

# Learning our ABCs

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# Outline

- Approximate Bayesian computation
- ABC with conjugate priors
- ABC and semi-automatic ABC with the g-and-k distribution

# Background and Motivation

## Full Posterior

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$$\pi(\theta|y_{obs}) = \frac{p(y_{obs}|\theta)\pi(\theta)}{p(y_{obs})}$$

## Partial Posterior

$$\pi(\theta|s_{obs}) = \frac{p(s_{obs}|\theta)\pi(\theta)}{p(s_{obs})}$$

where  $s_{obs} = S(y_{obs})$  is a vector of summary statistics (preferably sufficient) of lower dimension than the data

# ABC approximation (rejection algorithm)

$\pi_\epsilon(\theta|y_{obs})$ , is generated by repeatedly

- Generating  $\theta'$  from the prior distribution  $\pi(\cdot)$
- Generating  $y_i$  from the likelihood  $p(\cdot|\theta')$
- Accepting  $\theta'$  if  $\rho\{S(y_i), S(y_{obs})\} \leq \epsilon$

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Requires tuning of

- $S(\cdot)$ , the function to compute summary statistics
- $\rho$ , the distance function
- $\epsilon$ , the threshold

# ABC with local linear regression...

- Improve the previous algorithm by introducing a regression step to correct for discrepancy between  $S(y_{obs})$  and  $S(y_i)$
- For each simulated  $y_i$ , set

$$\theta_i = m(S(y_i)) + \eta_i$$

where  $m$  is the regression function and the  $\eta_i$  are centered random variables with common variance.

## ...and kernel

- Instead of accepting or rejecting a sample, assign each simulation  $(\theta_i, S(y_i))$  a weight with a kernel

$$K[\rho(S(y_i), S(y_{obs}))]$$

- Higher weights given for proximity to the observation
- We use the Epanechnikov kernel and the Euclidean distance function



# Principled summary statistic selection

- Best subset selection

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- Best subset selection
- Semi-automatic ABC
  - 1 Initial run of ABC to find a posterior region of non-negligible mass
  - 2 Simulate parameter values and summary statistics
  - 3 Run a linear regression of the summary statistics on each parameter. Use an information criterion such as BIC to determine which summary statistics can best be used to infer the parameter values
  - 4 Run ABC using this choice of summary statistics

# Beta prior, binomial likelihood

$$\theta \sim \text{Beta}(1, 1) \quad (1)$$

$$X|\theta \sim \text{Bin}(12, \theta) \quad (2)$$

$$\theta|X = 2 \sim \text{Beta}(3, 11) \quad (3)$$

# Beta prior, binomial likelihood

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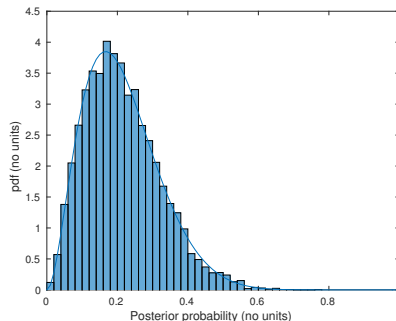
$$X|\theta \sim \text{Bin}(12, \theta) \quad (2)$$

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## ABC Algorithm

- Sample  $\theta \sim \text{Beta}(1, 1)$
- Sample  $X|\theta \sim \text{Bin}(12, \theta)$
- Accept  $\theta$  if  $X|\theta = 2$ , otherwise reject.

