Some recent advances on Approximate Bayesian Computation techniques

Jean-Michel Marin

University of Montpellier, CNRS
Alexander Grothendieck Montpellier Institute

9 December 2017

Thanks

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- Judith, Natesh, ...

Introduction

Bayesian parametric paradigm

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Likelihood function $f(\mathbf{y}|\theta)$ expensive or impossible to calculate

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Extremely difficult to sample from the posterior distribution

$$\pi(\theta|\mathbf{y}) \propto \pi(\theta) f(\mathbf{y}|\theta)$$

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If, with Christian, we work on ABC methods, we can be very grateful to our biologist colleagues!

Introduction

- some methodological aspects of ABC

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- our ABC random forests proposal

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- ABC and PAC-Bayes

Methodological aspects of ABC
Likelihood-free rejection sampler

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Likelihood-free rejection sampler

Rubin (1984) The Annals of Statistics
Tavaré et al. (1997) Genetics
Pritchard et al. (1999) Mol. Biol. Evol.

1) Set $i = 1$

Methodological aspects of ABC
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5) If $i \leqslant N$, return to 2)
```

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ABC target

$$\pi_\epsilon(\theta|\mathbf{y}) = \frac{\int \pi(\theta) f(\mathbf{z}|\theta) \mathbb{I}(\mathbf{z} \in A_{\epsilon,\mathbf{y}}) \mathrm{d}\mathbf{z}}{\int_{A_{\epsilon,\mathbf{y}} \times \Theta} \pi(\theta) f(\mathbf{z}|\theta) \mathrm{d}\mathbf{z}\mathrm{d}\theta}$$

$A_{\epsilon,\mathbf{y}} = \{\mathbf{z} | d(\eta(\mathbf{z}), \eta(\mathbf{y})) \leqslant \epsilon\}$ the acceptance set

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$$d(z,y) = |z-y|$$

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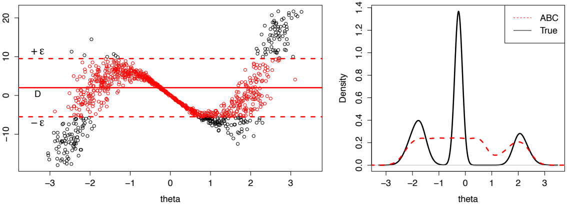

$$\epsilon = 7.5$$

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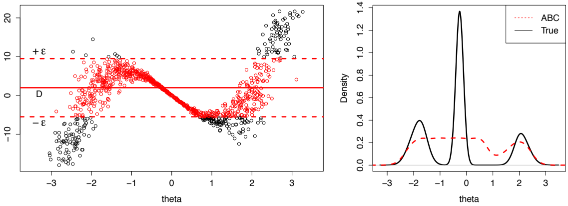

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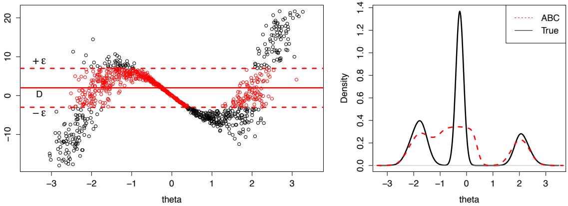

$\epsilon = 5$

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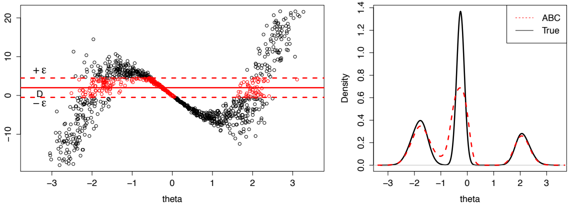

$\epsilon = 2.5$

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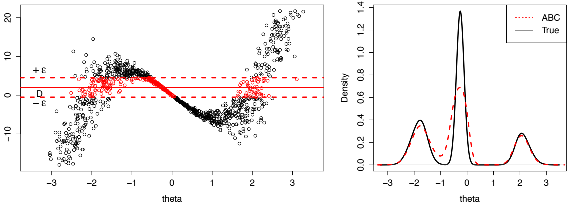

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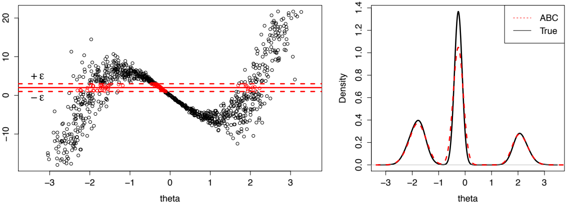

$\epsilon = 1$

Methodological aspects of ABC
A k-NN approximation

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ϵ corresponds to a quantile of the distances

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New insights into Approximate Bayesian Computation
Biau, Cérou, Guyader (2015) Annales de l'IHP

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- intuitive

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- simple to implement
- embarrassingly parallelisable

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New insights into Approximate Bayesian Computation
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- intuitive
- simple to implement
- embarrassingly parallelisable
- BUT curse of dimensionality: most of the simulations are at the boundary of the space as the number of summary statistics increases

Methodological aspects of ABC
Two views of the ABC approximation

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$\Longrightarrow$ **Wilkinson (2013) SAGMB** shows that ABC is exact but for a different model to that intended

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Two views of the ABC approximation

$\Longrightarrow$ **Wilkinson (2013) SAGMB** shows that ABC is exact but for a different model to that intended

$\Longrightarrow$ **Blum (2010) JASA** emphasizes that ABC is a kernel smoothing approximation of the likelihood function

$$\pi_\epsilon(\theta|\mathbf{y}) = \frac{\int \pi(\theta) f(\mathbf{z}|\theta)\mathbb{I}(\mathbf{z} \in A_{\epsilon,\mathbf{y}})\mathrm{d}\mathbf{z}}{\int_{A_{\epsilon,\mathbf{y}}\times\Theta} \pi(\theta) f(\mathbf{z}|\theta)\mathrm{d}\mathbf{z}\mathrm{d}\theta}$$

$$= \frac{\pi(\theta)\int f(\mathbf{z}|\theta) K(d(\eta(\mathbf{z}),\eta(\mathbf{y})))\mathrm{d}\mathbf{z}}{\int \pi(\theta) f(\mathbf{z}|\theta) K(d(\eta(\mathbf{z}),\eta(\mathbf{y})))\mathrm{d}\mathbf{z}\mathrm{d}\theta}$$

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More efficient algorithms

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Simulate all the θ's particles using the prior distribution

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$\Longrightarrow$ very inefficient

