both models.

[Marin, Pillai, X, & Rousseau, 2012]

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Fearnhead and Prangle (2010) study ABC and the selection of the summary statistic in close proximity to Wilkinson's proposal

- ABC considered as inferential method and calibrated as such
- randomised (or 'noisy') version of the summary statistics

$$\tilde{\eta}(\boldsymbol{y}) = \eta(\boldsymbol{y}) + \tau \varepsilon$$

derivation of a well-calibrated version of ABC, i.e. an algorithm that gives proper predictions for the distribution associated with this randomised summary statistic

Summary [of F&P/statistics)

optimality of the posterior expectation

$\mathbb{E}[\theta|y]$

of the parameter of interest as summary statistics $\eta(y)$! • use of the standard quadratic loss function

$$(\theta - \theta_0)^{\mathsf{T}} A(\theta - \theta_0)$$
.

recent extension to model choice, optimality of Bayes factor

 $B_{12}(y)$

[F&P, ISBA 2012 talk]

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[F&P, ISBA 2012 talk]

- Choice of summary statistics is paramount for ABC validation/performance
- At best, ABC approximates $\pi(. | \eta(\mathbf{y}))$
- Model selection feasible with ABC [with caution!]
- For estimation, consistency if $\{\theta; \mu(\theta) = \mu_0\} = \theta_0$
- ► For testing consistency if $\{\mu_1(\theta_1), \theta_1 \in \Theta_1\} \cap \{\mu_2(\theta_2), \theta_2 \in \Theta_2\} = \emptyset$

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[Marin et al., 2011]

ABC for model choice

Introduction

ABC

ABC as an inference machine

ABC for model choice BMC Principle Gibbs random fields (counterexample) Generic ABC model choice

Model choice consistency



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ABCe

BMC Principle

Several models

 M_1, M_2, \ldots

are considered simultaneously for dataset \boldsymbol{y} and model index $\boldsymbol{\mathcal{M}}$ central to inference.

Use of

- prior $\pi(\mathcal{M} = m)$, plus
- prior distribution on the parameter conditional on the value m of the model index, π_m(θ_m)

BMC Principle

Several models

 M_1, M_2, \ldots

are considered simultaneously for dataset \boldsymbol{y} and model index $\boldsymbol{\mathfrak{M}}$ central to inference.

Goal is to derive the posterior distribution of $\ensuremath{\mathcal{M}}$,

 $\pi(\mathcal{M} = m | \mathsf{data})$

a challenging computational target when models are complex.

Generic ABC for model choice

Algorithm 3 Likelihood-free model choice sampler (ABC-MC)

for t = 1 to T do

repeat

Generate *m* from the prior $\pi(\mathcal{M} = m)$ Generate θ_m from the prior $\pi_m(\theta_m)$ Generate *z* from the model $f_m(z|\theta_m)$ **until** $\rho\{\eta(z), \eta(y)\} < \epsilon$ Set $m^{(t)} = m$ and $\theta^{(t)} = \theta_m$ end for

[Grelaud & al., 2009; Toni & al., 2009]

Posterior probability $\pi(\mathcal{M}=m|\mathbf{y})$ approximated by the frequency of acceptances from model m

$$\frac{1}{T}\sum_{t=1}^{T}\mathbb{I}_{m^{(t)}=m}.$$

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Posterior probability $\pi(\mathcal{M}=m|\mathbf{y})$ approximated by the frequency of acceptances from model m

$$\frac{1}{T} \sum_{t=1}^{T} \mathbb{I}_{m^{(t)}=m}.$$

Extension to a weighted polychotomous logistic regression estimate of $\pi(\mathcal{M} = m | \mathbf{y})$, with non-parametric kernel weights [Cornuet et al., DIYABC, 2009]

Potts model

► Skip MRFs

Potts model

Distribution with an energy function of the form

$$\theta S(\mathbf{y}) = \theta \sum_{l \sim i} \delta_{y_l = y_i}$$

where $l \sim i$ denotes a neighbourhood structure

In most realistic settings, summation

$$Z_{\theta} = \sum_{\mathbf{x} \in \mathcal{X}} \exp\{\theta S(\mathbf{x})\}$$

involves too many terms to be manageable and numerical approximations cannot always be trusted

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Setup

Choice to be made between M neighbourhood relations

$$i \stackrel{m}{\sim} i' \qquad (0 \leqslant m \leqslant M - 1)$$

with

$$S_m(\mathbf{x}) = \sum_{\substack{i \in i' \\ i \sim i'}} \mathbb{I}_{\{x_i = x_{i'}\}}$$

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driven by the posterior probabilities of the models.

Computational target:

$$\mathbb{P}(\mathcal{M} = m | \mathbf{x}) \propto \int_{\Theta_m} f_m(\mathbf{x} | \theta_m) \pi_m(\theta_m) \, \mathrm{d}\theta_m \, \pi(\mathcal{M} = m)$$

If $S(\mathbf{x})$ sufficient statistic for the joint parameters $(\mathcal{M}, \theta_0, \dots, \theta_{M-1})$,

$$\mathbb{P}(\mathcal{M}=m|\mathbf{x})=\mathbb{P}(\mathcal{M}=m|S(\mathbf{x})).$$

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Computational target:

$$\mathbb{P}(\mathcal{M}=m|\mathbf{x}) \propto \int_{\Theta_m} f_m(\mathbf{x}|\theta_m) \pi_m(\theta_m) \, \mathrm{d}\theta_m \, \pi(\mathcal{M}=m)$$

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Sufficient statistics in Gibbs random fields

Each model *m* has its own sufficient statistic $S_m(\cdot)$ and $S(\cdot) = (S_0(\cdot), \ldots, S_{M-1}(\cdot))$ is also (model-)sufficient. Explanation: For Gibbs random fields,

$$\begin{aligned} \mathbf{x}|\mathcal{M} &= m \sim f_m(\mathbf{x}|\boldsymbol{\theta}_m) &= f_m^1(\mathbf{x}|S(\mathbf{x}))f_m^2(S(\mathbf{x})|\boldsymbol{\theta}_m) \\ &= \frac{1}{n(S(\mathbf{x}))}f_m^2(S(\mathbf{x})|\boldsymbol{\theta}_m) \end{aligned}$$

where

$n(S(\mathbf{x})) = \#\{\tilde{\mathbf{x}} \in \mathcal{X} : S(\tilde{\mathbf{x}}) = S(\mathbf{x})\}$ (c) S(x) is sufficient for the joint parameter

Each model *m* has its own sufficient statistic $S_m(\cdot)$ and $S(\cdot) = (S_0(\cdot), \ldots, S_{M-1}(\cdot))$ is also (model-)sufficient. Explanation: For Gibbs random fields,

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 \bigcirc *S*(*x*) is sufficient for the joint parameters

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Toy example

iid Bernoulli model versus two-state first-order Markov chain, i.e.

$$f_0(\mathbf{x}|\boldsymbol{\theta}_0) = \exp\left(\boldsymbol{\theta}_0 \sum_{i=1}^n \mathbb{I}_{\{\mathbf{x}_i=1\}}\right) / \{1 + \exp(\boldsymbol{\theta}_0)\}^n$$

versus

$$f_1(\mathbf{x}|\theta_1) = \frac{1}{2} \exp\left(\theta_1 \sum_{i=2}^n \mathbb{I}_{\{x_i = x_{i-1}\}}\right) / \{1 + \exp(\theta_1)\}^{n-1},$$

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with priors $\theta_0 \sim \mathcal{U}(-5,5)$ and $\theta_1 \sim \mathcal{U}(0,6)$ (inspired by "phase transition" boundaries).

