Approximate Bayesian Computation

Michael Gutmann

https://sites.google.com/site/michaelgutmann

University of Helsinki and Aalto University

December 2015

Content

Two parts:

- 1. The basics of approximate Bayesian computation (ABC)
- 2. ABC methods used in practice

What is ABC?

A set of methods for approximate Bayesian inference which can be used whenever sampling from the model is possible.

Michael Gutmann ABC 2 / 47

Part I

Basic ABC

Recap of Bayesian inference

- ▶ The ingredients for Bayesian parameter inference:
 - ▶ Observed data $\mathbf{y}^o \in \mathcal{Y} \subset \mathbb{R}^n$
 - A statistical model for the data generating process, $p_{y|\theta}$, parametrized by $\theta \in \Theta \subset \mathbb{R}^d$.
 - A prior probability density function (pdf) for the parameters θ , p_{θ}
- ▶ The mechanics of Bayesian inference:

$$p_{\theta|\mathbf{y}}(\theta|\mathbf{y}^{o}) \propto p_{\mathbf{y}|\theta}(\mathbf{y}^{o}|\theta) \qquad \qquad \times p_{\theta}(\theta)$$
 (1)

posterior
$$\propto$$
 likelihood function \times prior (2)

Often written without subscripts ("function overloading")

$$p(\theta|\mathbf{y}^o) \propto p(\mathbf{y}^o|\theta) \times p(\theta)$$
 (3)

Likelihood function

- ▶ Likelihood function: $L(\theta) = p(\mathbf{y}^{o}|\theta)$
 - For discrete random variables:

$$L(\theta) = p(\mathbf{y}^{o}|\theta) = \Pr(\mathbf{y} = \mathbf{y}^{o}|\theta)$$
 (4)

Probability that data generated from the model, when using parameter value θ , are equal to \mathbf{y}° .

► For continuous random variables:

$$L(\theta) = p(\mathbf{y}^{o}|\theta) = \lim_{\epsilon \to 0} \frac{\Pr(\mathbf{y} \in B_{\epsilon}(\mathbf{y}^{o})|\theta)}{\operatorname{Vol}(B_{\epsilon}(\mathbf{y}^{o}))}$$
(5)

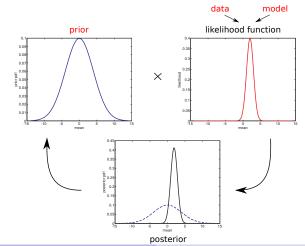
Proportional to the probability that the generated data are in a small ball $B_{\epsilon}(\mathbf{y}^{o})$ around \mathbf{y}^{o} .

 \blacktriangleright $L(\theta)$ indicates to which extent different values of the model parameters are consistent with the observed data.

$$p(heta) = rac{1}{\sqrt{2\pi \cdot 4^2}} \exp\left(-rac{ heta^2}{2 \cdot 4^2}
ight)$$

$$y^{o} = 2$$

$$p(y|\theta) = \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{(y-\theta)^2}{2}\right)$$



Different kinds of statistical models

- ▶ The statistical model was defined via the family of pdfs $p(\mathbf{y}|\boldsymbol{\theta})$.
- Statistical models can be specified in other ways as well.
- ► In this lecture: models which are specified via a mechanism (rule) for generating data
- Example: Instead of

$$p(y|\theta) = \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{(y-\theta)^2}{2}\right)$$
 (6)

we could have specified the model via

$$y = z + \theta$$
 $z = \sqrt{-2\log(\omega)}\cos(2\pi\nu)$ (7)

where ω and ν are independent random variables uniformly distributed on (0,1). Advantage?

