Approximate Bayesian Computation

Outline

- 1. What is Approximate Bayesian Computation?
- 2. When do we use ABC instead of other methods would we use it?
- 3. How do we use it?
 - a) Choices in the ABC-rejection algorithm
 - b) Short introduction to more advanced ABC

1. What is Approximate Bayesian Computation?

Bayesian inference is based on the idea of updating belief with new evidence

- **Belief**: Prior distribution. Parameters are random variables instead of fixed quantities (they have there own distribution)
- **Evidence**: Likelihood function tells you the probability of the evidence given the parameters

 θ : Mathematical model parameter, D: data

$$P(\theta|D) = \frac{P(D|\theta)P(\theta)}{P(D)}$$

 θ : Mathematical model parameter, D: Data

$$P(\theta|D) \propto P(D|\theta)P(\theta)$$

 θ : Mathematical model parameter, D: Data

$$P(\theta|D) \propto P(D|\theta)P(\theta)$$

Probability of data given θ (likelihood)

EVIDENCE

 θ : Mathematical model parameter, D: Data

Prior probability

BELIEF

$$P(\theta|D) \propto P(D|\theta)P(\theta)$$

Probability of data given θ (likelihood)

EVIDENCE

 θ : Mathematical model parameter, D: Data

Prior probability

Posterior $P(\theta|D) \propto P(D|\theta) P(\theta)$ probability

Probability of data given θ (likelihood)

EVIDENCE

 θ : Mathematical model parameter, D: Data

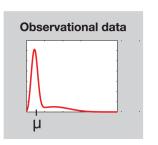


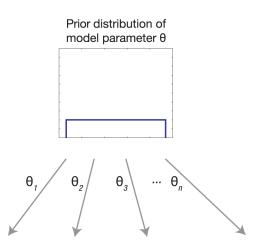
Posterior
$$\longrightarrow P(\theta|D) \propto P(D|\theta)P(\theta)$$
 probability

What if we can't use a likelihood function? How do we approximate $P(D|\theta)$?

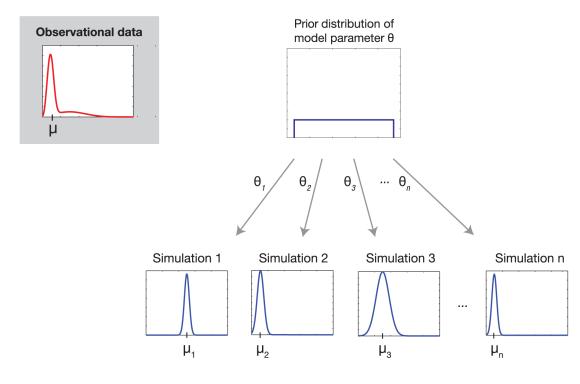
Probability of data given θ (likelihood) EVIDENCE