# Beta prior, binomial likelihood



**Figure:** 10,000 samples using ABC.

$p$  value for  $\chi^2$  goodness of fit test  $(50 \pm 30)\%$   
 $(10 \pm 10)$  rejects per accepted sample

# Normal-gamma prior, Normal likelihood

## Prior

$$\tau \sim \text{Gamma}(\alpha_0, \beta_0) \quad (4)$$

$$\mu|\tau \sim \text{N}(\mu_0, 1/(\nu_0\tau)) \quad (5)$$

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## Joint Posterior

$$\mu, \tau|X \sim \text{NGamma}(\mu_1, \nu_1, \alpha_1, \beta_1) \quad (7)$$



# Normal-gamma prior, Normal likelihood

## Marginal Posterior

$$\mu|X = \sqrt{\frac{\beta_1}{\alpha_1 \nu_1}} T_{2\alpha_1} + \mu_1 \quad (8)$$

and

$$\tau|X \sim \text{Gamma}(\alpha_1, \beta_1) \quad (9)$$

where  $T_{2\alpha} \sim t_{2\alpha}$ .

# Normal-gamma prior, Normal likelihood

## ABC Algorithm

- Sample  $\tau \sim \text{Gamma}(\alpha_0, \beta_0)$
- Sample  $\mu | \tau \sim \text{N}(\mu_0, 1/(\nu_0 \tau))$
- Sample  $n$  times  $Y | \mu, \tau \sim \text{N}(\mu, 1/\tau)$

# Normal-gamma prior, Normal likelihood

## ABC Algorithm

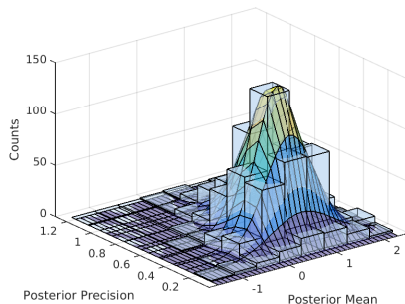
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- Sample  $\mu | \tau \sim \text{N}(\mu_0, 1/(\nu_0 \tau))$
- Sample  $n$  times  $Y | \mu, \tau \sim \text{N}(\mu, 1/\tau)$
- Conduct two tailed hypothesis tests, at some confidence level, on

$$\frac{\sqrt{n}(\bar{X} - \bar{Y})}{\sqrt{S_X^2 + S_Y^2}} \sim \text{N}(0, 1) \quad (10)$$

$$\frac{S_X^2}{S_Y^2} \sim F_{n-1, n-1} \quad (11)$$

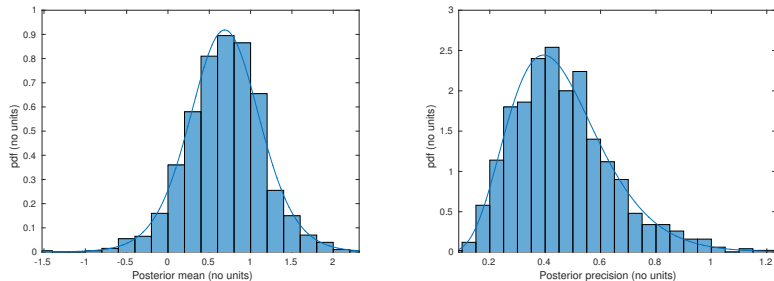
- Accept  $\mu, \tau$  if both null hypothesis are accepted, reject otherwise

# Normal-gamma prior, Normal likelihood



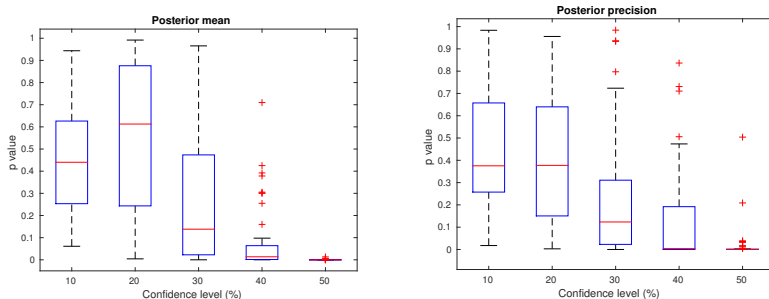
**Figure:** Joint histogram of 1000 samples from ABC. Confidence level set at 10%.