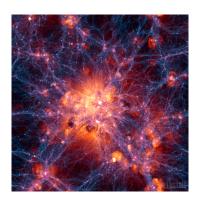
Simulator-based models

- ▶ Sampling from the model is straightforward. For example:
 - 1. Sampling ω_i and ν_i from the uniform random variables ω and ν .
 - 2. computing the nonlinear transformation $y_i = f(\omega_i, \nu_i, \theta) = \theta + \sqrt{-2\log(\omega_i)}\cos(2\pi\nu_i)$ produces samples $y_i \sim p(y|\theta)$.
- ▶ Enables direct modeling of how data are generated.
- Names for models specified via a data generating mechanism:
 - Generative models
 - ▶ Implicit models
 - Stochastic simulation models
 - Simulator-based models

Simulator-based models are used in:

- Astrophysics:
 Simulating the formation of galaxies, stars, or planets
- Evolutionary biology:
 Simulating the evolution of life
- Health science:
 Simulating the spread of an infectious disease

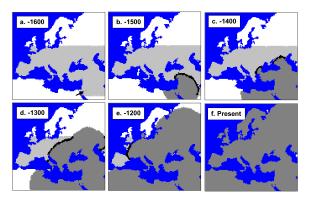




Dark matter density simulated by the Illustris collaboration (Figure from http://www.illustris-project.org)

Examples (evolutionary biology)

- Simulation of different hypothesized evolutionary scenarios
- ► Interaction between early modern humans (Homo sapiens) and their Neanderthal contemporaries in Europe

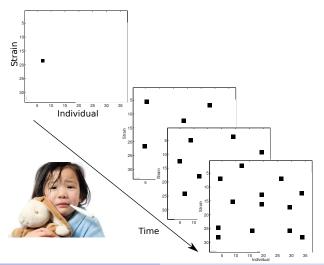


Immigration of Modern Humans into Europe from the Near East. Light gray: Neanderthal population. Dark: Homo sapiens. from (Currat and Excoffier, *Plos Biology*, 2004, 10.1371/journal.pbio.0020421). The numbers in the figures indicate generations. See also Pinhasi et al, The genetic history of Europeans, *Trends in Genetics*, 2012

10 / 47

Examples (health science)

 Simulation of bacterial transmission dynamics in child day care centers (Numminen et al, Biometrics, 2013)

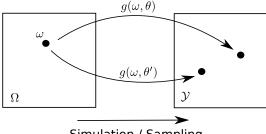


Formal definition of a simulator-based model

- Let $(\Omega, \mathcal{F}, \mathcal{P})$ be a probability space.
- A simulator-based model is a collection of (measurable) functions $g(.,\theta)$ parametrized by θ ,

$$\omega \in \Omega \mapsto \mathbf{y} = g(\omega, \theta) \in \mathcal{Y}$$
 (8)

▶ For any fixed θ , $\mathbf{y}_{\theta} = g(., \theta)$ is a random variable.



Simulation / Sampling

Advantages of simulator-based models

- Direct implementation of hypotheses of how the observed data were generated.
- ▶ Neat interface with physical or biological models of data.
- Modeling by replicating the mechanisms of nature which produced the observed/measured data. ("Analysis by synthesis")
- Possibility to perform experiments in silico.

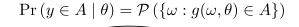
Disadvantages of simulator-based models

- ► Generally elude analytical treatment.
- ▶ Can be easily made more complicated than necessary.
- ▶ Statistical inference is difficult . . . but possible!
- This lecture is about inference for simulator-based models —

Family of pdfs induced by the simulator

- ▶ For any fixed θ , the output of the simulator $\mathbf{y}_{\theta} = g(., \theta)$ is a random variable.
- ▶ Generally, it is impossible to write down the pdf of \mathbf{y}_{θ} analytically in closed form.
- ▶ No closed-form formulae available for $p(\mathbf{y}|\boldsymbol{\theta})$.
- ▶ Simulator defines the model pdfs $p(\mathbf{y}|\theta)$ implicitly.

