

Approximate Bayesian Computation

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Intractability

- Statistical inference:
 - Given some data (e.g. forensic evidence at a crime scene)
 - Set up random process model that could have produced it
 - Infer unknowns parameters in the model (e.g. identity of perpetrator)
- Standard methods (e.g. maximum likelihood, Bayes) based on probability calculations under the model
- Can be intractable: impossible or impractically time consuming!
- Especially for complex modern models

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ABC idea

- Often models are **generative**
- i.e. can simulate data from model given parameters
- Can be used for inference without probability calculations!
- Simulate data under many parameter values
- Accept parameters giving data "close" to observations
- Gives approximation to exact inference
- Main idea of approximate Bayesian computation (ABC)
- One of several likelihood-free methods

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Example applications

- Population genetics
- Infectious disease epidemiology
- Systems biology / molecular dynamics
- Ecology
- Astrophysics / high energy physics
- Finance
- Agent based models
- Weather / climate

Overview of talk

- Recap of Bayesian inference
- Example of intractable likelihoods
- Introduction to ABC
- Summary statistics I
- Example analysis
- Summary statistics II
- Post-processing
- Efficient ABC algorithms
- Software
- Other likelihood-free methods
- More methodology
- Pros and cons
- References

Likelihood

- Observed data y_{obs}
- Model proposed with density $\pi(y|\theta)$
- \blacksquare We wish to infer parameters θ
- The likelihood function is $L(\theta) = \pi(y_{\text{obs}}|\theta)$
- Maximum likelihood finds θ maximising $L(\theta)$

• n.b. for discrete data use probabilities instead of densities

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- We must specify a **prior distribution** $\pi(\theta)$
 - Beliefs about parameters before data observed
- We're interested in the **posterior distribution** $\pi(\theta|y_{\text{obs}})$
 - Beliefs updated to take data into account
- Posterior depends on prior and likelihood through Bayes theorem:

$$\pi(\theta|y_{\rm obs}) = \pi(\theta)\pi(y_{\rm obs}|\theta)/Z$$

i.e. posterior \propto prior \times likelihood

• where $Z = \int \pi(\theta)\pi(y_{\rm obs}|\theta)d\theta$ (normalising constant)

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Monte Carlo

- Direct calculation of posterior generally infeasible
- Common alternative approach is **Monte Carlo**
- Monte Carlo aims to produce a sample $\theta_1, \theta_2, \ldots$ from the posterior distribution
- Can then estimate posterior quantities (point estimates, interval estimates, quantiles etc)
- Or produce density estimates (histograms, contour plots etc)

Monte Carlo methods

- Many standard Monte Carlo algorithms:
 - Rejection sampling
 - Importance sampling
 - Markov chain Monte Carlo (MCMC)
 - Sequential Monte Carlo (SMC)
- All require many evaluations of the likelihood function
- Not feasible for intractable likelihoods evaluation not possible or very slow
- n.b. some Monte Carlo methods only require unbiased estimates of the likelihood function
- Helps with some cases of intractable likelihood

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Examples of intractable likelihoods

Computer models

- Some models exist as computer simulation programs
- Equation for likelihood not available (and would be extremely complicated)
- Example: agent based models
- Each agent obeys simple rules, interact to form a complex system
- Applications include
 - ecology (e.g. agents represent animals)
 - systems biology (e.g. agents represent cells)
 - economics (e.g. agents represent firms)

Partial observation

- Suppose we have a tractable probability model $\pi(x, y|\theta)$ for complete data (x, y)
- However we only observe that $y = y_{obs}$ (i.e. partial data)
- So x is an unobserved latent variable
- Likelihood is

$$L(\theta) = \pi(y_{\text{obs}}|\theta) = \int \pi(x, y_{\text{obs}}|\theta) dx$$

■ Integral typically intractable, especially if x high dimensional

Partial observation: examples

- Epidemic models
 - x is times of all infections/recoveries, y is final number affected
- Biochemical networks
 - \blacksquare x is all reaction times, y is partial measurements of one species
- Population genetics
 - x is coalescent/mutation/recombination history, y is observed sequences



