Bayesian Inference by Density Ratio Estimation

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Task

Perform Bayesian inference for models where

1. the likelihood function is too costly to compute
2. sampling – simulating data – from the model is possible

Program

Background

Previous work

Proposed approach

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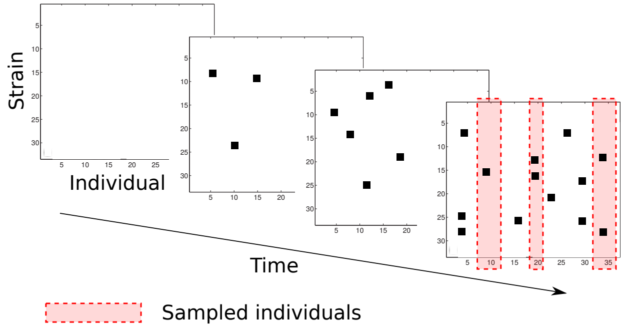
Simulator-based models

- Goal: Inference for models that are specified by a mechanism for generating data
  - e.g. stochastic dynamical systems
  - e.g. computer models / simulators of some complex physical or biological process
- Such models occur in multiple and diverse scientific fields.
- Different communities use different names:
  - Simulator-based models
  - Stochastic simulation models
  - Implicit models
  - Generative (latent-variable) models
  - Probabilistic programs

Examples

Simulator-based models are widely used:

- Evolutionary biology:
  Simulating evolution
- Neuroscience:
  Simulating neural circuits
- Ecology:
  Simulating species migration
- Health science:
  Simulating the spread of an infectious disease

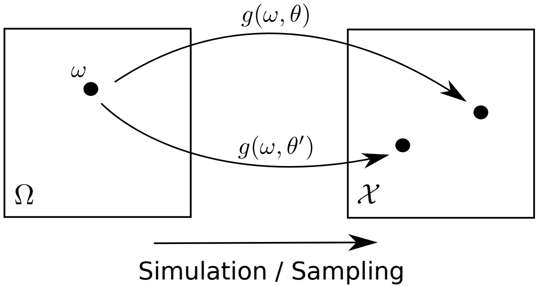


Definition of simulator-based models

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

$$\boldsymbol{\omega} \in \Omega \mapsto \boldsymbol{x} = g(\boldsymbol{\omega}, \boldsymbol{\theta}) \in \mathcal{X} \tag{1}$$

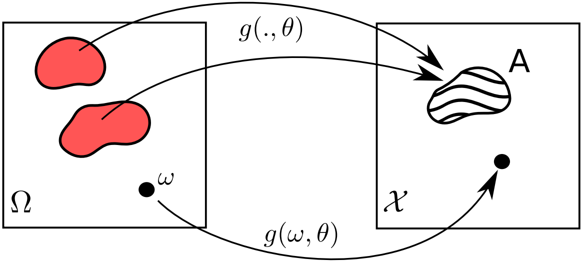
- For any fixed $\boldsymbol{\theta}$, $\boldsymbol{x}_{\boldsymbol{\theta}} = g(., \boldsymbol{\theta})$ is a random variable.



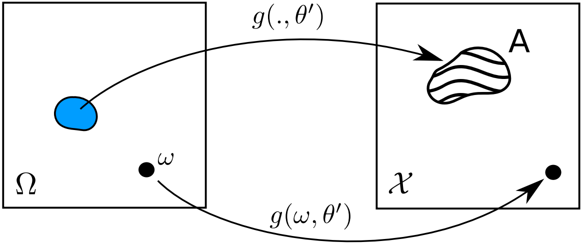
Implicit definition of the model pdfs

$$\Pr(x \in A \mid \theta) = \mathcal{P}(\{\omega : g(\omega, \theta) \in A\})$$

Parameter value θ



Parameter value θ'



Advantages of simulator-based models

- Direct implementation of hypotheses of how the observed data were generated.
- Neat interface with scientific models (e.g. from physics or biology).
- Modelling by replicating the mechanisms of nature that 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.