If $\eta_1(\mathbf{x})$ sufficient statistic for model m = 1 and parameter θ_1 and $\eta_2(\mathbf{x})$ sufficient statistic for model m = 2 and parameter θ_2 , $(\eta_1(\mathbf{x}), \eta_2(\mathbf{x}))$ is not always sufficient for (m, θ_m)

(C) Potential loss of information at the testing level

If $\eta_1(\mathbf{x})$ sufficient statistic for model m = 1 and parameter θ_1 and $\eta_2(\mathbf{x})$ sufficient statistic for model m = 2 and parameter θ_2 , $(\eta_1(\mathbf{x}), \eta_2(\mathbf{x}))$ is not always sufficient for (m, θ_m)

© Potential loss of information at the testing level

Sample

$$\mathbf{x} = (x_1, \ldots, x_n)$$

from either a Poisson $\mathfrak{P}(\lambda)$ or from a geometric $\mathfrak{G}(p)$ Sum

$$S = \sum_{i=1}^{n} x_i = \eta(\mathbf{x})$$

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sufficient statistic for either model but not simultaneously

Limiting behaviour of B_{12} $(T \rightarrow \infty)$

ABC approximation

$$\widehat{B_{12}}(\mathbf{y}) = \frac{\sum_{t=1}^{T} \mathbb{I}_{m^t=1} \mathbb{I}_{\rho\{\eta(z^t),\eta(\mathbf{y})\}\leqslant\epsilon}}{\sum_{t=1}^{T} \mathbb{I}_{m^t=2} \mathbb{I}_{\rho\{\eta(z^t),\eta(\mathbf{y})\}\leqslant\epsilon}},$$

where the (m^t, z^t) 's are simulated from the (joint) prior As \mathcal{T} goes to infinity, limit

$$B_{12}^{\epsilon}(\mathbf{y}) = \frac{\int \mathbb{I}_{\rho[\eta(z),\eta(\mathbf{y})] \leqslant \epsilon} \pi_1(\theta_1) f_1(z|\theta_1) \, dz \, d\theta_1}{\int \mathbb{I}_{\rho[\eta(z),\eta(\mathbf{y})] \leqslant \epsilon} \pi_2(\theta_2) f_2(z|\theta_2) \, dz \, d\theta_2}$$

$$= \frac{\int \mathbb{I}_{\rho[\eta,\eta(\mathbf{y})] \leqslant \epsilon} \pi_1(\theta_1) f_1^{\eta}(\eta|\theta_1) \, d\eta \, d\theta_1}{\int \mathbb{I}_{\rho[\eta,\eta(\mathbf{y})] \leqslant \epsilon} \pi_2(\theta_2) f_2^{\eta}(\eta|\theta_2) \, d\eta \, d\theta_2},$$

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where $f_1^{\eta}(\eta|\theta_1)$ and $f_2^{\eta}(\eta|\theta_2)$ distributions of $\eta(z)$

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$$\widehat{B_{12}}(\mathbf{y}) = \frac{\sum_{t=1}^{T} \mathbb{I}_{m^t=1} \mathbb{I}_{\rho\{\eta(z^t),\eta(\mathbf{y})\} \leqslant \epsilon}}{\sum_{t=1}^{T} \mathbb{I}_{m^t=2} \mathbb{I}_{\rho\{\eta(z^t),\eta(\mathbf{y})\} \leqslant \epsilon}},$$

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$$\begin{split} B_{12}^{\epsilon}(\mathbf{y}) &= \frac{\int \mathbb{I}_{\rho\{\eta(z),\eta(\mathbf{y})\}\leqslant\epsilon} \pi_1(\theta_1) f_1(z|\theta_1) \, \mathrm{d}z \, \mathrm{d}\theta_1}{\int \mathbb{I}_{\rho\{\eta(z),\eta(\mathbf{y})\}\leqslant\epsilon} \pi_2(\theta_2) f_2(z|\theta_2) \, \mathrm{d}z \, \mathrm{d}\theta_2} \\ &= \frac{\int \mathbb{I}_{\rho\{\eta,\eta(\mathbf{y})\}\leqslant\epsilon} \pi_1(\theta_1) f_1^{\eta}(\eta|\theta_1) \, \mathrm{d}\eta \, \mathrm{d}\theta_1}{\int \mathbb{I}_{\rho\{\eta,\eta(\mathbf{y})\}\leqslant\epsilon} \pi_2(\theta_2) f_2^{\eta}(\eta|\theta_2) \, \mathrm{d}\eta \, \mathrm{d}\theta_2} \,, \end{split}$$

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where $f_1^\eta(\eta|\theta_1)$ and $f_2^\eta(\eta|\theta_2)$ distributions of $\eta(z)$

Limiting behaviour of B_{12} ($\epsilon \rightarrow 0$)

When ϵ goes to zero,

$$B_{12}^{\eta}(\mathbf{y}) = \frac{\int \pi_1(\boldsymbol{\theta}_1) f_1^{\eta}(\eta(\mathbf{y})|\boldsymbol{\theta}_1) \, \mathrm{d}\boldsymbol{\theta}_1}{\int \pi_2(\boldsymbol{\theta}_2) f_2^{\eta}(\eta(\mathbf{y})|\boldsymbol{\theta}_2) \, \mathrm{d}\boldsymbol{\theta}_2}$$

C Bayes factor based on the sole observation of $\eta(y)$

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Limiting behaviour of B_{12} ($\epsilon \rightarrow 0$)

When ϵ goes to zero,

$$B_{12}^{\eta}(\mathbf{y}) = \frac{\int \pi_1(\boldsymbol{\theta}_1) f_1^{\eta}(\boldsymbol{\eta}(\mathbf{y})|\boldsymbol{\theta}_1) \, \mathrm{d}\boldsymbol{\theta}_1}{\int \pi_2(\boldsymbol{\theta}_2) f_2^{\eta}(\boldsymbol{\eta}(\mathbf{y})|\boldsymbol{\theta}_2) \, \mathrm{d}\boldsymbol{\theta}_2}$$