Likelihood-free inference

- General idea:
 - Simulate data y from various parameter values θ
 - Consider closest matches of y to y_{obs}
 - Use corresponding parameters for inference
- Can be implemented in many different ways
- Many approaches suggested in various fields over last 40+ years
- ABC puts this idea into a Bayesian framework

Likelihood-free inference timeline

- 1970s Various applications Hoel and Mitchell, Ross etc
- 1984 Inference for implicit models Diggle and Gratton
- 1984 Bayesian inference by simulating data Rubin
- 1989 **Simulated method of moments** *McFadden* (Econometrics)
- 1992 GLUE Beven and Binley (Hydrology)
- 1993 Indirect inference Gourieroux et al (Econometrics)
- 1997 **ABC** Tavaré et al/Fu and Li (Population genetics)
- 2005 Convolution filter Rossi and Vila
- 2006 **Iterated filtering** *lonides et al*
- 2010 Synthetic likelihood Wood
- ...and many more!

ABC algorithm - simplest version

Input: observed data y_{obs} , threshold $h \ge 0$

For i = 1, 2, ..., N:

- 1 Sample parameter vector θ_i from prior $\pi(\theta)$
- 2 Simulate data from $\pi(y|\theta_i)$
- If $d(y, y_{\text{obs}}) \leq h$ accept θ_i

where $d(y, y_{obs})$ is a distance function e.g. Euclidean

Output: accepted θ_i values

This is a rejection sampling algorithm

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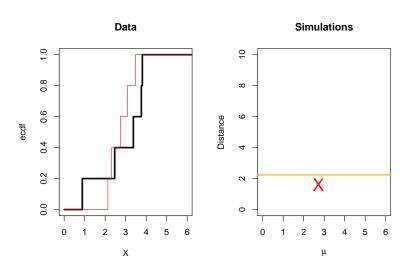
ABC target distribution

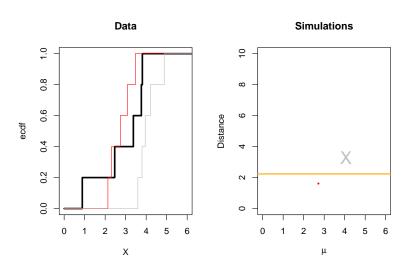
- Consider a proposed (θ, y) pair
- Sampled from $\pi(\theta)\pi(y|\theta) = \pi(\theta,y)$
- Acceptance is conditional on $y \approx y_{\text{obs}}$
- So accepted pairs drawn from $\pi(\theta, y|y \approx y_{\text{obs}})$
- And θ from $\pi(\theta|y \approx y_{\text{obs}})$
- An approx to exact posterior $\pi(\theta|y=y_{\text{obs}})$
- Taking h = 0 only accepts when $y = y_{obs}$
- Samples from exact posterior, but typically not practical (acceptances impossible/rare)

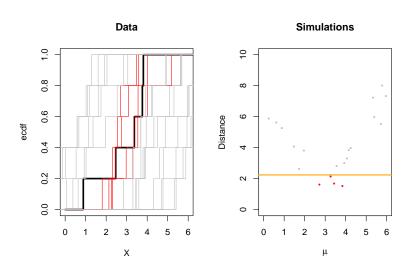
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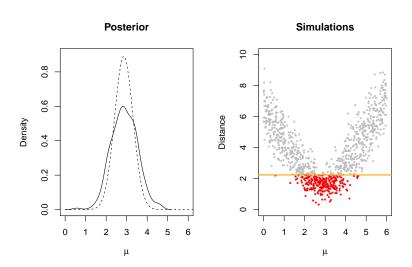
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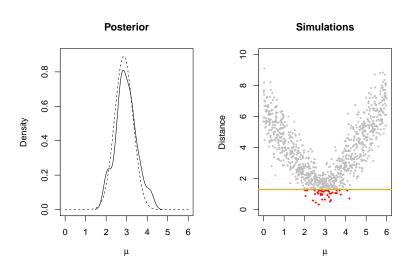
- Model: 5 draws from $N(\mu, 1)$
- Data is ordered draws: $y_1 \le y_2 \le ... \le y_5$
- Prior: Uniform(0,6)