1. Sample θ^* from the prior distribution $P(\theta)$

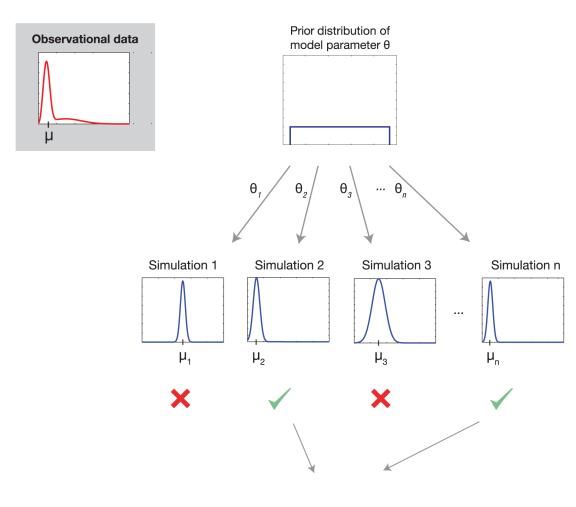




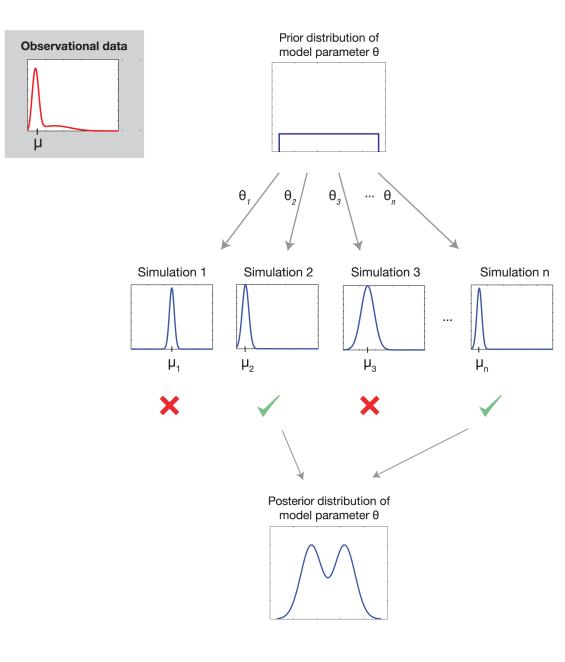
- 1. Sample θ^* from the prior distribution $P(\theta)$
- 2. Simulate a dataset D^* from your model using θ^*



- 1. Sample θ^* from the prior distribution $P(\theta)$
- 2. Simulate a dataset D^* from your model using θ^*
- 3. If $d(D, D^*) \le \epsilon$ accept θ^* , otherwise reject



- 1. Sample θ^* from the prior distribution $P(\theta)$
- 2. Simulate a dataset D^* from your model using θ^*
- 3. If $d(D, D^*) \le \epsilon$ accept θ^* , otherwise reject
- 4. Repeat until you have accepted *N* accepted samples



- 1. Sample θ^* from $P(\theta)$
- 2. Simulate a dataset D^* from your model using θ^*
- 3. Calculate the summary statistic for the observed data $\mu = S(D)$ and simulated data $\mu = S(D^*)$
- 4. If $d(S(D), S(D^*)) \le \epsilon$ accept θ^* , otherwise reject
- 5. Repeat until you have accepted *N* accepted samples

- 1. Sample θ^* from $P(\theta)$
- 2. Simulate a dataset D^* from your model using θ^*
- 3. Calculate the summary statistic for the observed data $\mu = S(D)$ and simulated data $\mu = S(D^*)$
- 4. If $d(S(D), S(D^*)) \le \epsilon$ accept θ^* , otherwise reject
- 5. Repeat until you have accepted *N* accepted samples

Summary statistic for model trajectory

Distance measure between model trajectory and data

 θ : Mathematical model parameter, D: Data

$$P(\theta|D) \propto P(D|\theta)P(\theta)$$

Probability of data given θ (likelihood)

EVIDENCE

 θ : Mathematical model parameter, D: Data

$$P(\theta|D) \propto P(D|\theta)P(\theta)$$

$$P(D|\theta) \approx P(d(S(D), S(D^*)) \leq \epsilon)$$

1. What is Approximate Bayesian Computation?

A method to approximate the posterior probability $P(\theta|D)$ without a likelihood function

2. When do we use ABC instead of other methods?

2. When do we use ABC instead of other methods?

- Data quality is poor, which means we have to aggregate it
- The likelihood function might be costly to evaluate (it takes a long time)
 - Large data sets
 - Complicated likelihood function

2. When do we use ABC instead of other methods?

- Data quality is poor, which means we have to aggregate it
- The likelihood function might be costly to evaluate (it takes a long time)
 - Large data sets
 - Complicated likelihood function

- Intuitive method of model fitting
 - Parameter -> model trajectory -> accept or reject

3. How do we use ABC?

a. Choices in the ABC- rejection algorithm

Choice of summary statistic(s) S(D)

- This is how we choose whether to accept or reject parameter values
- Sufficient summary statistic will give the same result as the likelihood
- "no other statistic that can be calculated from the same sample provides any additional information as to the value of the parameter"
- If we haven't written down a likelihood then we can't know if our summary statistics are sufficient...

Choice of summary statistic(s) S(D)

- This is how we choose whether to accept or reject parameter values
- Sufficient summary statistic will give the same result as the likelihood
- "no other statistic that can be calculated from the same sample provides any additional information as to the value of the parameter"
- In practice
 - Look at published model fitting studies using ABC methods for ideas for sufficient statistics
 - Check with simulated data!