C Bayes factor based on the sole observation of $\eta(\boldsymbol{y})$

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Limiting behaviour of B_{12} (under sufficiency)

If $\eta(\boldsymbol{y})$ sufficient statistic in both models,

$$f_i(\mathbf{y}|\mathbf{\theta}_i) = g_i(\mathbf{y})f_i^{\eta}(\eta(\mathbf{y})|\mathbf{\theta}_i)$$

Thus

$$B_{12}(\mathbf{y}) = \frac{\int_{\Theta_1} \pi(\theta_1) g_1(\mathbf{y}) f_1^{\eta}(\eta(\mathbf{y})|\theta_1) d\theta_1}{\int_{\Theta_2} \pi(\theta_2) g_2(\mathbf{y}) f_2^{\eta}(\eta(\mathbf{y})|\theta_2) d\theta_2} \\ = \frac{g_1(\mathbf{y}) \int \pi_1(\theta_1) f_1^{\eta}(\eta(\mathbf{y})|\theta_1) d\theta_1}{g_2(\mathbf{y}) \int \pi_2(\theta_2) f_2^{\eta}(\eta(\mathbf{y})|\theta_2) d\theta_2} = \frac{g_1(\mathbf{y})}{g_2(\mathbf{y})} B_{12}^{\eta}(\mathbf{y}).$$

[Didelot, Everitt, Johansen & Lawson, 2011]

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© No discrepancy only when cross-model sufficiency

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If $\eta(\boldsymbol{y})$ sufficient statistic in both models,

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Thus

$$B_{12}(\mathbf{y}) = \frac{\int_{\Theta_1} \pi(\theta_1) g_1(\mathbf{y}) f_1^{\eta}(\eta(\mathbf{y})|\theta_1) d\theta_1}{\int_{\Theta_2} \pi(\theta_2) g_2(\mathbf{y}) f_2^{\eta}(\eta(\mathbf{y})|\theta_2) d\theta_2} \\ = \frac{g_1(\mathbf{y}) \int \pi_1(\theta_1) f_1^{\eta}(\eta(\mathbf{y})|\theta_1) d\theta_1}{g_2(\mathbf{y}) \int \pi_2(\theta_2) f_2^{\eta}(\eta(\mathbf{y})|\theta_2) d\theta_2} = \frac{g_1(\mathbf{y})}{g_2(\mathbf{y})} B_{12}^{\eta}(\mathbf{y}).$$

[Didelot, Everitt, Johansen & Lawson, 2011]

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© No discrepancy only when cross-model sufficiency

Poisson/geometric example (back)

Sample

$$\mathbf{x} = (x_1, \ldots, x_n)$$

from either a Poisson $\mathcal{P}(\lambda)$ or from a geometric $\mathcal{G}(\textbf{\textit{p}})$ Discrepancy ratio

$$\frac{g_1(\mathbf{x})}{g_2(\mathbf{x})} = \frac{S! n^{-S} / \prod_i x_i!}{1 / \binom{n+S-1}{S}}$$

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Poisson/geometric discrepancy

Range of $B_{12}(\mathbf{x})$ versus $B_{12}^{\eta}(\mathbf{x})$: The values produced have nothing in common.



Creating an encompassing exponential family

 $f(\mathbf{x}|\boldsymbol{\theta}_1,\boldsymbol{\theta}_2,\boldsymbol{\alpha}_1,\boldsymbol{\alpha}_2) \propto \exp\{\boldsymbol{\theta}_1^\mathsf{T}\boldsymbol{\eta}_1(\mathbf{x}) + \boldsymbol{\theta}_2^\mathsf{T}\boldsymbol{\eta}_2(\mathbf{x}) + \boldsymbol{\alpha}_1 t_1(\mathbf{x}) + \boldsymbol{\alpha}_2 t_2(\mathbf{x})\}$

leads to a sufficient statistic $(\eta_1(\mathbf{x}), \eta_2(\mathbf{x}), t_1(\mathbf{x}), t_2(\mathbf{x}))$ [Didelot, Everitt, Johansen & Lawson, 2011]

Creating an encompassing exponential family

 $f(\mathbf{x}|\boldsymbol{\theta}_1,\boldsymbol{\theta}_2,\boldsymbol{\alpha}_1,\boldsymbol{\alpha}_2) \propto \exp\{\boldsymbol{\theta}_1^\mathsf{T}\boldsymbol{\eta}_1(\mathbf{x}) + \boldsymbol{\theta}_2^\mathsf{T}\boldsymbol{\eta}_2(\mathbf{x}) + \boldsymbol{\alpha}_1 t_1(\mathbf{x}) + \boldsymbol{\alpha}_2 t_2(\mathbf{x})\}$

leads to a sufficient statistic $(\eta_1(\mathbf{x}), \eta_2(\mathbf{x}), t_1(\mathbf{x}), t_2(\mathbf{x}))$ [Didelot, Everitt, Johansen & Lawson, 2011]

In the Poisson/geometric case, if $\prod_i x_i!$ is added to S, no discrepancy
Creating an encompassing exponential family

 $f(\mathbf{x}|\boldsymbol{\theta}_1,\boldsymbol{\theta}_2,\boldsymbol{\alpha}_1,\boldsymbol{\alpha}_2) \propto \exp\{\boldsymbol{\theta}_1^\mathsf{T}\boldsymbol{\eta}_1(\mathbf{x}) + \boldsymbol{\theta}_2^\mathsf{T}\boldsymbol{\eta}_2(\mathbf{x}) + \boldsymbol{\alpha}_1 t_1(\mathbf{x}) + \boldsymbol{\alpha}_2 t_2(\mathbf{x})\}$

leads to a sufficient statistic $(\eta_1(\mathbf{x}), \eta_2(\mathbf{x}), t_1(\mathbf{x}), t_2(\mathbf{x}))$ [Didelot, Everitt, Johansen & Lawson, 2011]

Only applies in genuine sufficiency settings...

 $\textcircled{\textbf{C}}$ Inability to evaluate information loss due to summary statistics

The ABC approximation to the Bayes Factor is based solely on the summary statistics....

In the Poisson/geometric case, if $\mathbb{E}[y_i] = \theta_0 > 0$,

$$\lim_{n \to \infty} B_{12}^{\eta}(\mathbf{y}) = \frac{(\theta_0 + 1)^2}{\theta_0} e^{-\theta_0}$$

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MA example



Evolution [against ε] of ABC Bayes factor, in terms of frequencies of visits to models MA(1) (left) and MA(2) (right) when ε equal to 10, 1, .1, .01% quantiles on insufficient autocovariance distances. Sample of 50 points from a MA(2) with $\theta_1 = 0.6, \, \theta_2 = 0.2$. True Bayes factor equal to 17.71.