# Normal-gamma prior, Normal likelihood



**Figure:** Marginal histogram of 100- samples from ABC. Confidence level set at 10%.

# Normal-gamma prior, Normal likelihood



**Figure:**  $p$  values for the  $\chi^2$  goodness of fit test. The test was conducted 50 times with different observations.

# Normal-gamma prior, Normal likelihood

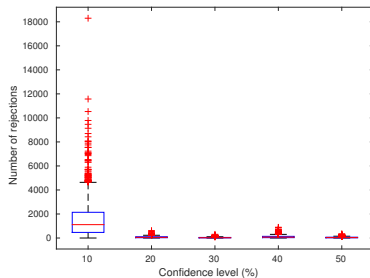


Figure: Rejections per accepted sample

- Threshold not too big, not too small.
- Ideally comparison through sufficient statistics.
- Posterior can be unknown.
- Unable to simulate from improper priors.



## $g$ -and- $k$ distribution

- Easy to simulate from, but evaluating likelihood can be costly

$$F^{-1}(x, \theta) = A + B \left( 1 + c \frac{1 - \exp(-g \cdot z(x))}{1 + \exp(-g \cdot z(x))} \right) (1 + z(x)^2)^k z(x)$$

- $\theta = (A, B, c, g, k)$
- $c$  taken as fixed at 0.8
- Suitable choice of summary statistics not immediately obvious

# Simulating data

- Generate  $10^4$  ‘observations’ under ‘true’  
 $\theta = (A = 3, B = 1, g = 2, k = 0.5)$
- Simulate  $10^5$  parameters from  $\mathcal{U}[0, 10]^4$
- Simulate  $10^4$  observations from  $g$ -and- $k$  distribution for each simulated parameter vector
- Use order statistics as summary statistics

## Summary statistic selection

$m$	$l$	$mean$
60	1	24,016
60	2	9,470
60	3	1,090
<b>60</b>	<b>4</b>	<b>-5,794</b>
100	1	25,253
100	2	10,835
100	3	2,946
100	4	-3,447
140	1	24,813
140	2	10,965
140	3	3,360
140	4	-2,734

**Table:** The BIC resulting from inferring the parameter values from the order statistics for a variety of number of order statistics ( $m$ ), and powers of these ( $l$ )

# Fitted vs true parameter values

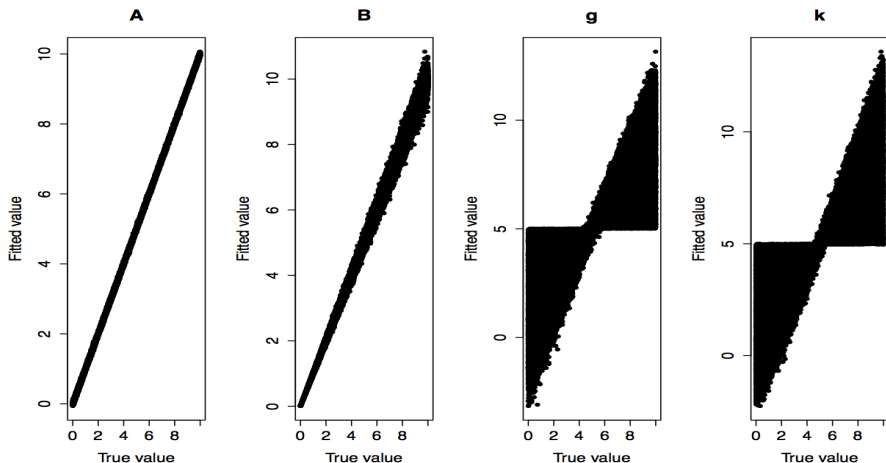
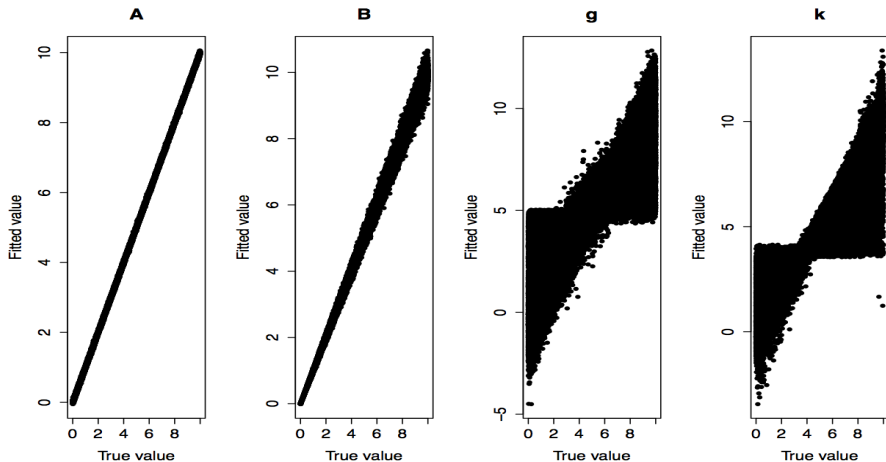


