Non-linear regression models for Approximate Bayesian Computation (ABC)

Michael Blum <u>Olivier François</u> TIMC-IMAG, Faculty of Medicine U. Grenoble Accept/Reject ABC methods suffer from the curse of dimensionality

ABC is wasteful. A typical usage may involve millions of simulations, and it retains only a few thousands.

Be more tolerant and recycle the wasted data by using regression-based ABC (Beaumont et al 2002)

Linear regression-based ABC can sometimes be improved

# abc of ABC

Using stochastic simulations with known parameters,  $\theta \sim \pi(\theta)$ , we compute a subset of summary statistics, s, and we compare them to the observed subset, s<sub>obs</sub>

$$\mathsf{P}_{\varepsilon}(\theta \mid \mathsf{D}) \quad \alpha \quad \mathsf{P}(\mid \mid \mathsf{s} - \mathsf{s}_{obs} \mid \mid < \varepsilon \mid \theta) \quad \pi(\theta)$$

Problematic if s is of large dimension

Beaumont et al (2002) increase the tolerance  $\epsilon$ , and correct the posterior distribution by performing linear regression



 $\varphi$  = model parameter, s = summary statistic (here in one dimension)

### Linear regression improves ABC



# Blum and OF (2009) suggest the use of non-linear conditional heteroscedastic regression models



# One example in population genetics

Given n = 100 DNA sequences at a particular locus, and having observed 10 polymorphic sites at this locus,

Estimate  $\theta$  the scaled mutation rate (or the population size).

# Generating model for s

- 1. Draw  $\theta$  from a vague prior
- 2. Simulate L<sub>n</sub> the length of the sample genealogy
- 3. Generate s ~ Poisson( $\theta L_{p}/2$ )

Replicated 2,000 times

#### Results : Distance to the (exact) posterior distribution



<u>Reducing the dimensionality</u> of the set of summary statistics

This may be achieved by many regression models, like ridge regression, gam's or projection pursuit.

We choose feedforward neural networks (Ripley 1996; Bishop 2006)

Why neural nets?

Their first layer allows for a nonlinear projection on a subspace of much lower dimensionality

Regression is performed using the reduced number of projection variables

Automatic choice of (new) summary statistics

# Neural nets

Build *H* linear combinations of summary statistics (H < D = dimension of s)

$$S_h = W_{0h} + \sum_{k=1...D} W_{kh} S^k$$
,  $h = 1,...,H$ 

Perform non-linear regression on the *H* projections

$$\theta = w_{00} + \sum_{h=1...H} w_{h0} \varphi(S_h) + error$$
$$= g_w(s) + error$$

# <u>Fitting NN</u>

Weighted (ie local) penalized least-squares criterion

$$\sum_{i=1...n} (\theta_{i} - g_{w}(s_{i}))^{2} K_{\varepsilon}(||s_{i} - s_{obs}||) + \lambda ||w||^{2}$$

Weight decay,  $\lambda$ , is determined by cross-validation

# Posterior sampling correction:

$$\theta_{i}^{*} = \theta_{i} + g_{w}(s_{obs}) - g_{w}(s_{i}), \quad i = 1,...,M$$

# Michael's example (adding useless statistics)



# A second example (Heggland and Frigessi, 2004)

M/G/1 queue: single server model

Arrival times ~ Unif( $\theta_1, \theta_2$ )

Service time ~  $Exp(\theta_3)$ 

Observation: n = 50 inter-departure times, y

Goal: Estimate the service rate  $\theta_{3}$ 

Summary statistics: 20%, 10% and 5% quantiles (percentiles) of y

Dimension of s = 5, 10, 20

Tolerance rate = 50%

5 summary statistics





# Model choice

# Computing posterior probabilities for K models $M_1, \dots, M_K$

Neural nets extend the multinomial logistic regression approach of Beaumont (2007)

Logistic outputs + entropy criterion

# Other extensions

Adaptive NCH model (Blum and OF 2009)

Based on the estimation of support of the posterior density (with SVM) and iterated IS

# <u>Conclusions</u>

Regression-based ABC is a post-simulation approach

Easy to implement and pragmatic

R functions available (CRAN package soon)

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