MA example



Evolution [against ϵ] of ABC Bayes factor, in terms of frequencies of visits to models MA(1) (left) and MA(2) (right) when ϵ equal to 10, 1, .1, .01% quantiles on insufficient autocovariance distances. Sample of 50 points from a MA(1) model with $\theta_1 = 0.6$. True Bayes factor B_{21} equal to .004.

Besides specific models like Gibbs random fields, using distances over the data itself escapes the discrepancy... [Toni & Stumpf, 2010; Sousa & al., 2009]

...and so does the use of more informal model fitting measures [Ratmann & al., 2009]

...or use another type of approximation like empirical likelihood [Mengersen et al., 2012, see Kerrie's ASC 2012 talk]

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ABC model choice consistency

Introduction

ABC

ABC as an inference machine

ABC for model choice

Model choice consistency Formalised framework Consistency results Summary statistics



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ABC_{el}

Central question to the validation of ABC for model choice:

When is a Bayes factor based on an insufficient statistic T(y) consistent?

Note/warnin: \bigcirc drawn on $\mathbf{T}(\mathbf{y})$ through $B_{12}^{\mathsf{T}}(\mathbf{y})$ necessarily differs from \bigcirc drawn on \mathbf{y} through $B_{12}(\mathbf{y})$ [Marin, Pillai, X, & Rousseau, arXiv, 2012]

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Comparison suggested by referee of PNAS paper [thanks!]: [X, Cornuet, Marin, & Pillai, Aug. 2011] Model \mathfrak{M}_1 : $\mathbf{y} \sim \mathcal{N}(\theta_1, 1)$ opposed to model \mathfrak{M}_2 : $\mathbf{y} \sim \mathcal{L}(\theta_2, 1/\sqrt{2})$, Laplace distribution with mean θ_2 and scale parameter $1/\sqrt{2}$ (variance one).

Comparison suggested by referee of PNAS paper [thanks!]: [X, Cornuet, Marin, & Pillai, Aug. 2011] Model \mathfrak{M}_1 : $\mathbf{y} \sim \mathcal{N}(\theta_1, 1)$ opposed to model \mathfrak{M}_2 : $\mathbf{y} \sim \mathcal{L}(\theta_2, 1/\sqrt{2})$, Laplace distribution with mean θ_2 and scale parameter $1/\sqrt{2}$ (variance one). Four possible statistics

- 1. sample mean \overline{y} (sufficient for \mathfrak{M}_1 if not \mathfrak{M}_2);
- 2. sample median med(y) (insufficient);
- 3. sample variance var(y) (ancillary);
- 4. median absolute deviation mad(y) = med(|y med(y)|);

A benchmark if toy example

 $\begin{array}{ll} \mbox{Comparison suggested by referee of PNAS paper [thanks!]:} & [X, \mbox{ Cornuet, Marin, \& Pillai, Aug. 2011]} \\ \mbox{Model } \mathfrak{M}_1: \ y \sim \mathcal{N}(\theta_1, 1) \mbox{ opposed} \\ \mbox{to model } \mathfrak{M}_2: \ y \sim \mathcal{L}(\theta_2, 1/\sqrt{2}), \mbox{ Laplace distribution with mean } \theta_2 \\ \mbox{ and scale parameter } 1/\sqrt{2} \mbox{ (variance one).} \end{array}$

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Starting from sample

$$\mathbf{y}=(y_1,\ldots,y_n)$$

the observed sample, not necessarily iid with true distribution

$$\mathbf{y} \sim \mathbb{P}^n$$

Summary statistics

$$\mathbf{T}(\mathbf{y}) = \mathbf{T}^n = (T_1(\mathbf{y}), T_2(\mathbf{y}), \cdots, T_d(\mathbf{y})) \in \mathbb{R}^d$$

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with *true* distribution $\mathbf{T}^n \sim G_n$.

\bigodot Comparison of

- under \mathfrak{M}_1 , $\mathbf{y} \sim F_{1,n}(\cdot | \mathbf{\theta}_1)$ where $\mathbf{\theta}_1 \in \Theta_1 \subset \mathbb{R}^{p_1}$
- under \mathfrak{M}_2 , $\mathbf{y} \sim F_{2,n}(\cdot|\theta_2)$ where $\theta_2 \in \Theta_2 \subset \mathbb{R}^{p_2}$

turned into

- under \mathfrak{M}_1 , $\mathbf{T}(\mathbf{y}) \sim \mathcal{G}_{1,n}(\cdot|\mathbf{\theta}_1)$, and $\theta_1|\mathbf{T}(\mathbf{y}) \sim \pi_1(\cdot|\mathbf{T}^n)$
- under \mathfrak{M}_2 , $\mathbf{T}(\mathbf{y}) \sim \mathcal{G}_{2,n}(\cdot|\mathbf{\theta}_2)$, and $\theta_2|\mathbf{T}(\mathbf{y}) \sim \pi_2(\cdot|\mathbf{T}^n)$

A collection of asymptotic "standard" assumptions:

[A1] is a standard central limit theorem under the true model **[A2]** controls the large deviations of the estimator \mathbf{T}^n from the estimand $\mu(\theta)$

[A3] is the standard prior mass condition found in Bayesian asymptotics (*d_i* effective dimension of the parameter)
[A4] restricts the behaviour of the model density against the true

density

[Think CLT!]

Assumptions

A collection of asymptotic "standard" assumptions:

[Think CLT!]

[A1] There exist

- ▶ a sequence $\{v_n\}$ converging to $+\infty$,
- a distribution Q,
- ▶ a symmetric, $d \times d$ positive definite matrix V_0 and
- ▶ a vector $\mu_0 \in \mathbb{R}^d$

such that

$$v_n V_0^{-1/2} (\mathbf{T}^n - \mu_0) \stackrel{n \to \infty}{\leadsto} Q$$
, under G_n

Assumptions

A collection of asymptotic "standard" assumptions:

[Think CLT!]

[A2] For i = 1, 2, there exist sets $\mathcal{F}_{n,i} \subset \Theta_i$, functions $\mu_i(\theta_i)$ and constants $\epsilon_i, \tau_i, \alpha_i > 0$ such that for all $\tau > 0$,

$$\sup_{\theta_i \in \mathcal{F}_{n,i}} \frac{G_{i,n} \Big[|\mathbf{T}^n - \mu_i(\theta_i)| > \tau |\mu_i(\theta_i) - \mu_0| \wedge \varepsilon_i |\theta_i \Big]}{(|\tau \mu_i(\theta_i) - \mu_0| \wedge \varepsilon_i)^{-\alpha_i}} \lesssim v_n^{-\alpha_i}$$

with

$$\pi_i(\mathcal{F}_{n,i}^c) = o(v_n^{-\tau_i}).$$

Assumptions

A collection of asymptotic "standard" assumptions:

[Think CLT!]