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various sequential Monte Carlo algorithms have been constructed as an alternative

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Sisson et al. (2007) PNAS
Beaumont, Cornuet, Marin and Robert (2009) Biometrika
Del Moral et al. (2012) Statistics and Computing
Marin, Pudlo and Sedki (2012) IEEE Proceedings of WSC
Filippi et al. (2013) SAGMB

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More efficient algorithms

The key idea is to decompose the difficult problem of sampling from $\pi_\epsilon(\theta, z|y)$ into a series of simpler subproblems

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Time 0 sampling from $\pi_{\epsilon_0}(\theta, \mathbf{z}|\mathbf{y})$ with large ϵ_0

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Likelihood free MCMC sampler **Majoram et al. (2003) PNAS**

Methodological aspects of ABC
Regression adjustments

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Beaumont et al. (2002) Genetics
local linear regression adjustment of the parameter values

Methodological aspects of ABC
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Beaumont et al. (2002) Genetics
local linear regression adjustment of the parameter values

Blum and Francois (2010) Statistics and Computing
heteroscedastic models, feed-forward neural networks

Methodological aspects of ABC
Summary statistics

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Best subset selection

- **Joyce and Marjoram (2008) SAGMB**, τ-sufficiency
- **Nunes and Balding (2010) SAGMB**, entropy

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Summary statistics

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Projection

- **Fearnhead and Prangle (2012) JRSS B** introduce semi-automatic ABC

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Regularization techniques

- **Blum, Nunes, Prangle and Fearnhead (2013) Statistical Science** use ridge regression
- **Saulnier, Gascuel, Alizon (2017) Plos Computational Biology** use LASSO

Methodological aspects of ABC
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A k-NN approximation of the posterior probabilities

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ABC likelihood-free methods for model choice in Gibbs random fields **Grelaud, Robert, Marin, Rodolphe and Taly (2009) Bayesian Analysis**

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Lack of confidence in approximate Bayesian computation model choice Robert, Cornuet, Marin, Pillai (2011) PNAS

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Relevant statistics for Bayesian model choice Marin, Pillai, Robert, Rousseau (2014) JRSS B

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We investigate some ABC model choice techniques that use others machine learning procedures

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Estimation of demo-genetic model probabilities with Approximate Bayesian Computation using linear discriminant analysis on summary statistics **Estoup, Lombaert, Marin, Guillemaud, Pudlo, Robert, Cornuet (2012) Molecular Ecology**

Methodological aspects of ABC
Sofwares

abc R package several ABC algorithms for performing parameter estimation and model selection

abctools R package tuning ABC analyses
https://journal.r-project.org/archive/2015-2/nunes-prangle.pdf

abcrf R package ABC via random forests

EasyABC R package several algorithms for performing efficient ABC sampling schemes, including 4 sequential sampling schemes and 3 MCMC schemes

Methodological aspects of ABC

Sofwares

DIY-ABC software performs parameter estimation and model selection for population genetics models

ABC-SysBio python package parameter inference and model selection for dynamical systems

ABCtoolbox programs various ABC algorithms including rejection sampling, MCMC without likelihood, a particle-based sampler, and ABC-GLM

PopABC software package for inference of the pattern of demographic divergence, coalescent simulation, bayesian model choice

Methodological aspects of ABC
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Infering population history with DIY ABC: a user-friedly approach Approximate Bayesian Computation **Cornuet, Santos, Beaumont, Robert, Marin, Balding, Guillemaud, Estoup (2008) Bioinformatics**

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Infering population history with DIY ABC: a user-friedly approach Approximate Bayesian Computation **Cornuet, Santos, Beaumont, Robert, Marin, Balding, Guillemaud, Estoup (2008) Bioinformatics**

DIYABC v2.0: a software to make Approximate Bayesian Computation inferences about population history using Single Nucleotide Polymorphism, DNA sequence and microsatellite data **Cornuet, Pudlo, Veyssier, Dehne-Garcia, Gautier, Leblois, Marin, Estoup (2014) Bioinformatics**