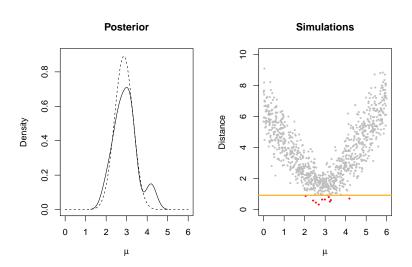








ABC algorithm example



Tuning ABC

- ABC has several tuning choices
- e.g. threshold *h* and distance function *d*
- Affect quality of approximate results
- Some key choices discussed next

ABC algorithm - effect of h

- h too large
 - Some accepted simulations are far from observations
 - Distribution of accepted θ s poor approx of posterior
- h too small
 - Distribution of accepted θ s better approx
 - But too few acceptances to learn distribution well!
- \blacksquare So choosing h is a trade-off between two source of error

Choice of *h* in practice

- Often rather than choose *h* in advance, the number *k* of desired acceptances is specified (e.g. 200)
- Then h is chosen to achieve k acceptances
- So chosen after distances computed
- This seems a good pragmatic approach
- Also some asymptotic theory available
- Blum (2010) "Approximate Bayesian Computation: A Nonparametric Perspective" (on h)
- Biau et al (2014) "New insights into Approximate Bayesian Computation" (on *k*)

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Choice of *d* in practice

■ Euclidean distance often used i.e.

$$d(a,b) = \left[\sum_{i}(a_i - b_i)^2\right]^{1/2}$$

(where *i* indexes data components)

- Not sensible if data on widely different scales
- A popular alternative is weighted Euclidean distance,

$$d(a,b) = \left[\sum_{i} \left(\frac{a_{i}-b_{i}}{\sigma_{i}}\right)^{2}\right]^{1/2}$$

- Here σ_i could be standard deviation of *i*th data component samples
- Many other distances possible impact on results modest in general

Choice of *d* for repeated observations

- Special case: data is IID (e.g. repeated time series)
- Recent work has found good ABC distance measures here:
 - Kernel MMD (Park et al 2016)
 - Wasserstein distance (Bernton et al 2017)
 - Kullback-Leibler divergence (Jiang et al 2018)



Summary statistics in ABC

- Earlier algorithm accepts when $d(y, y_{obs}) \le h$
- In practice the data is usually reduced to a vector of summary statistics s = S(y)
- Acceptance occurs when $d(s, s_{obs}) \le h$ (where $s_{obs} = S(y_{obs})$)
- Clearly necessary for non-numeric data such as genetic sequences
- Also turns out to be necessary more generally

Need for summary statistics

- Beaumont et al (2002), reviewing early work on ABC:

 "A crucial limitation of the... method is that only a small number of summary statistics can usually be handled.

 Otherwise, either acceptance rates become prohibitively low or the tolerance... must be increased, which can distort the approximation."
- Crucial that only a small number of summaries used
- Recognised from earliest work on ABC

Curse of dimensionality

- Quote is about a curse of dimensionality problem in ABC
- Informal statement:
 - More summary statistics means more opportunities for mismatches between S(y) and $S(y_{obs})$
 - So distances $d(S(y), S(y_{obs}))$ typically larger
 - Need large h, which causes approximation error
- Formal statement:
 - ABC converges to correct posterior as $h \to 0$, $N \to \infty$
 - Asymptotic rate of convergence worsens with dim y
 - Proved (at least partially) for most varieties of ABC

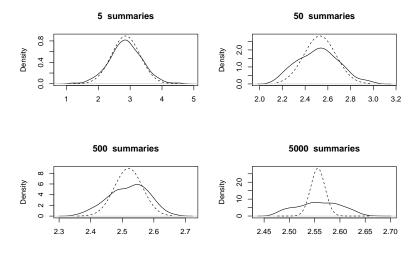
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Curse of dimensionality example

- Same example as before but with higher dimensional data
- Model: d draws from $N(\mu, 1)$
- Data is ordered draws: $y_1 \le y_2 \le ... \le y_d$
- Uniform prior on [0,6]
- \blacksquare $N = 10^4$ ABC iterations
- k = 200 acceptances
- Density estimate of ABC output compared to true posterior

Curse of dimensionality example

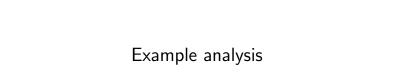


Need for summary statistics

- Dimension of data usually high so must be replaced with low-dimensional summaries
- Now ABC approximates $\pi(\theta|s_{obs})$
- i.e. posterior conditional on observed summaries
- We want this to be similar to $\pi(\theta|y_{obs})$
- lacktriangle So we want **informative summaries** about heta
- How to meet both requirements?