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[A3] If $\inf\{|\mu_i(\theta_i) - \mu_0|; \theta_i \in \Theta_i\} = 0$, defining (u > 0)

$$S_{n,i}(u) = \left\{ \theta_i \in \mathcal{F}_{n,i}; |\mu_i(\theta_i) - \mu_0| \leqslant u \, v_n^{-1} \right\},\$$

there exist constants $d_i < au_i \wedge lpha_i - 1$ such that

$$\pi_i(S_{n,i}(u)) \sim u^{d_i} v_n^{-d_i}, \quad \forall u \lesssim v_n$$

A collection of asymptotic "standard" assumptions:

[Think CLT!]

[A4] If $\inf\{|\mu_i(\theta_i) - \mu_0|; \theta_i \in \Theta_i\} = 0$, for any $\varepsilon > 0$, there exist $U, \delta > 0$ and $(E_n)_n$ such that, if $\theta_i \in S_{n,i}(U)$

 $E_n \subset \{t; g_i(t|\theta_i) < \delta g_n(t)\}$ and $G_n(E_n^c) < \epsilon$.

A collection of asymptotic "standard" assumptions:

[Think CLT!]

Again (sumup)

[A1] is a standard central limit theorem under the true model **[A2]** controls the large deviations of the estimator T^n from the estimand $\mu(\theta)$

[A3] is the standard prior mass condition found in Bayesian asymptotics (*d_i* effective dimension of the parameter)[A4] restricts the behaviour of the model density against the true density

Understanding d_i in **[A3]**: defined only when $\mu_0 \in {\mu_i(\theta_i), \theta_i \in \Theta_i}$,

$$\pi_i(\theta_i: |\mu_i(\theta_i) - \mu_0| < n^{-1/2}) = O(n^{-d_i/2})$$

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is the effective dimension of the model Θ_i around μ_0

Understanding d_i in **[A3]**: when $\inf\{|\mu_i(\theta_i) - \mu_0|; \theta_i \in \Theta_i\} = 0$,

$$\frac{m_i(\mathbf{T}^n)}{g_n(\mathbf{T}^n)} \sim v_n^{-d_i} ,$$

thus

$$\log(m_i(\mathbf{T}^n)/g_n(\mathbf{T}^n)) \sim -d_i \log v_n$$

and $v_n^{-d_i}$ penalization factor resulting from integrating θ_i out (see effective number of parameters in DIC)

Understanding d_i in **[A3]**: In regular models, d_i dimension of $\mathbf{T}(\Theta_i)$, leading to BIC In non-regular models, d_i can be smaller

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Asymptotic marginals

Asymptotically, under [A1]–[A4]

$$m_i(t) = \int_{\Theta_i} g_i(t|\Theta_i) \, \pi_i(\Theta_i) \, \mathrm{d}\Theta_i$$

is such that (i) if $\inf\{|\mu_i(\theta_i) - \mu_0|; \theta_i \in \Theta_i\} = 0$,

$$C_l v_n^{d-d_i} \leqslant m_i(\mathbf{T}^n) \leqslant C_u v_n^{d-d_i}$$

and (ii) if $\inf\{|\mu_i(\theta_i) - \mu_0|; \theta_i \in \Theta_i\} > 0$

$$m_i(\mathbf{T}^n) = o_{\mathbb{P}^n}[v_n^{d-\tau_i} + v_n^{d-\alpha_i}].$$

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Under same assumptions,

if $\inf\{|\mu_i(\theta_i) - \mu_0|; \theta_i \in \Theta_i\} = 0$,

the posterior distribution of $\mu_i(\theta_i)$ given \mathbf{T}^n is consistent at rate $1/v_n$ provided $\alpha_i \wedge \tau_i > d_i$.

Consequence of above is that asymptotic behaviour of the Bayes factor is driven by the asymptotic mean value of \mathbf{T}^n under both models. And only by this mean value!

Consequence of above is that asymptotic behaviour of the Bayes factor is driven by the asymptotic mean value of T^n under both models. And only by this mean value! Indeed, if

 $inf\{|\mu_0 - \mu_2(\theta_2)|; \theta_2 \in \Theta_2\} = inf\{|\mu_0 - \mu_1(\theta_1)|; \theta_1 \in \Theta_1\} = 0$

then

$$C_l v_n^{-(d_1-d_2)} \leqslant m_1(\mathbf{T}^n) / m_2(\mathbf{T}^n) \leqslant C_u v_n^{-(d_1-d_2)},$$

where C_I , $C_u = O_{\mathbb{P}^n}(1)$, irrespective of the true model. © Only depends on the difference $d_1 - d_2$: no consistency Consequence of above is that asymptotic behaviour of the Bayes factor is driven by the asymptotic mean value of T^n under both models. And only by this mean value! Else, if

 $\mathsf{inf}\{|\mu_0-\mu_2(\theta_2)|;\theta_2\in\Theta_2\}>\mathsf{inf}\{|\mu_0-\mu_1(\theta_1)|;\theta_1\in\Theta_1\}=0$

then

$$\frac{m_1(\mathbf{T}^n)}{m_2(\mathbf{T}^n)} \ge C_u \min\left(v_n^{-(d_1-\alpha_2)}, v_n^{-(d_1-\tau_2)}\right)$$

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Consistency theorem

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$$\inf\{|\mu_0-\mu_2(\theta_2)|; \theta_2 \in \Theta_2\} = \inf\{|\mu_0-\mu_1(\theta_1)|; \theta_1 \in \Theta_1\} = 0,$$

Bayes factor

$$B_{12}^{\mathsf{T}} = \mathsf{O}(v_n^{-(d_1-d_2)})$$

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irrespective of the true model. It is inconsistent since it always picks the model with the smallest dimension

If \mathbb{P}^n belongs to one of the two models and if μ_0 cannot be attained by the other one :

$$\begin{split} 0 &= \min\left(\inf\{|\mu_0 - \mu_i(\theta_i)|; \theta_i \in \Theta_i\}, i = 1, 2\right) \\ &< \max\left(\inf\{|\mu_0 - \mu_i(\theta_i)|; \theta_i \in \Theta_i\}, i = 1, 2\right), \end{split}$$

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then the Bayes factor B_{12}^{T} is consistent

Bayes factor driven by the means $\mu_i(\theta_i)$ and the relative position of μ_0 wrt both sets { $\mu_i(\theta_i)$; $\theta_i \in \Theta_i$ }, i = 1, 2.