Methodological aspects of ABC Sofwares

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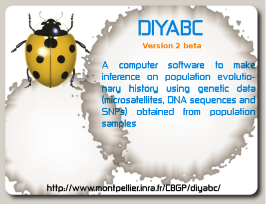

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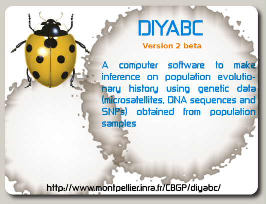

Asian ladybug

Methodological aspects of ABC Sofwares

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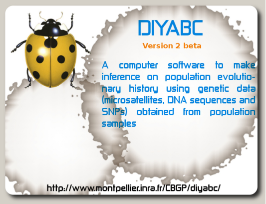

DIYABC

Version 2 beta

A computer software to make inference on population evolutionary history using genetic data (microsatellites, DNA sequences and SNPs) obtained from population samples

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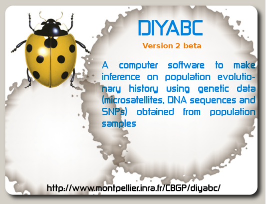

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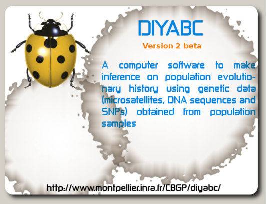

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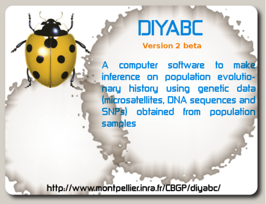

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Pigmies populations
Four human populations, to study the out-of-Africa colonization

Methodological aspects of ABC
Frontline news from population geneticists country

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DIYABC (2014) paper has now around 300 citations

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- sequential methods are difficult to calibrate and do not give reproducible results
- post hoc adjustments are crucial but they underestimate the amount of uncertainty
- available techniques to select the summary statistics do not give reproducible results

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Despite all these works, two major difficulties

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Despite all these works, two major difficulties

- to ensure reliability of the method, the number of simulations should be large
- choice of the summaries statistics is still a problem

Methodological aspects of ABC
Use modern machine learning tools

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Exploiting a large number of summary statistics is not an issue for some machine learning methods

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Idea: learn on a huge reference table using random forests

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Analysis of a random forest model
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Consistency of random forests
Scornet, Biau, Vert (2015) The Annals of Statistics

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This work stands at the interface between Bayesian inference and machine learning techniques

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As an alternative, Papamakarios and Murray (2016) propose to approximate the whole posterior distribution by using Mixture Density Networks (MDN, Bishop, 1994)

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Fast e-free Inference of Simulation Models with Bayesian Conditional Density Estimation
Papamakarios and Murray (2016) NIPS

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The MDN strategy consists in using Gaussian mixture models with parameters calibrated thanks to neural networks

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Idea: iteratively learn an efficient proposal prior (approximating the posterior distribution), then to use this proposal to train the posterior, both steps making use of MDN

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The MDN strategy consists in using Gaussian mixture models with parameters calibrated thanks to neural networks

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The number of mixture components and the number of hidden layers of the networks require calibration

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Use modern machine learning tools

Deep Learning for Population Genetic Inference
Sheehan and Song (2016) PLOS Computational Biology

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Use modern machine learning tools

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Deep learning makes use of multilayer neural networks to learn a feature-based function from the input (hundreds of correlated summary statistics) to the output (population genetic parameters of interest).

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Deep learning makes use of multilayer neural networks to learn a feature-based function from the input (hundreds of correlated summary statistics) to the output (population genetic parameters of interest).

Unsupervised pretraining using autoencoders very interesting, but requires a lot of calibration

ABC random forests
Model choice

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Reliable ABC model choice via random forests Pudlo, Marin, Estoup, Cornuet, Gauthier and Robert (2016) Bioinformatics