Sufficient statistics

- Sufficient statistics satisfy $\pi(\theta|s_{obs}) = \pi(\theta|y_{obs})$
- Low dimensional sufficient statistics would be ideal for ABC
- However they essentially only exist for exponential family models
- Very few intractable likelihood models are in this class
- So generally we must use **insufficient statistics** and accept some loss of information



Application

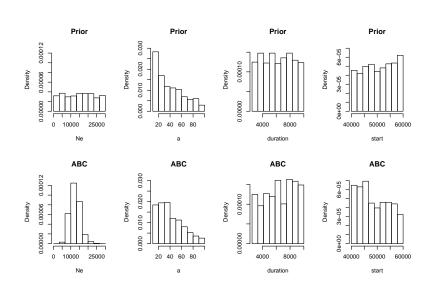
- We analyse the "human" dataset from the abc R package
- Population genetic data from Italy population (16 individuals)
- A coalescent model investigated with a population bottleneck. Parameters are:
 - Ne: Effective population size
 - a: Intensity of bottleneck (ratio of pop size before and during)
 - duration: Bottleneck duration
 - start: Start of bottleneck
- Data is genetic sequences from various regions of genome
- 3 summary statistics used, believed to be informative about demographic history
 - Average nucleotide diversity, $\bar{\pi}$
 - Mean of Tajima's D
 - Variance of Tajima's D

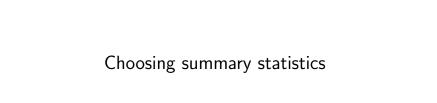
ABC setup

- $\sim N = 50,000$ ABC iterations
- k = 500 acceptances (1%)
- Weighted Euclidean distance used

```
library(abc)
data(human)
## Initialise data
sumstats = subset(stat.3pops.sim, models=="bott")
params = par.italy.sim
sumstats.obs = stat.voight[2,]
## Tuning choice
mytol = 500/nrow(sumstats) # i.e. 500 acceptances
## Do ABC
abc.out = abc(target=sumstats.obs, param=params,
              sumstat=sumstats, tol=mytol,
              method="rejection")
```

ABC output histograms





Recap

- lacktriangle We typically have high dimensional data y
- Want summary statistics S(y) which are:
 - (1) Low dimensional
 - (2) Informative about θ
- How to choose these?

Choosing summary statistics

- One option is to make a subjective choice
- More automatic methods have been proposed:
 - Subset selection

Find best subset of many *candidate summaries*. e.g. run ABC for each subset on test datasets and minimise error.

- **Projection**Find projections of many *data features* z(y) which are informative about θ . e.g. fit $\theta \sim N(Az(y), \Sigma)$ or use machine learning
- Auxiliary model Use a tractable auxiliary model. e.g. let S(y) be its MLEs.
- These methods typically do better than subjective choice
- But no obvious best method
- Lots of user input still required in choosing/tuning/testing method

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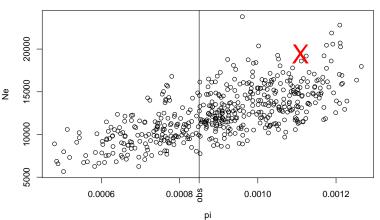


Idea

- ABC accepts a sample $\theta_1, \theta_2, \dots, \theta_k$
- The associated summary statistics are $s_1, s_2, ..., s_k$
- Can we **correct** θ_i to take account of the difference between s_i and s_{obs} ?