Number of particles (N)

The more the better, but computation time must be taken into account

Tolerance value ϵ

- Determines whether you accept or reject parameter(s) based on how closely the model prediction matches you data
 - Too small and the algorithm will take a long time to run
 - Too big and the final distribution of particles will be too wide

• The magnitude of the tolerance value ϵ will depend on your distance measure

For example, if the summary of the data S(D) is the cumulative number of cases, we could have:

- $S(D) = 100\ 000$ (from the data)
- $S(D^*) = 99 \ 900 \ (model \ prediction)$
- If the distance measure d() is the sum of squared difference
- then the $d(S(D), S(D^*)) = 10000$

The prediction was 100 people short of the data, distance measure is 10 000. Hence here a reasonable choice of tolerance might be $\epsilon = 10~000$.

3. How do we use ABC?
b. Short introduction to more advanced ABC

Improvements to ABC rejection algorithm: ABC-Sequential Monte Carlo (ABC-SMC)

- Instead of one tolerance ϵ , there is a vector of tolerances $\epsilon_1, \dots, \epsilon_T$
- 1. We perform ABC rejection with a very large tolerance ϵ_1 and store our N accepted parameter values as population 1.

Improvements to ABC rejection algorithm: ABC-Sequential Monte Carlo (ABC-SMC)

- Instead of one tolerance ϵ , there is a vector of tolerances $\epsilon_1, \dots, \epsilon_T$
- 1. We perform ABC rejection with a very large tolerance ϵ_1 and store our N accepted parameter values as population 1.
- 2. Then we propose parameters by re-sampling parameters from population 1 and perturb the parameters by a small amount. Accept/reject according ϵ_2 .
- 3. Add **weight** to each parameter value according to the prior distribution, how likely you were to obtain that value from perturbation and the previous weights.

Improvements to ABC rejection algorithm: ABC-Sequential Monte Carlo (ABC-SMC)

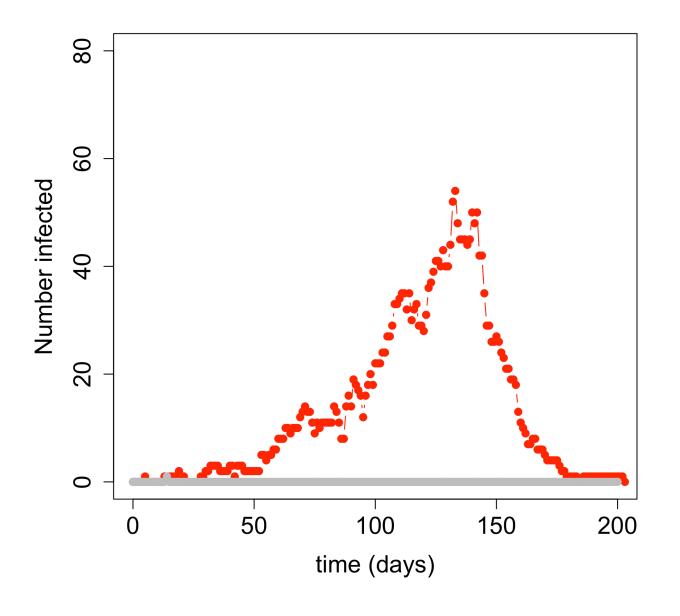
- Instead of one tolerance ϵ , there is a vector of tolerances $\epsilon_1, \dots, \epsilon_T$
- 1. We perform ABC rejection with a very large tolerance ϵ_1 and store our N accepted parameter values as population 1.
- 2. Then we propose parameters by re-sampling parameters from population 1 and perturb the parameters by a small amount. Accept/reject according ϵ_2 .
- 3. Add weight to each parameter value according to the prior distribution, how likely you were to obtain that value from perturbation and the previous weights.
 - Repeat steps 2-3 T times, sampling from the previous population. Each time decrease the tolerance value.

ABC-SMC: Stochastic model extension

- ABC rejection or ABC-SMC algorithm can be inefficient for stochastic models
- You can reject a parameter set because it gave a result which was very different to the data by chance
 - E.g. in stochastic epidemic models, by chance, an epidemic would not take off