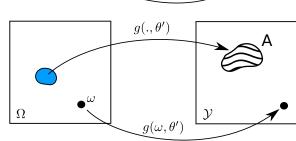
Implicit definition of the model pdfs



 $g(.,\theta)$

Parameter value θ

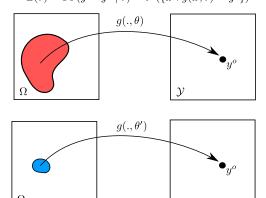
Parameter value θ'



 $g(\omega, \theta)$

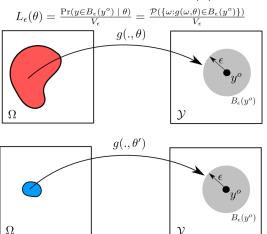
Implicit definition of the likelihood function

► The implicit definition of the model pdfs implies an implicit definition of the likelihood function. For discrete random variables: $L(\theta) = \Pr(y = y^o \mid \theta) = \mathcal{P}(\{\omega : g(\omega, \theta) = y^o\})$



Implicit definition of the likelihood function

▶ For continuous random variables: $L(\theta) = \lim_{\epsilon \to 0} L_{\epsilon}(\theta)$



Implicit definition of the likelihood function

- ► To compute the likelihood function, we need to compute the probability that the simulator generates data close to \mathbf{y}^o , $\Pr(\mathbf{y} = \mathbf{y}^o | \boldsymbol{\theta})$ or $\Pr(\mathbf{y} \in B_{\epsilon}(\mathbf{y}^o) | \boldsymbol{\theta})$
- No analytical expression available.
- ▶ But we can empirically test whether simulated data equals \mathbf{y}^o or is in $B_{\epsilon}(\mathbf{y}^o)$.
- This property will be exploited to perform inference for simulator-based models.

Exact inference for discrete random variables

- For discrete random variables, we can perform exact Bayesian inference without knowing the likelihood function.
- ▶ Idea: the posterior is obtained by conditioning $p(\theta, \mathbf{y})$ on the event $\mathbf{y} = \mathbf{y}^o$:

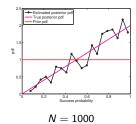
$$p(\theta|\mathbf{y}^{o}) = \frac{p(\theta, \mathbf{y}^{o})}{p(\mathbf{y}^{o})} = \frac{p(\theta, \mathbf{y} = \mathbf{y}^{o})}{p(\mathbf{y} = \mathbf{y}^{o})}$$
(9)

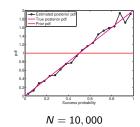
- ▶ Given tuples (θ_i, \mathbf{y}_i) where
 - $m{ heta}_i \sim p_{ heta}$ (iid from the prior)
 - $\mathbf{y}_i = g(\omega_i, \theta_i)$ (obtained by running the simulator) retain only those where $\mathbf{y}_i = \mathbf{y}^o$.
- ► The θ_i from the retained tuples are samples from the posterior $p(\theta|\mathbf{y}^o)$.

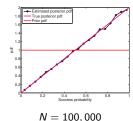
- ▶ Posterior inference of the success probability θ in a Bernoulli trial.
- ▶ Data: y^o = 1
- Prior: $p_{\theta} = 1$ on (0, 1)
- Data generating process:
 - ▶ Given $\theta_i \sim p_\theta$
 - $\sim \omega_i \sim U(0,1)$
 - $y_i = \begin{cases} 1 & \text{if } \omega_i < \theta_i \\ 0 & \text{otherwise} \end{cases}$

- % Observed data
 yobs = 1;
 % Number of samples to generate from the posterior
 N = 10000;
 % Sample from prior, uniform on (0,1)
 theta = rand(1,N);
 % Run the "simulator"
 omega = rand(1,N);
 ysim = omega<theta;
 % Check for simulated data which are equal to observed data
 index = (ysim==yobs);
 % Samples from the posterior
 thetaPost = theta(index);</pre>
- ▶ Retain those θ_i for which $y_i = y^o$.