Illustration: human dataset

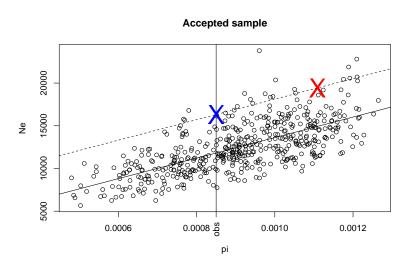




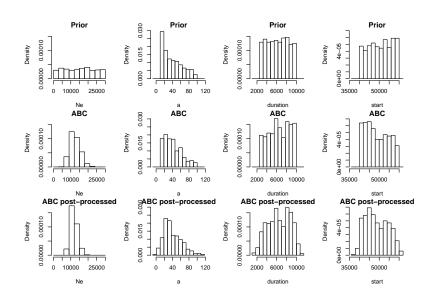
Approach

- Fit a model to the accepted (θ_i, s_i) pairs
- e.g. regression $\theta \sim N(As + b, \Sigma)$ (Beaumont et al 2002)
- So $E(\theta|s) = As + b$
- Now correct θ_i to $\theta_i E(\theta|s_i) + E(\theta|s_{obs})$
- i.e. to $\theta_i + A(s_{obs} s_i)$

Illustration: human dataset



Example: human dataset



Variations

- Regression correction can be applied to output of most ABC algorithms
- Methods using more flexible regression models have been proposed
- e.g. heteroskedastic regression, neural networks (Blum and François 2010)
- Similar ideas for ABC model choice (Beaumont et al 2008)

Usefulness

- Originally hoped post-processing would reduce curse of dimensionality
- However it's been proved that the rate of convergence issue is essentially unchanged (Blum 2010)
- Nonetheless post-processing sometimes improves results greatly in practice (Blum et al 2013)
- Li and Fearnhead (2018) give some asymptotic support for use in case of large data
- But Frazier et al (2018) argue it's poor under misspecified models

More efficient ABC algorithms

Inefficiency of rejection ABC

- Always samples θ from prior distribution
- Typically posterior is much more concentrated than prior
- Therefore most simulations will be very poor
- We'd like to propose better θ values
- Ideally learn good proposal distribution during algorithm

ABC importance sampling

```
Input: y_{\text{obs}}, h \ge 0, d(\cdot, \cdot), importance density g(\theta)
For i = 1, 2, ..., N:
```

- **1** Sample parameter vector θ_i from $g(\theta)$
- 2 Simulate data from $\pi(y|\theta_i)$
- 3 If $d(y, y_{\text{obs}}) \le h$ accept θ_i with weight $w_i = \pi(\theta)/g(\theta)$

Output: accepted (θ_i, w_i) pairs

Monte Carlo inference now possible as for standard importance sampling

Issue: need a sensible choice of g

ABC-SMC (very rough overview)

- Run standard ABC with threshold h_1
- Use output to choose importance density $g(\theta)$
- Run ABC importance sampling with threshold $h_2 < h_1$
- And so on
- Adaptively learns $g(\theta)$
- Various schemes along these lines
- (Technical point: some are population Monte Carlo methods and others are true SMC algorithms)

ABC-MCMC

- o Initialise some θ_0 and simulate corresponding y. Let t=0.
- 1 Propose θ' from $q(\cdot|\theta_t)$ e.g. $\theta' \sim N(\theta_t, \Sigma)$
- 2 Simulate y' from model conditional on θ'
- $\textbf{3} \ \mathsf{Calculate} \ \alpha = \min \left[1, \frac{\pi(\theta') q(\theta'|\theta_t) \mathbb{1} \left[d(s(y'), s_{\mathsf{obs}}) \leq h \right]}{\pi(\theta_t) q(\theta_t|\theta') \mathbb{1} \left[d(s(y), s_{\mathsf{obs}}) \leq h \right]} \right]$
- 4 With probability lpha accept

Acceptance: Let $\theta_{t+1} = \theta'$ and y = y'Rejection: Let $\theta_{t+1} = \theta_t$ and leave y unchanged

- 5 Increment t and return to 1
- Discard initial results as burn-in
- Remainder can be used as Monte Carlo sample

Comparison of ABC algorithms

- All sample from same approximate distribution given h etc.
- So can choose based on efficiency/convenience
- ABC rejection
 - Least efficient
 - But simple to implement, esp parallelisation
 - Simulations can be reused for other analyses e.g. checking performance on simulated datasets
 - Model choice version easy
- ABC-SMC
 - Allows adaptation of h
 - Complicated to code
 - Some parallelisation possible
 - Lots of tuning choices
 - Model choice version easy

Comparison of ABC algorithms, continued

ABC-MCMC

- Must fix *h* in advance (some research on varying it)
- Parallelisation not possible
- Several tuning choices
- Model choice version tricky
- Some convergence theory exists (which shows alternative "one-hit" MCMC kernel is more efficient)