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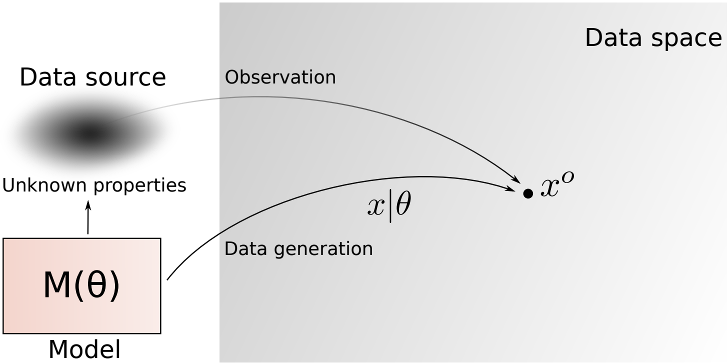
Main reason: *Likelihood function is intractable*

The likelihood function $L(\boldsymbol{\theta})$

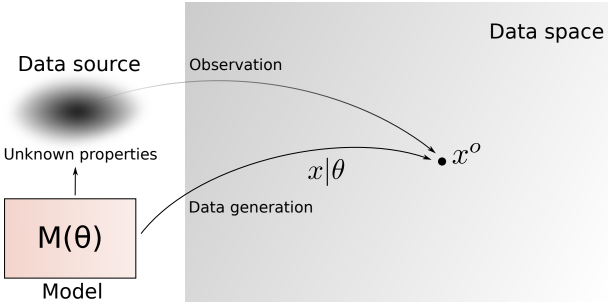
- Probability that the model generates data like $\boldsymbol{x}^o$ when using parameter value $\boldsymbol{\theta}$
- Generally well defined but intractable for simulator-based / implicit models



Program

Three foundational issues

1. How should we assess whether $\boldsymbol{x}_{\boldsymbol{\theta}} \equiv \boldsymbol{x}^o$?
2. How should we compute the probability of the event $\boldsymbol{x}_{\boldsymbol{\theta}} \equiv \boldsymbol{x}^o$?
3. For which values of $\boldsymbol{\theta}$ should we compute it?



Likelihood: Probability that the model generates data like $\boldsymbol{x}^o$ for parameter value $\boldsymbol{\theta}$

Approximate Bayesian computation

1. How should we assess whether $\boldsymbol{x_\theta} \equiv \boldsymbol{x}^o$?
   $\Rightarrow$ Check whether $||T(\boldsymbol{x_\theta}) - T(\boldsymbol{x}^o)|| \leq \epsilon$
2. How should we compute the proba of the event $\boldsymbol{x_\theta} \equiv \boldsymbol{x}^o$?
   $\Rightarrow$ By counting
3. For which values of $\boldsymbol{\theta}$ should we compute it?
   $\Rightarrow$ Sample from the prior (or other proposal distributions)

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Difficulties:

- Choice of $T()$ and ϵ
- Typically high computational cost

For recent review, see: Lintusaari et al (2017) "Fundamentals and recent developments in approximate Bayesian computation", Systematic Biology

Synthetic likelihood

(Simon Wood, Nature, 2010)

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2. How should we compute the proba of the event $\boldsymbol{x}_{\boldsymbol{\theta}} \equiv \boldsymbol{x}^o$?
   - $\Rightarrow$ Compute summary statistics $\boldsymbol{t}_{\boldsymbol{\theta}} = T(\boldsymbol{x}_{\boldsymbol{\theta}})$
   - $\Rightarrow$ Model their distribution as a Gaussian
   - $\Rightarrow$ Compute likelihood function with $T(\boldsymbol{x}^o)$ as observed data
3. For which values of $\boldsymbol{\theta}$ should we compute it?
   - $\Rightarrow$ Use obtained "synthetic" likelihood function as part of a Monte Carlo method

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Difficulties:

- Choice of $T()$
- Gaussianity assumption may not hold
- Typically high computational cost

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Overview of some of my work

1. How should we assess whether $\boldsymbol{x}_{\boldsymbol{\theta}} \equiv \boldsymbol{x}^o$?
   - $\Rightarrow$ Use classification (Gutmann et al, 2014, 2017)
2. How should we compute the proba of the event $\boldsymbol{x}_{\boldsymbol{\theta}} \equiv \boldsymbol{x}^o$?
3. For which values of $\boldsymbol{\theta}$ should we compute it?
   - $\Rightarrow$ Use Bayesian optimisation (Gutmann and Corander, 2013-2016)
     Compared to standard approaches: speed-up by a factor of 1000 more

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Basic idea

(Dutta et al, 2016, arXiv:1611.10242)

- Frame posterior estimation as ratio estimation problem

$$p(\boldsymbol{\theta}|\mathbf{x}) = \frac{p(\boldsymbol{\theta})p(\mathbf{x}|\boldsymbol{\theta})}{p(\mathbf{x})} = p(\boldsymbol{\theta})r(\mathbf{x}, \boldsymbol{\theta}) \tag{2}$$

$$r(\mathbf{x}, \boldsymbol{\theta}) = \frac{p(\mathbf{x}|\boldsymbol{\theta})}{p(\mathbf{x})} \tag{3}$$