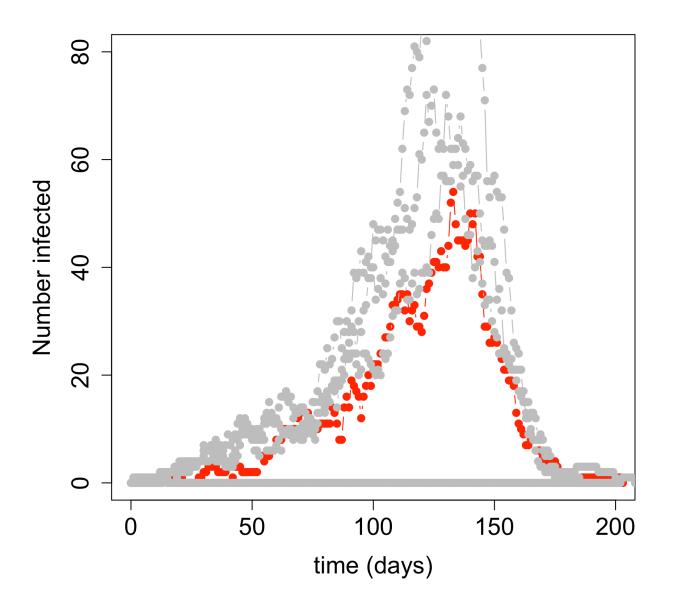
Number infected time (days)

DataStochastic model simulation



Data Stochastic model simulation

Reject parameter value because $dig(S(D),S(D^*)ig)>\epsilon$



DataStochastic model simulation

$$d(S(D), S(D^*)) \le \epsilon$$
 in 19 other model simulations!

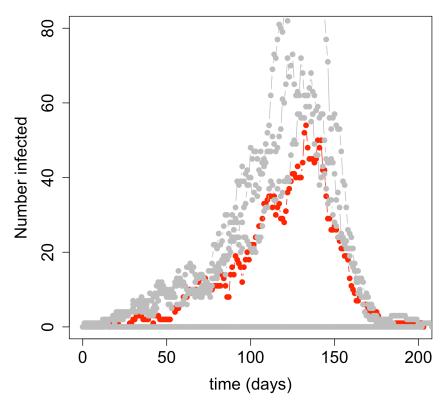
ABC-SMC: Stochastic model extension

 The ABC-SMC extension for stochastic models is to simulate the data set B times and calculate the number of times the parameter set would be accepted. Add this measure to our weights.

ABC-SMC: Stochastic model extension

 The ABC-SMC extension for stochastic models is to simulate the data set B times and calculate the number of times the parameter set would be accepted. Add this measure to our weights.

This parameter value would be accepted 19 times out of B=20 simulations.



In summary: ABC

- Can be used when data quality is poor, likelihood is complex or unknown and is an intuitive model fitting technique
- **But** you have to specify a suitable summary statistic(s)
- ABC can be slow, there are many extensions: ABC-SMC, ABC-PMC etc.

Reading

General introductions

- McKinley, Trevelyan J.; Vernon, Ian; Andrianakis, Ioannis; McCreesh, Nicky; Oakley, Jeremy E.; Nsubuga, Rebecca N.; Goldstein, Michael; White, Richard G. Approximate Bayesian Computation and Simulation-Based Inference for Complex Stochastic Epidemic Models. Statist. Sci. 33 (2018), no. 1, 4--18. doi:10.1214/17-STS618. https://projecteuclid.org/euclid.ss/1517562021
- Sunnåker M, Busetto AG, Numminen E, Corander J, Foll M, et al. (2013) Approximate Bayesian Computation. PLOS Computational Biology 9(1): e1002803.https://doi.org/10.1371/journal.pcbi.1002803
- Hartig, F., Calabrese, J. M., Reineking, B., Wiegand, T. and Huth, A. (2011), Statistical inference for stochastic simulation models theory and application. Ecology Letters, 14: 816-827. doi:10.1111/j.1461-0248.2011.01640.x
- Toni T, Welch D, Strelkowa N, Ipsen A, Stumpf MPH. (2009). Approximate Bayesian computation scheme for parameter inference and model selection in dynamical systems. J. R. Soc. Interface 6 187-202; DOI: 10.1098/rsif.2008.0172.

Reading

Examples of ABC

- Conlan, A.J., McKinley, T.J., Karolemeas, K., Pollock, E.B., Goodchild, A.V., Mitchell, A.P., Birch, C.P., Clifton-Hadley, R.S. and Wood, J.L., (2012). Estimating the hidden burden of bovine tuberculosis in Great Britain. *PLoS Computational Biology*, 8(10), p.e1002730.
- McKinley, T., Cook, A. R. and Deardon, R. (2009). Inference in epidemic models without likelihoods. *Int. J. Biostat.* **5**.
- Beaumont MA, Zhang W, and Balding DJ. (2002) Approximate Bayesian Computation in Population Genetics. GENETICS. 162 (4) 2025-2035.