Software options

- python: "ABCPy" and "PyABC" (many algorithms, very up to date)
- python: "ABCSysBio" (sequential ABC algorithm, systems biology)
- R: "abc" package (rejection sampling)
- R: "easyABC" package (multiple algorithms)
- standalone: "DIY-ABC" (rejection sampling, population genetics)
- standalone: "pop-ABC" (rejection sampling, population genetics)
- **.** . . .
- Or code your own!
 - Especially feasible for rejection ABC as algorithm v simple



Other likelihood-free methods

- Indirect inference
 - Tries to find θ minimising average distance $d(s, s_{obs})$
 - Can be viewed as maximum likelihood analogue of ABC
- Synthetic likelihood
- Likelihood-free expectation propagation
- History matching
- Conditional density estimation (e.g. via random forests or deep learning)
- Bayesian optimisation of estimated likelihoods
- Likelihood ratio estimation



Summary

- ABC is a likelihood-free method for inference
- Useful for generative models with intractable likelihood
- Idea is to find θ values that produce $S(y) \approx S(y_{\text{obs}})$
- These approximate posterior
- Informative low-dimensional summaries crucial for method to work well
- Lots of algorithms/methodology exists to improve the method
- Research in more general likelihood-free methods very active!

Strengths

- The **only** way to do inference in some situations!
- Lots of freedom in what model can be used
 - Just need to be able to simulate data in reasonable time
- Simplicity
 - Simplest ABC algorithm very easy to understand/implement

Weaknesses

- Tuning requirements
 - Acceptance threshold, summary statistics, algorithm specific choices...
- Results are approximate
 - And it's hard to quantify how approximate
- Computationally expensive
 - Since very large number of simulations often required
- Only possible for a small number of parameters (up to around 10)
 - ABC curse of dimensionality limits number of summary statistics
 - Identifiability generally requires at least one summary statistic for each parameter



Review papers

- Beaumont et al "Approximate Bayesian computation in evolution and ecology" (2010)
- Bertorelle et al "ABC as a flexible framework to estimate demography over space and time: some cons, many pros" (2010)
- Csillery et al "Approximate Bayesian computation (ABC) in practice" (2010)
- Marin et al "Approximate Bayesian computational methods" (2011)
- Sunnaker et al "Approximate Bayesian computation" (2013) (basis of the ABC wikipedia page!)
- Baragatti and Pudlo "An overview on approximate Bayesian computation" (2014)
- Lintusaari et al "Fundamentals and recent developments in approximate Bayesian computation" (2017)
- Handbook of ABC (2018)

Bonus material!

ABC for model choice

Bayesian model choice

- Suppose there are several proposed models for the data
- i.e. $M_1, M_2, ..., M_k$
- We'll usually consider k = 2 or 3
- Each has a pdf $\pi(y|\theta, M_i)$ and a prior $\pi(\theta|M_i)$
- n.b. θ may represent **different** set of parameters for each model
- We also have prior model weights $\pi(M_1), \pi(M_2), \ldots$
- We want posterior models weights $\pi(M_1|y_{\text{obs}}), \ldots$
- Maybe also parameter estimates $\pi(\theta|y_{\text{obs}}, M_1), \ldots$
- All based on Bayes theorem

Difficulties with Bayesian model choice

Computational

Likelihood-based calculation of posterior model weights notoriously hard in sufficiently complicated problems Motivates methods like reversible-jump MCMC etc

Robustness

Results can be very sensitive to details of prior distributions Sensitivity analysis required

■ Interpretation

Depends on whether we assume one model really is correct Or that we search for the best approximation

■ However still useful in practice!