For ABC, this implies the most likely statistics \mathbf{T}^n are ancillary statistics with different mean values under both models

Else, if \mathbf{T}^n asymptotically depends on some of the parameters of the models, it is possible that there exists $\theta_i \in \Theta_i$ such that $\mu_i(\theta_i) = \mu_0$ even though model \mathfrak{M}_1 is misspecified

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Toy example: Laplace versus Gauss [1]

lf

$$\mathbf{T}^{n} = n^{-1} \sum_{i=1}^{n} X_{i}^{4}, \quad \mu_{1}(\theta) = 3 + \theta^{4} + 6\theta^{2}, \quad \mu_{2}(\theta) = 6 + \cdots$$

and the true distribution is Laplace with mean $\theta_0 = 1$, under the Gaussian model the value $\theta^* = 2\sqrt{3} - 3$ also leads to $\mu_0 = \mu(\theta^*)$ [here $d_1 = d_2 = d = 1$]
Toy example: Laplace versus Gauss [1]

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© A Bayes factor associated with such a statistic is inconsistent

Toy example: Laplace versus Gauss [1]

lf

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Toy example: Laplace versus Gauss [1]

lf

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Fourth moment

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Toy example: Laplace versus Gauss [0]

When

$$\mathbf{T}(\mathbf{y}) = \left\{ \bar{y}_n^{(4)}, \bar{y}_n^{(6)} \right\}$$

and the true distribution is Laplace with mean $\theta_0 = 0$, then $\mu_0 = 6$, $\mu_1(\theta_1^*) = 6$ with $\theta_1^* = 2\sqrt{3} - 3$ $[d_1 = 1 \text{ and } d_2 = 1/2]$

thus

$$B_{12} \sim n^{-1/4} \rightarrow 0$$
: consistent

Under the Gaussian model $\mu_0 = 3$, $\mu_2(\theta_2) \ge 6 > 3 \ \forall \theta_2$

 $B_{12} \rightarrow +\infty$: consistent

Toy example: Laplace versus Gauss [0]

When

$$\mathbf{T}(\mathbf{y}) = \left\{ \bar{y}_n^{(4)}, \bar{y}_n^{(6)} \right\}$$

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: consistent

Toy example: Laplace versus Gauss [0]

When

$$\mathbf{T}(\mathbf{y}) = \left\{ \bar{y}_n^{(4)}, \bar{y}_n^{(6)} \right\}$$



Fourth AND sixth moments

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After running ABC, i.e. creating *reference tables* of (θ_i, x_i) from both joints, straightforward derivation of ABC estimates $\hat{\theta}_1$ and $\hat{\theta}_2$. Evaluation of $\mathbb{E}^1_{\hat{\theta}_1}[\mathcal{T}(X)]$ and $\mathbb{E}^2_{\hat{\theta}_2}[\mathcal{T}(X)]$ allows for detection of different means under both models via Monte Carlo simulations

Toy example: Laplace versus Gauss



Normalised χ^2 without and with mad

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A population genetic illustration

Two populations (1 and 2) having diverged at a fixed known time in the past and third population (3) which diverged from one of those two populations (models 1 and 2, respectively).

Observation of 50 diploid individuals/population genotyped at 5, 50 or 100 independent microsatellite loci.



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Observation of 50 diploid individuals/population genotyped at 5, 50 or 100 independent microsatellite loci.

Stepwise mutation model: the number of repeats of the mutated gene increases or decreases by one. Mutation rate μ common to all loci set to 0.005 (single parameter) with uniform prior distribution

 $\mu \sim \mathcal{U}[0.0001, 0.01]$

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Summary statistics associated to the $(\delta_{\mu})^2$ distance

 $x_{l,i,j}$ repeated number of allele in locus l = 1, ..., L for individual i = 1, ..., 100 within the population j = 1, 2, 3. Then

$$(\delta_{\mu})_{j_{1},j_{2}}^{2} = \frac{1}{L} \sum_{l=1}^{L} \left(\frac{1}{100} \sum_{i_{1}=1}^{100} x_{l,i_{1},j_{1}} - \frac{1}{100} \sum_{i_{2}=1}^{100} x_{l,i_{2},j_{2}} \right)^{2}$$

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For two copies of locus *I* with allele sizes x_{l,i,j_1} and x_{l,i',j_2} , most recent common ancestor at coalescence time τ_{j_1,j_2} , gene genealogy distance of $2\tau_{j_1,j_2}$, hence number of mutations Poisson with parameter $2\mu\tau_{j_1,j_2}$. Therefore,

$$\mathbb{E}\left\{\left(x_{l,i,j_{1}}-x_{l,i',j_{2}}\right)^{2}|\tau_{j_{1},j_{2}}\right\}=2\mu\tau_{j_{1},j_{2}}$$

and

$$\begin{array}{c|c} & \text{Model 1} & \text{Model 2} \\ \hline \mathbb{E} \left\{ (\delta_{\mu})_{1,2}^2 \right\} & 2\mu_1 t' & 2\mu_2 t' \\ \hline \mathbb{E} \left\{ (\delta_{\mu})_{1,3}^2 \right\} & 2\mu_1 t & 2\mu_2 t' \\ \hline \mathbb{E} \left\{ (\delta_{\mu})_{2,3}^2 \right\} & 2\mu_1 t' & 2\mu_2 t \end{array}$$

Thus,

- ▶ Bayes factor based only on distance $(\delta_{\mu})_{1,2}^2$ not convergent: if $\mu_1 = \mu_2$, same expectation
- ► Bayes factor based only on distance $(\delta_{\mu})_{1,3}^2$ or $(\delta_{\mu})_{2,3}^2$ not convergent: if $\mu_1 = 2\mu_2$ or $2\mu_1 = \mu_2$ same expectation
- if two of the three distances are used, Bayes factor converges: there is no (μ₁, μ₂) for which all expectations are equal

A population genetic illustration



Posterior probabilities that the data is from model 1 for 5, 50 and 100 loci

When \mathfrak{M}_1 submodel of \mathfrak{M}_2 , and if the true distribution belongs to the smaller model \mathfrak{M}_1 , Bayes factor is of order

$$v_n^{-(d_1-d_2)}$$

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When \mathfrak{M}_1 submodel of \mathfrak{M}_2 , and if the true distribution belongs to the smaller model \mathfrak{M}_1 , Bayes factor is of order

$$v_n^{-(d_1-d_2)}$$

If summary statistic only informative on a parameter that is the same under both models, i.e if $d_1 = d_2$, then

© the Bayes factor is not consistent

When \mathfrak{M}_1 submodel of \mathfrak{M}_2 , and if the true distribution belongs to the smaller model \mathfrak{M}_1 , Bayes factor is of order

$$v_n^{-(d_1-d_2)}$$

Else, $d_1 < d_2$ and Bayes factor is going to ∞ under \mathfrak{M}_1 . If true distribution not in \mathfrak{M}_1 , then

© Bayes factor is consistent only if $\mu_1 \neq \mu_2 = \mu_0$

- Model selection feasible with ABC
- Choice of summary statistics is paramount
- \blacktriangleright At best, ABC $\rightarrow \pi(. \mid \textbf{T}(y))$ which concentrates around μ_0

- For estimation : $\{\theta; \mu(\theta) = \mu_0\} = \theta_0$
- For testing $\{\mu_1(\theta_1), \theta_1 \in \Theta_1\} \cap \{\mu_2(\theta_2), \theta_2 \in \Theta_2\} = \emptyset$

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Empirical likelihood (EL)

Introduction

ABC

ABC as an inference machine

ABC for model choice

Model choice consistency

ABC_{el} ABC and EL Composite likelihood Illustrations



Empirical likelihood (EL)

▶ help!