- ▶ The method produces samples from the posterior.
- Monte Carlo error when summarizing the samples as an empirical distribution or computing expectations via sample averages.
- ▶ Histogram for *N* simulated tuples (θ_i, y_i)







The good and the bad

- ▶ The method produces samples from $p(\theta|\mathbf{y}^o)$.
- This is good.
- But only applicable to discrete random variables.
- And even for discrete random variables: Computationally not feasible in higher dimensions
- ▶ Reason: The probability of the event $\mathbf{y}_{\theta} = \mathbf{y}^{\circ}$ becomes smaller and smaller as the dimension of the data increases.
- Out of N simulated tuples only a small fraction will be accepted.
 - The small number of accepted samples do not represent the posterior well.
 - Large Monte Carlo errors
- This is bad.

ARC

Approximations to make inference feasible

- ► Settle for approximate yet computationally feasible inference.
- Introduce two types of approximations:
 - 1. Instead of working with the whole data, work with lower dimensional summary statistics \mathbf{t}_{θ} and \mathbf{t}^{o} ,

$$\mathbf{t}_{\boldsymbol{\theta}} = T(\mathbf{y}_{\boldsymbol{\theta}}) \qquad \mathbf{t}^{\boldsymbol{o}} = T(\mathbf{y}^{\boldsymbol{o}}). \tag{10}$$

- 2. Instead of checking $\mathbf{t}_{\theta} = \mathbf{t}^{o}$, check whether $\Delta_{\theta} = d(\mathbf{t}^{o}, \mathbf{t}_{\theta})$ is less than ϵ . (d may or may not be a metric)
- In other words:
 - 1. Replace $\Pr(\mathbf{y} \in B_{\epsilon'}(\mathbf{y}^o) \mid \boldsymbol{\theta})$ with $\Pr(\Delta_{\boldsymbol{\theta}} \leq \epsilon \mid \boldsymbol{\theta})$
 - 2. Do not take the limit $\epsilon \to 0$
- ▶ Defines an approximate likelihood function $\tilde{L}_{\epsilon}(\theta)$,

$$\tilde{L}_{\epsilon}(\theta) \propto \Pr\left(\Delta_{\theta} \le \epsilon \mid \theta\right)$$
 (11)

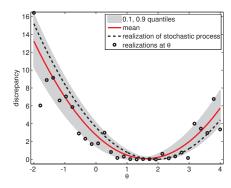
- Inference of the mean θ of a Gaussian of variance one.
- $Pr(\mathbf{y} = \mathbf{y}^o | \boldsymbol{\theta}) = 0.$
- ▶ Discrepancy Δ_{θ} :

$$\Delta_{\theta} = (\hat{\mu}^{\circ} - \hat{\mu}_{\theta})^{2},$$

$$\hat{\mu}^{\circ} = \frac{1}{n} \sum_{i=1}^{n} y_{i}^{\circ},$$

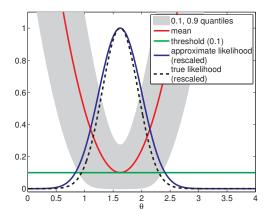
$$\hat{\mu}_{\theta} = \frac{1}{n} \sum_{i=1}^{n} y_{i},$$

$$y_{i} \sim \mathcal{N}(\theta, 1)$$



Discrepancy Δ_{θ} is a random variable.

Probability that Δ_{θ} is below some threshold ϵ approximates the likelihood function.



- ▶ Here, $T(\mathbf{y}) = \frac{1}{n} \sum_{i=1}^{n} y_i$ is a sufficient statistics for inference of the mean θ
- ▶ The only approximation is $\epsilon > 0$.
- ▶ In general, the summary statistics will not be sufficient.