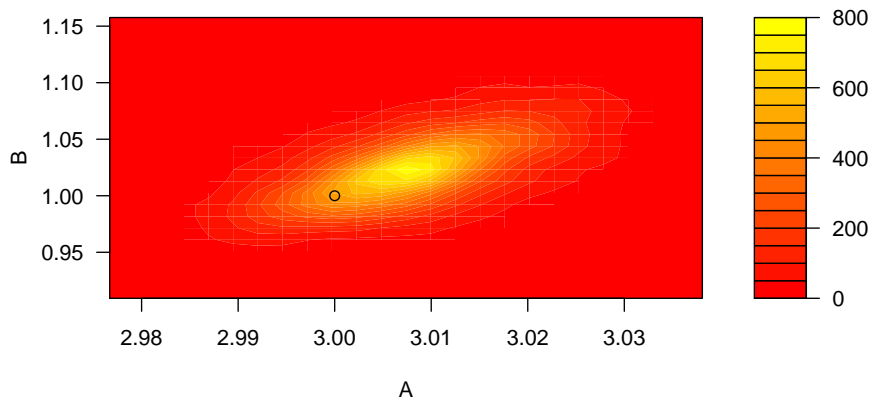
Figure: Inference of parameter values using order statistics  $s$

# Fitted vs true parameter values



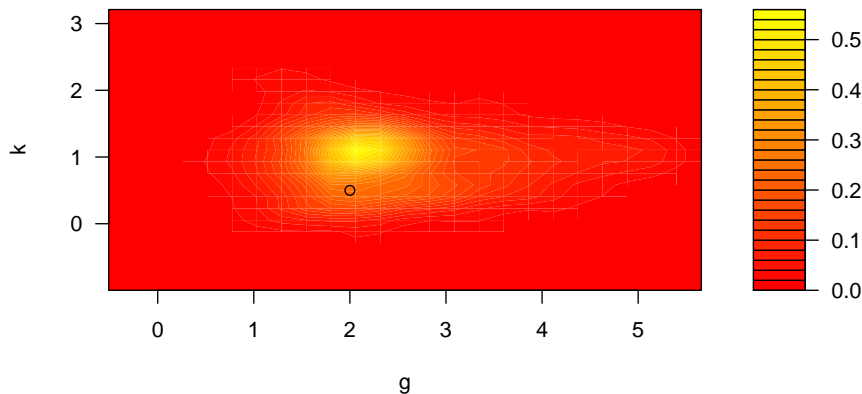
**Figure:** Inference of parameter values using order statistics on summary statistics and transformations ( $s, s^2, s^3, s^4$ )