Dataset x made of n independent replicates $x = (x_1, \ldots, x_n)$ of some $X \sim F$

Generalized moment condition model

$$\mathbb{E}_{F}\big[h(X,\phi)\big]=0,$$

where h is a known function, and ϕ an unknown parameter

Corresponding empirical likelihood $L_{el}(\phi|x) = \max_{p} \prod_{i=1}^{n} p_{i}$ for all p such that $0 \leq p_{i} \leq 1$, $\sum_{i} p_{i} = 1$, $\sum_{i} p_{i}h(x_{i}, \phi) = 0$.

[Owen, 1988, Bio'ka; Owen, 2001]

Empirical likelihood (EL)

▶ help!

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Corresponding empirical likelihood

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[Owen, 1988, Bio'ka; Owen, 2001]

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Convergence of EL [3.4]

Theorem 3.4 Let X, Y_1, \ldots, Y_n be independent rv's with common distribution F_0 . For $\theta \in \Theta$, and the function $h(X, \theta) \in \mathbb{R}^s$, let $\theta_0 \in \Theta$ be such that

 $\operatorname{Var}(h(Y_i, \theta_0))$

is finite and has rank q > 0. If θ_0 satisfies

 $\mathbb{E}(h(X,\theta_0))=0,$

then

$$-2\log\left(\frac{L_{\rm el}(\theta_0|Y_1,\ldots,Y_n)}{n^{-n}}\right) \to \chi^2_{(q)}$$

in distribution when $n \to \infty$.

[Owen, 2001]

"... The interesting thing about Theorem 3.4 is what is not there. It includes no conditions to make $\hat{\theta}$ a good estimate of θ_0 , nor even conditions to ensure a unique value for θ_0 , nor even that any solution θ_0 exists. Theorem 3.4 applies in the just determined, over-determined, and under-determined cases. When we can prove that our estimating equations uniquely define θ_0 , and provide a consistent estimator $\hat{\theta}$ of it, then confidence regions and tests follow almost automatically through Theorem 3.4.".

[Owen, 2001]

Act as if EL was an exact likelihood

[Lazar, 2003]

for $i = 1 \rightarrow N$ do generate ϕ_i from the prior distribution $\pi(\cdot)$ set the weight $\omega_i = L_{el}(\phi_i | x_{obs})$ end for return (ϕ_i, ω_i) , $i = 1, \dots, N$

Output weighted sample of size N

Raw ABC_{el}sampler

Act as if EL was an exact likelihood

[Lazar, 2003]

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Performance evaluated through effective sample size

$$extsf{ESS} = 1 \Big/ \sum_{i=1}^{N} \left\{ \left. \omega_i \right/ \sum_{j=1}^{N} \omega_j
ight\}^2$$

Raw ABC_{el}sampler

Act as if EL was an exact likelihood

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More advanced algorithms can be adapted to EL:
 E.g., adaptive multiple importance sampling (AMIS) of
 Cornuet et al. to speed up computations

[Cornuet et al., 2012]

Moment condition in population genetics?

EL does not require a fully defined and often complex (hence debatable) parametric model

Main difficulty

Derive a constraint

$$\mathbb{E}_{F}[h(X, \phi)] = 0,$$

on the parameters of interest ϕ when X is made of the genotypes of the sample of individuals at a given locus

E.g., in phylogeography, φ is composed of

- dates of divergence between populations,
- ratio of population sizes,
- mutation rates, etc.

None of them are moments of the distribution of the allelic states of the sample

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 \bigcirc *h* made of pairwise composite scores (whose zero is the pairwise maximum likelihood estimator)

Pairwise composite likelihood

The intra-locus pairwise likelihood

$$\ell_2(\mathbf{x}_{\mathbf{k}}|\boldsymbol{\Phi}) = \prod_{i < j} \ell_2(\mathbf{x}_k^i, \mathbf{x}_k^j | \boldsymbol{\Phi})$$

with x_k^1, \ldots, x_k^n : allelic states of the gene sample at the k-th locus

The pairwise score function

$$abla_{\mathrm{d}} \log \ell_2(\mathbf{x_k} | \mathrm{d}) = \sum_{i < j}
abla_{\mathrm{d}} \log \ell_2(\mathbf{x}_k^i, \mathbf{x}_k^j | \mathrm{d})$$

Composite likelihoods are often much narrower than the original likelihood of the model

Safe with EL because we only use position of its mode

Pairwise likelihood: a simple case

Assumptions

- sample ⊂ closed, panmictic population at equilibrium
- marker: microsatellite
- mutation rate: $\theta/2$

if x_k^i et x_k^j are two genes of the sample,

 $\ell_2(x_k^i,x_k^j|\theta)$ depends only on $\delta=x_k^i-x_k^j$

 $\ell_{2}(\delta|\theta) = \frac{1}{\sqrt{1+2\theta}} \rho(\theta)^{|\delta|}$ with $\rho(\theta) = \frac{\theta}{1+\theta+\sqrt{1+2\theta}}$ Pairwise score function $\partial_{\theta} \log \ell_{2}(\delta|\theta) = \frac{1}{1+2\theta} + \frac{|\delta|}{\theta\sqrt{1+2\theta}}$

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$$\begin{split} \ell_{2}(\delta|\theta) &= \frac{1}{\sqrt{1+2\theta}} \rho\left(\theta\right)^{|\delta|} \\ \text{with} \\ \rho(\theta) &= \frac{\theta}{1+\theta+\sqrt{1+2\theta}} \\ \text{Pairwise score function} \end{split}$$

 $\partial_{\theta} \log \ell_2(\delta|\theta) =$ $-\frac{1}{1+2\theta} + \frac{|\delta|}{\theta\sqrt{1+2\theta}}$

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Pairwise likelihood: 2 diverging populations



Assumptions

 τ: divergence date of pop. a and b

• $\theta/2$: mutation rate Let x_k^i and x_k^j be two genes coming resp. from pop. *a* and *b* Set $\delta = x_k^i - x_k^j$. Then $\ell_2(\delta|\theta, \tau) = \frac{e^{-\tau\theta}}{\sqrt{1+2\theta}} \sum_{k=-\infty}^{+\infty} \rho(\theta)^{|k|} I_{\delta-k}(\tau\theta).$ where $I_n(z)$ *n*th-order modified Bessel function of the first kind

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Pairwise likelihood: 2 diverging populations