Rejection ABC algorithm

- The two approximations made yield the rejection algorithm for approximate Bayesian computation (ABC):
 - 1. Sample $\theta_i \sim p_{\theta}$
 - 2. Simulate a data set \mathbf{y}_i by running the simulator with θ_i $(\mathbf{y}_i = g(\omega_i, \theta_i))$
 - 3. Compute the discrepancy $\Delta_i = d(T(\mathbf{y}^o), T(\mathbf{y}_i))$
 - 4. Retain θ_i if $\Delta_i \leq \epsilon$
- ▶ This is *the* basic ABC algorithm.
- ▶ It produces samples $\theta \sim \tilde{p}_{\epsilon}(\theta|\mathbf{y}^{o})$,

$$\tilde{p}_{\epsilon}(\theta|\mathbf{y}^{o}) \propto p_{\theta}(\theta)\tilde{L}_{\epsilon}(\theta)$$
 (12)

$$\widetilde{L}_{\epsilon}(\boldsymbol{\theta}) \propto \Pr\left(\underbrace{d(T(\mathbf{y}^{o}), T(\mathbf{y}))}_{\Delta c} \le \epsilon \mid \boldsymbol{\theta}\right)$$
 (13)

Part II

ABC methods used in practice

Brief recap

- ► Simulator-based models: Models which are specified by a data generating mechanism.
- ▶ By construction, we can sample from simulator-based models. Likelihood function can generally not be written down.
- ▶ Rejection ABC: Trial and error scheme to find parameter values which produce simulated data resembling the observed data.
- Simulated data resemble the observed data if some discrepancy measure is small.

Critique of the rejection ABC algorithm

- ▶ The rejection ABC algorithm works.
- ▶ But it is computationally not efficient.
- ▶ The probability of the event $\Delta_{\theta} \leq \epsilon$ is usually small when $\theta \sim p_{\theta}$. In particular for small ϵ .

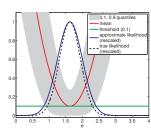
Critique of the rejection ABC algorithm

▶ In the Gaussian example, the probability for $\Delta_{\theta} \leq \epsilon$ can be computed in closed form $\Delta_{\theta} = (\hat{\mu}^{o} - \hat{\mu}_{\theta})^{2}$

$$\Pr(\Delta_{\theta} \leq \epsilon) = \Phi\left(\sqrt{\textit{n}}(\hat{\mu}^{\textit{o}} - \theta) + \sqrt{\textit{n}\epsilon}\right) - \Phi\left(\sqrt{\textit{n}}(\hat{\mu}^{\textit{o}} - \theta) - \sqrt{\textit{n}\epsilon}\right)$$

$$\Phi(x) = \int_{-\infty}^{x} \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{1}{2}u^2\right) du$$

- ▶ For $n\epsilon$ small: $\tilde{L}_{\epsilon}(\theta) \propto \Pr(\Delta_{\theta} \leq \epsilon) \propto \sqrt{\epsilon}L(\theta)$
- For small ε good approximation of the likelihood function.
- ▶ But for small ϵ , $\Pr(\Delta_{\theta} \leq \epsilon) \approx 0$: Very few samples will be accepted



Two widely used algorithms

- Two widely used algorithms which improve upon rejection ABC:
 - 1. Regression ABC (Beaumont et al, Genetics, 2002)
 - 2. Sequential Monte Carlo ABC (Sisson et al, PNAS, 2007)
- ▶ Both use rejection ABC as a building block.
- Sequential Monte Carlo (SMC) ABC is also known as Population Monte Carlo (PMC) ABC.

Two widely used algorithms

- ▶ Regression ABC consists in running rejection ABC with a relatively large ϵ and then adjusting the obtained samples so that they are closer to samples from the true posterior.
- ▶ Sequential Monte Carlo ABC consists in sampling θ from an adaptively constructed proposal distribution $\phi(\theta)$ rather than from the prior in order to avoid simulating many data sets which are not accepted.

Basic idea of regression ABC

- ▶ The summary statistics $\mathbf{t}_{\theta} = T(\mathbf{y}_{\theta})$ and θ have a joint distribution.
- Let \mathbf{t}_i be the summary statistics for simulated data $\mathbf{y}_i = g(\boldsymbol{\omega}_i, \boldsymbol{\theta}_i)$.
- We can learn a regression model between the summary statistics (covariates) and the parameters (response variables)

$$\theta_i = f(\mathbf{t}_i) + \boldsymbol{\xi}_i \tag{14}$$

where ξ_i is the error term (zero mean random variable).