- Estimating $r(\mathbf{x}, \boldsymbol{\theta})$ is the difficult part since $p(\mathbf{x}|\boldsymbol{\theta})$ unknown.
- Estimate $\hat{r}(\mathbf{x}, \boldsymbol{\theta})$ yields estimate of the likelihood function and posterior

$$\hat{L}(\boldsymbol{\theta}) \propto \hat{r}(\mathbf{x}^o, \boldsymbol{\theta}), \qquad \hat{p}(\boldsymbol{\theta}|\mathbf{x}^o) = p(\boldsymbol{\theta})\hat{r}(\mathbf{x}^o, \boldsymbol{\theta}). \tag{4}$$

Estimating density ratios in general

- Relatively well studied problem (Textbook by Sugiyama et al, 2012)
- Bregman divergence provides general framework
  (Gutmann and Hirayama, 2011; Sugiyama et al, 2011)
- Here: density ratio estimation by logistic regression

Density ratio estimation by logistic regression

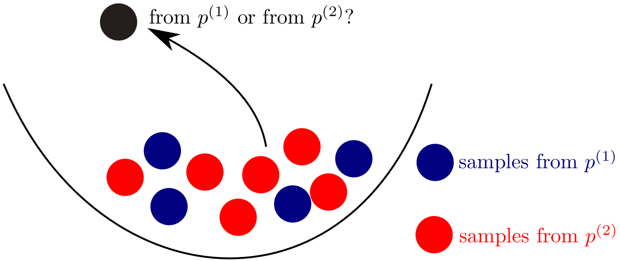
- Samples from two data sets

$$\mathbf{x}_i^{(1)} \sim p^{(1)}, \quad i = 1, \ldots, n^{(1)} \tag{5}$$

$$\mathbf{x}_i^{(2)} \sim p^{(2)}, \quad i = 1, \ldots, n^{(2)} \tag{6}$$

- Probability that a test data point $\mathbf{x}$ was sampled from $p^{(1)}$

$$\mathbb{P}(\mathbf{x} \sim p^{(1)} | \mathbf{x}, h) = \frac{1}{1 + \nu \exp(-h(\mathbf{x}))}, \qquad \nu = \frac{n^{(2)}}{n^{(1)}} \tag{7}$$



Density ratio estimation by logistic regression

- Estimate h by minimising

$$\mathcal{J}(h) = \frac{1}{n}\left\{\sum_{i=1}^{n^{(1)}} \log\left[1 + \nu \exp\left(-h_i^{(1)}\right)\right] + \sum_{i=1}^{n^{(2)}} \log\left[1 + \frac{1}{\nu}\exp\left(h_i^{(2)}\right)\right]\right\}$$

$$h_i^{(1)} = h\left(\mathbf{x}_i^{(1)}\right) \qquad h_i^{(2)} = h\left(\mathbf{x}_i^{(2)}\right)$$

$$n = n^{(1)} + n^{(2)}$$

- Objective is the re-scaled negated log-likelihood.
- For large $n^{(1)}$ and $n^{(2)}$

$$\hat{h} = \mathrm{argmin}_h\, \mathcal{J}(h) = \log \frac{p^{(1)}}{p^{(2)}}$$

without any constraints on h

Estimating the posterior

- Property was used to estimate unnormalised models
  (Gutmann & Hyvärinen, 2010, 2012)
- It was used to estimate likelihood ratios
  (Pham et al, 2014; Cranmer et al, 2015)
- For posterior estimation, we use
  - data generating pdf $p(\boldsymbol{x}|\boldsymbol{\theta})$ for $p^{(1)}$
  - marginal $p(\boldsymbol{x})$ for $p^{(2)}$ (Other choices for $p(\boldsymbol{x})$ possible too)
  - sample sizes entirely under our control