ABC model choice

- Some or all models may have intractable likelihoods
- Human dataset example:
 - 3 coalescent models compared representing different demographic histories
 - 1 Model 1: bottleneck
 - 2 Model 2: constant population
 - 3 Model 3: exponential population growth
 - Each model has different number of parameters
- ABC algorithms can be adapted to this problem

ABC model choice: rejection sampling

```
Input: y_{\text{obs}}, h, d(\cdot, \cdot), S(\cdot)

For i = 1, 2, ..., N:

1 Sample model m_i from model prior

2 Sample parameter vector \theta_i from prior \pi(\theta|m_i)

3 Simulate data from \pi(y|\theta_i, m_i)

4 If d(S(y), s_{\text{obs}}) \leq h accept (m_i, \theta_i)

Output: accepted (m_i, \theta_i) values
```

Estimate posterior weight of model M_i by its frequency in output

Example: human dataset

- Equal prior model weights
- \blacksquare N = 150,000 ABC iterations
- k = 500 acceptances (0.3%)
- Results for 3 sets of observed data: Hausa (Cameroon),
 Chinese and Italian (each 16 individuals)
- Same ABC simulations used for each analysis
- Output proportions:

Population	Bottleneck	Constant	Exp growth
Hausa	0.012	0.288	0.702
Chinese	0.776	0.226	0.000
Italian	0.966	0.036	0.000

■ Especially important to do sensitivity analyses etc. See abc package vignette for worked details.

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Summary statistics for ABC model choice

- Can't simply use good parameter inference summaries
- Example: suppose x_1, x_2, \ldots, x_n iid $N(\mu, 1)$ Then sample mean good to infer μ But sample variance needed for model comparison
- Various summary statistic selection methods can be generalised to model choice

ABC model choice and classification

- ABC model choice similar to classification
- We simulate data-label pairs (y_i, m_i)
- Aim is to infer label for a further point y_{obs}
- Many statistics/machine learning methods for this
- Could be used to choose ABC summary statistics (Prangle et al 2013)
- Or to replace ABC entirely (Pudlo et al 2014 advocate random forest classifiers instead)



Why weight distances

- So far ABC simulations are accepted or rejected
- Discards some information about distance of accepted simulations
- Instead we can weight close matches higher
- We introduce a ABC kernel K(x)
- Then $K([s s_{obs}]/h)$ maps summaries s to a weight
- h affects the scale, acting as a "bandwidth"
- Examples:
 - Uniform kernel: $K(x) = \begin{cases} 1 & \text{for } x^T x \leq 1 \\ 0 & \text{otherwise} \end{cases}$
 - Gaussian kernel: $K(x) = \exp(-x^T x)$
- So uniform kernel gives an accept/reject algorithm
- (n.b. can easily include weight terms in kernels)

ABC algorithm with kernel

```
Input: y_{\text{obs}}, h \ge 0, S(\cdot), ABC kernel K(x).
```

For
$$i = 1, 2, ..., N$$
:

- 1 Sample parameter vector θ_i from prior $\pi(\theta)$
- 2 Simulate data from $\pi(y|\theta_i)$

3 Let
$$w_i = K([S(y) - s_{obs}]/h)$$

Output: accepted (θ_i, w_i) pairs

Use for Monte Carlo as in importance sampling

n.b. distance $d(\cdot, \cdot)$ no longer used $-K(\cdot)$ performs similar role.

Kernels in other ABC algorithms

- Same idea can be used in all the algorithms described earlier
- Can help ABC-MCMC/ABC-SMC work well
- Alternatively can modify algorithms to accept with probability w_i
- Little theory on best choice of kernel
- Practice suggests it's not as important to results as summary statistics

Effect of kernel

- Assume *K* is a pdf
- Then ABC samples from posterior for a misspecified model

summary statistics \sim model of interest + hz

- \blacksquare where z is an independent draw from $K(\cdot)$
- See "Approximate Bayesian computation (ABC) gives exact results under the assumption of model error" Wilkinson 2013
- Can occasionally allow exact inference if model can be expressed in this form
- Or can be used to capture effect of model misspecification

Sequential ABC analysis

Motivation

- Time series setting
- We have data at every time point
- If model has a helpful structure we can do inference sequentially
- i.e. analyse data at t = 1 by ABC, then data at t = 2, ...
- Each step has low dimensional data! So low approximation error
- Can be done by an ABC version of particle filtering
- For a review see Jasra (2014) "Approximate Bayesian computation for a class of time series models"

Challenges

- Sequential ABC is promising
- Algorithms have been developed with good theoretical properties
- But still challenging in practice
- Can be very computationally demanding
- Prone to getting "stuck" at outlying observations
- Tuning well is difficult
- Data at each time point could be complicated, requiring introduction of summaries