▶ The training data for the regression are typically tuples (θ_i, \mathbf{t}_i) produced by rejection-ABC with some sufficiently large ϵ .

Basic idea of regression ABC

Fitting the regression model to the training data (θ_i, \mathbf{t}_i) yields an estimated regression function \hat{f} and the residuals $\hat{\boldsymbol{\xi}}_i$,

$$\hat{\boldsymbol{\xi}}_i = \boldsymbol{\theta}_i - \hat{\boldsymbol{f}}(\mathbf{t}_i) \tag{15}$$

▶ Regression ABC consists in replacing θ_i with θ_i^* ,

$$\boldsymbol{\theta}_{i}^{*} = \hat{f}(\mathbf{t}^{o}) + \hat{\boldsymbol{\xi}}_{i} = \hat{f}(\mathbf{t}^{o}) + \boldsymbol{\theta}_{i} - \hat{f}(\mathbf{t}_{i})$$
 (16)

- ▶ Corresponds to an adjustment of θ_i .
- ▶ If the relation between **t** and θ is learned correctly, the θ_i^* correspond to samples from an approximation with $\epsilon = 0$.

Basic idea of sequential Monte Carlo ABC

- We may modify the rejection ABC algorithm and use $\phi(\theta)$ instead of the prior p_{θ} .
 - 1. Sample $\theta_i \sim \phi(\theta)$
 - 2. Simulate a data set \mathbf{y}_i by running the simulator with θ_i $(\mathbf{y}_i = g(\omega_i, \theta_i))$
 - 3. Compute the discrepancy $\Delta_i = d(T(\mathbf{y}^o), T(\mathbf{y}_i))$
 - **4**. Retain θ_i if $\Delta_i \leq \epsilon$
- ▶ The retained samples follow a distribution proportional to $\phi(\theta)\tilde{L}_{\epsilon}(\theta)$

Basic idea of sequential Monte Carlo ABC

▶ Parameters θ_i weighted with w_i ,

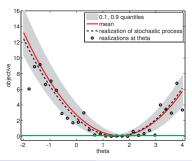
$$w_i = \frac{p_{\theta}(\theta_i)}{\phi(\theta_i)},\tag{17}$$

follow a distribution proportional to $p_{\theta}(\theta)\tilde{L}_{\epsilon}(\theta)$.

- Can be used to iteratively morph the prior into a posterior:
 - Use a sequence of shrinking thresholds ϵ_t
 - ▶ Run rejection ABC with ϵ_0 .
 - ▶ Define ϕ_t at iteration t based on the weighted samples from the previous iteration (e.g Gaussian mixture with means equal to the θ_i from the previous iteration).
- More efficient than rejection ABC: $\phi_t(\theta)$ is close to the approximate posterior in the final iterations.

Another approach

- ▶ Evaluating Δ_{θ} is computationally costly. We are only interested in small Δ_{θ} (thresholding!)
- We could increase the computational efficiency by evaluating Δ_{θ} predominantly where it tends to be small.
- ▶ Use a combination of probabilistic modeling of Δ_{θ} and optimization to figure out where to evaluate Δ_{θ} .