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A 2-dim score function

$$\begin{split} & \partial_\tau \log \ell_2(\delta|\theta,\tau) = -\theta + \\ & \frac{\theta}{2} \frac{\ell_2(\delta-1|\theta,\tau) + \ell_2(\delta+1|\theta,\tau)}{\ell_2(\delta|\theta,\tau)} \end{split}$$

$$\begin{aligned} &\partial_{\theta} \log \ell_{2}(\delta|\theta,\tau) = \\ &-\tau - \frac{1}{1+2\theta} + \frac{q(\delta|\theta,\tau)}{\ell_{2}(\delta|\theta,\tau)} + \\ &\frac{\tau}{2} \frac{\ell_{2}(\delta-1|\theta,\tau) + \ell_{2}(\delta+1|\theta,\tau)}{\ell_{2}(\delta|\theta,\tau)} \end{aligned}$$

where

$$q(\delta|\theta,\tau) := \\ \frac{\mathrm{e}^{-\tau\theta}}{\sqrt{1+2\theta}} \frac{\rho'(\theta)}{\rho(\theta)} \sum_{k=-\infty}^{\infty} |k| \rho(\theta)^{|k|} I_{\delta-k}(\tau\theta)$$

Example: normal posterior



Sample sizes are of 25 (column 1), 50 (column 2) and 75 (column 3) observations
Example: normal posterior



Sample sizes are of 25 (column 1), 50 (column 2) and 75 (column 3) observations

Example: Superposition of gamma processes

Example of superposition of *N* renewal processes with waiting times τ_{ij} (i = 1, ..., M), $j = 1, ...) \sim \mathcal{G}(\alpha, \beta)$, when *N* is unknown. Renewal processes

$$\zeta_{i1} = \tau_{i1}, \ \zeta_{i2} = \zeta_{i1} + \tau_{i2}, \ \dots$$

with observations made of first *n* values of the ζ_{ij} 's,

$$z_1 = \min\{\zeta_{ij}\}, \ z_2 = \min\{\zeta_{ij}; \zeta_{ij} > z_1\}, \ \ldots,$$

ending with

$$z_n = \min{\{\zeta_{ij}; \zeta_{ij} > z_{n-1}\}}.$$
[Cox & Kartsonaki, B'ka, 2012]

Example: Superposition of gamma processes (ABC)

Interesting testing ground for ABC_{el} since data (z_t) neither iid nor Markov

Recovery of an iid structure by

- 1. simulating a pseudo-dataset, $(z_1^{\star}, \dots, z_n^{\star})$, as in regular ABC,
- 2. deriving sequence of indicators (v_1, \ldots, v_n) , as

$$z_1^{\star} = \zeta_{\nu_1 1}, \ z_2^{\star} = \zeta_{\nu_2 j_2}, \ \dots$$

3. exploiting that those indicators are distributed from the prior distribution on the v_t 's leading to an iid sample of $\mathcal{G}(\alpha, \beta)$ variables



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 exploiting that those indicators are distributed from the prior distribution on the ν_t's leading to an iid sample of G(α, β) variables



Pop'gen': A first experiment



Dataset:

- 50 genes per populations,
- 100 microsat. loci

Assumptions:

- N_e identical over all populations
- $\blacktriangleright \ \varphi = (\log_{10} \theta, \log_{10} \tau)$
- uniform prior over $(-1., 1.5) \times (-1., 1.)$

Comparison of the original ABC with ABC_{el}

ESS=7034





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Comparison of the original ABC with ABC_{el}

ESS=7034





ABC vs. $\mathsf{ABC}_{\mathsf{el}}$ on 100 replicates of the 1st experiment

Accuracy:

	log	ξ ₁₀ θ	$\log_{10} \tau$		
	ABC	ABC _{el}	ABC	ABC _{el}	
(1)	0.097	0.094	0.315	0.117	
(2)	0.071	0.059	0.272	0.077	
(3)	0.68	0.81	1.0	0.80	

(1) Root Mean Square Error of the posterior mean

- (2) Median Absolute Deviation of the posterior median
- (3) Coverage of the credibility interval of probability 0.8

Computation time: on a recent 6-core computer (C++/OpenMP)

- ABC \approx 4 hours
- ► $ABC_{el} \approx 2 \text{ minutes}$



Dataset:

- ▶ 50 genes per populations,
- 100 microsat. loci

Assumptions:

- *N_e* identical over all populations
- non-informative uniform

Comparison of the original ABC with $\mbox{ABC}_{\rm el}$

histogram = ABC_{el} curve = original ABC vertical line = "true" parameter

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- ▶ 50 genes per populations,
- 100 microsat. loci

Assumptions:

- N_e identical over all populations
- $\phi =$ $(\log_{10} \theta, \log_{10} \tau_1, \log_{10} \tau_2)$ pon-informative uniform

Comparison of the original ABC with ABC_{el}



histogram = ABC_{el} curve = original ABC vertical line = "true" parameter



Dataset:

- ▶ 50 genes per populations,
- 100 microsat. loci

Assumptions:

- *N_e* identical over all populations
- ► $\phi =$ (log₁₀ θ , log₁₀ τ_1 , log₁₀ τ_2) ► non-informative uniform

Comparison of the original ABC with ABC_{el}



histogram = ABC_{el} curve = original ABC vertical line = "true" parameter

ABC vs. $\mathsf{ABC}_{\mathsf{el}}$ on 100 replicates of the 2nd experiment

Accuracy:

	$\log_{10} \theta$		$\log_{10} \tau_1$		$\log_{10} \tau_2$	
	ABC	ABC _{el}	ABC	ABC _{el}	ABC	ABC _{el}
(1)	.0059	.0794	.472	.483	29.3	4.76
(2)	.048	.053	.32	.28	4.13	3.36
(3)	.79	.76	.88	.76	.89	.79

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- (1) Root Mean Square Error of the posterior mean
- (2) Median Absolute Deviation of the posterior median
- (3) Coverage of the credibility interval of probability 0.8

Computation time: on a recent 6-core computer (C++/OpenMP)

- ABC \approx 6 hours
- ► $ABC_{el} \approx 8$ minutes

On large datasets, $\mathsf{ABC}_{\mathsf{el}}$ gives more accurate results than ABC

ABC simplifies the dataset through summary statistics Due to the large dimension of x, the original ABC algorithm estimates

 $\pi\left(\theta \mid \eta(x_{\text{obs}})\right),$

where $\eta(x_{obs})$ is some (non-linear) projection of the observed dataset on a space with smaller dimension \hookrightarrow Some information is lost

ABC_{el}**simplifies the model** through a generalized moment condition model.

 \hookrightarrow Here, the moment condition model is based on pairwise composition likelihood

Personal Call

My son Joachim, 19, is looking for a summer internship as a salesman in the US in the summer 2013, requirement of his business school (léseg) curriculum. Any help in this matter appreciated!



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