# Inference on A and B parameters



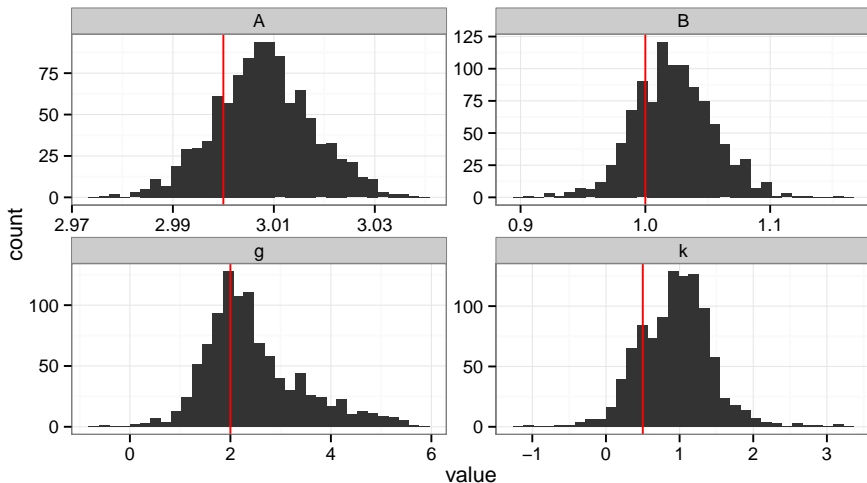
**Figure:** ABC with semi-automatic summary statistic selection, local linear regression correction, tolerance 0.01 (chosen by cross-validation)

# Inference on $g$ and $k$ parameters



**Figure:** ABC with semi-automatic summary statistic selection, local linear regression correction, tolerance 0.01 (chosen by cross-validation)

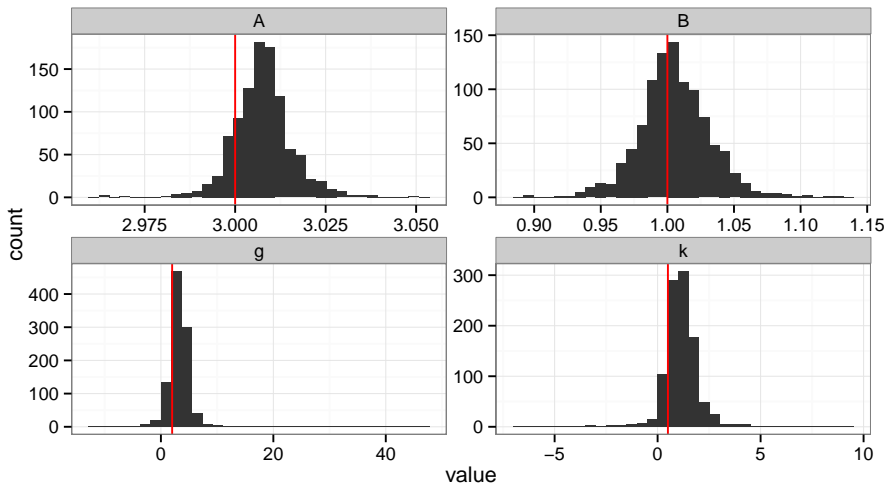
# Inference on all parameters



**Figure:** ABC with semi-automatic summary statistic selection, local linear regression correction, tolerance 0.01 (chosen by cross-validation)



# Comparison with standard ABC



**Figure:** ABC using 60 order statistics as summary statistics, local linear regression correction, tolerance 0.01 (chosen by cross-validation)

# Conclusions

- Semi-automatic selection of summary statistics can be useful
- Not a panacea
  - ▶ Still need to choose summary statistics for step 1
  - ▶ Need to choose set of explanatory variables for linear model
  - ▶ Still need to tune  $\epsilon$ ,  $\rho$  (and  $K$ )
- Plenty more to explore ... (over to Paul, Giuseppe and Marcin)