Learning a model of the discrepancy

▶ The approximate likelihood function $\tilde{L}_{\epsilon}(\theta)$ is determined by the distribution of the discrepancy Δ_{θ}

$$\tilde{L}_{\epsilon}(oldsymbol{ heta}) \propto \Pr\left(\Delta_{oldsymbol{ heta}} \leq \epsilon \mid oldsymbol{ heta}
ight)$$

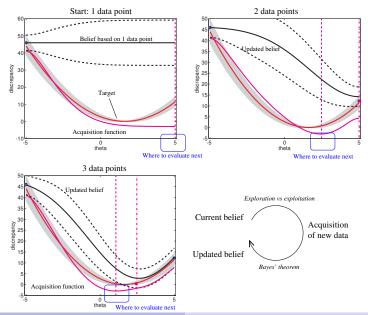
- ▶ If we knew the distribution of Δ_{θ} we could compute $\tilde{L}_{\epsilon}(\theta)$.
- ▶ In recent work, we proposed to learn a model of Δ_{θ} and to approximate $\tilde{L}_{\epsilon}(\theta)$ by $\hat{L}_{\epsilon}(\theta)$,

$$\widetilde{L}_{\epsilon}(\boldsymbol{\theta}) \propto \widehat{\mathsf{Pr}}\left(\Delta_{\boldsymbol{\theta}} \leq \epsilon \mid \boldsymbol{\theta}\right),$$
 (18)

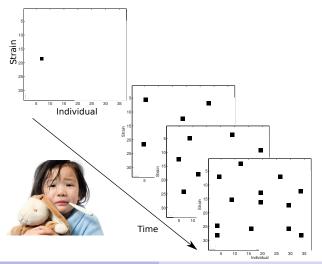
where $\widehat{\Pr}$ is the probability under the model of Δ_{θ} . (Gutmann and Corander, *Journal of Machine Learning Research*, in press, 2015)

▶ Model is learned more accurately in regions where Δ_{θ} tends to be small, using techniques from Bayesian optimization.

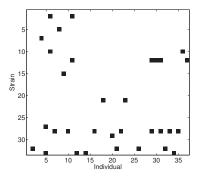
Bayesian optimization



► Inference about bacterial transmission dynamics in child day care centers (Numminen et al, *Biometrics*, 2013)



Data: Colonization states of sampled attendees of 29 child day care centers (DCCs) in Oslo greater area.

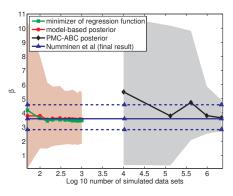


Example data from a DCC. Each square indicates an attendee colonized with a strain of the bacterium *Streptococcus pneumoniae*.

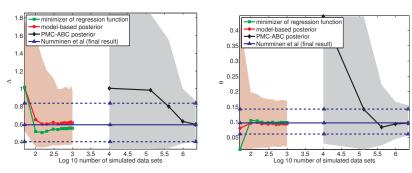
- Simulator-based model: latent continuous-time Markov chain for the transmission dynamics in a DCC and an observation model (Numminen et, Biometrics, 2013).
- ▶ The model has three parameters:
 - \triangleright β : rate of infections within a DCC
 - Λ: rate of infections outside a DCC
 - \blacktriangleright θ : possibility to be infected with multiple strains
- Likelihood is intractable (data at a single time point are available only).

- Comparison of the model-based approach with a sequential/population Monte Carlo ABC approach.
- ▶ Roughly equal results using 1000 times fewer simulations.
- ► The minimizer of the regression function under the model does not involve choosing a threshold €.

Posterior means: solid lines with markers, credibility intervals: shaded areas or dashed lines.



 Comparison of the model-based approach with a sequential/population Monte Carlo ABC approach.



Posterior means are shown as solid lines with markers, credibility intervals as shaded areas or dashed lines.

Summary

- ► The topic was Bayesian inference for models specified via a simulator (implicit / generative models).
- Introduced approximate Bayesian computation (ABC).
- Principle of ABC: Find parameter values which yield simulated data resembling the observed data.
- Covered three classical algorithms:
 - Rejection ABC
 - Regression ABC
 - 3. Sequential Monte Carlo ABC
- Introduced recent work which uses Bayesian optimization to increase the efficiency of the inference.
- ▶ Not covered: How to choose the summary statistics / the discrepancy measure between simulated and observed data.

Michael Gutmann ARC 47 / 47