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Input ABC reference table involving model index and summary statistics, table used as learning set

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For $i = 1, \dots, M$

- **a)** Generate m_i from the prior $\pi(\mathscr{M} = m)$
- **b)** Generate θ'_{m_i} from the prior $\pi_{m_i}(\cdot)$
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Output a random forest classifier to infer model indexes $\widehat{m(\eta(\mathbf{y}))}$

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Random forest predicts a MAP model index, from the observed dataset

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frequency of trees associated with majority model is no proper substitute to the true posterior probability

ABC random forests
Model choice

Estimate of the posterior probability of the selected model

$$\mathbb{P}[\mathscr{M} = \widehat{m(\eta(\mathbf{y}))} | \eta(\mathbf{y})]$$

random comes from $\mathscr{M}$ (bayesian)!

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Model choice

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$$\mathbb{P}[\mathscr{M} = \widehat{m(\eta(\mathbf{y}))}|\eta(\mathbf{y})] = 1 - \mathbb{E}\left[\mathbb{I}(\mathscr{M} \neq \widehat{m(\eta(\mathbf{y}))})|\eta(\mathbf{y})\right]$$

ABC random forests
Model choice

A second random forest in regression

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A second random forest in regression

1) compute the value of $\mathbb{I}(\mathscr{M} \neq \widehat{\mathrm{m}(\eta(\mathbf{z}))})$ for the trained random forest $\hat{\mathrm{m}}$ and for all terms in the ABC reference table using the out-of-bag classifiers

ABC random forests
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on same reference table out-of-bag magic trick avoid overfitting!

ABC random forests
Parameter inference

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ABC random forests for Bayesian parameter inference **Raynal, Marin, Pudlo, Ribatet, Robert and Estoup (2017) Preprint reviewed and recommended by Peer Community In Evolutionary Biology**

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Output some regression RF predictors to infer posterior expectations, quantiles, variances and covariances

ABC random forests
Parameter inference

Expectations Construct d regression RF, one per dimension

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Quantiles very nice trick to estimate the cdf, no new forest
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Covariances new forests for which the responses variables are the products of out-of-bag errors

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We constructed forests able to estimate everywhere in the space of summary statistics but we are interested only in one point, the observed dataset

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construct local random forest, thesis of Louis Raynal

ABC and PAC-Bayes

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Bayesian and PAC-Bayesian frameworks have learned from each other

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PAC-Bayesian Theory Meets Bayesian Inference
Germain, Bach, Lacoste, Lacoste-Julien (2016) NIPS

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The Safe Bayesian: Learning the Learning Rate via the Mixability Gap Grünwald (2012) ALT

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The ABC toolbox seems unable to bring anything to the PAC-Bayesian framework

ABC and PAC-Bayes

On the other hand

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On the other hand

ABC concerns are machine learning concerns

ABC and PAC-Bayes

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Use PAC-Bayes learning on the ABC reference table

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Contrary to the standard context

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ABC and PAC-Bayes

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Probably approximate Bayesian computation: nonasymptotic convergence of ABC under misspecification Ridgway (2017) Preprint

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Convergence of the ABC posterior under model misspecification
Use of concentration inequalities, PAC-Bayesian analysis

End

Yesterday with Benjamin and Pascal in a Chinese restaurant, the bill arrives... with a cake and a hidden message:

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This year, take comfort in your rituals, but be open to new experiences

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A clear sign, I should try to use some PAC-Bayesian results

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Thank you very much for your attention