Estimating the posterior

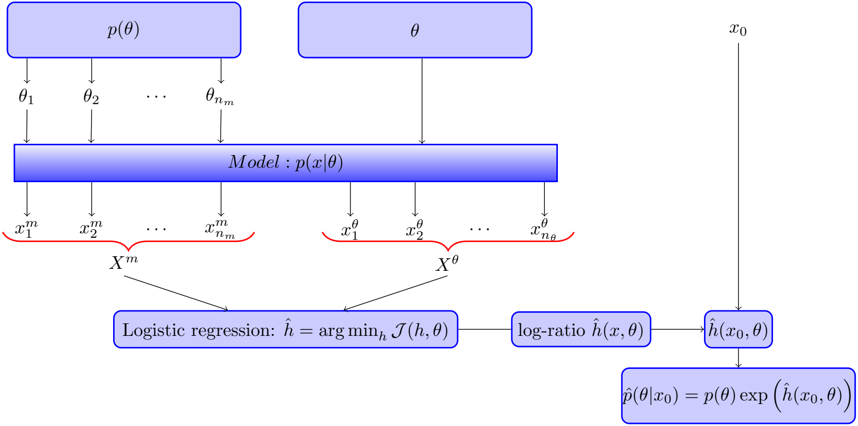
- Logistic regression gives (point-wise in $\boldsymbol{\theta}$)

$$\hat{h}(\mathbf{x}, \boldsymbol{\theta}) \to \log \frac{p(\mathbf{x}|\boldsymbol{\theta})}{p(\mathbf{x})} = \log r(\mathbf{x}, \boldsymbol{\theta}) \tag{8}$$

- Estimated posterior and likelihood function:

$$\hat{p}(\boldsymbol{\theta}|\mathbf{x}^o) = p(\boldsymbol{\theta}) \exp(\hat{h}(\mathbf{x}^o, \boldsymbol{\theta})) \quad \hat{L}(\boldsymbol{\theta}) \propto \exp(\hat{h}(\mathbf{x}^o, \boldsymbol{\theta})) \tag{9}$$

Estimating the posterior



(Dutta et al, 2016, arXiv:1611.10242)

Auxiliary model

- We need to specify a model for h.
- For simplicity: linear model

$$h(\boldsymbol{x}) = \sum_{i=1}^{b} \beta_i \psi_i(\boldsymbol{x}) = \beta^\top \psi(\boldsymbol{x}) \tag{10}$$

  where $\psi_i(\boldsymbol{x})$ are summary statistics
- More complex models possible

Exponential family approximation

- Logistic regression yields

$$\hat{h}(\boldsymbol{x};\boldsymbol{\theta}) = \hat{\beta}(\boldsymbol{\theta})^\top \psi(\boldsymbol{x}), \quad \hat{r}(\boldsymbol{x},\boldsymbol{\theta}) = \exp(\hat{\beta}(\boldsymbol{\theta})^\top \psi(\boldsymbol{x})) \tag{11}$$

- Resulting posterior

$$\hat{p}(\boldsymbol{\theta}|\boldsymbol{x}^o) = p(\boldsymbol{\theta}) \exp(\hat{\beta}(\boldsymbol{\theta})^\top \psi(\boldsymbol{x}^o)) \tag{12}$$

- Implicit exponential family approximation of $p(\boldsymbol{x}|\boldsymbol{\theta})$

$$\hat{r}(\boldsymbol{x},\boldsymbol{\theta}) = \frac{\hat{p}(\boldsymbol{x}|\boldsymbol{\theta})}{\hat{p}(\boldsymbol{x})} \tag{13}$$

$$\hat{p}(\boldsymbol{x}|\boldsymbol{\theta}) = \hat{p}(\boldsymbol{x}) \exp(\hat{\beta}(\boldsymbol{\theta})^\top \psi(\boldsymbol{x})) \tag{14}$$

- Implicit because $\hat{p}(\boldsymbol{x})$ never explicitly constructed.

Remarks

- Vector of summary statistics $\psi(\boldsymbol{x})$ should include a constant for normalisation of the pdf (log partition function)
- Normalising constant is estimated via the logistic regression
- Simple linear model leads to a generalisation of synthetic likelihood
- L_1 penalty on β for weighing and selecting summary statistics

Application to ARCH model

- Model:

$$x^{(t)} = \theta_1 x^{(t-1)} + e^{(t)} \tag{15}$$

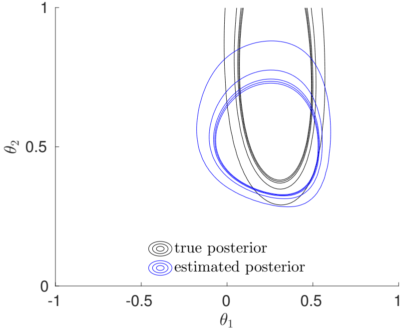
$$e^{(t)} = \xi^{(t)} \sqrt{0.2 + \theta_2 (e^{(t-1)})^2} \tag{16}$$

  $\xi^{(t)}$ and $e^{(0)}$ independent standard normal r.v., $x^{(0)} = 0$
- 100 time points
- Parameters: $\theta_1 \in (-1, 1), \quad \theta_2 \in (0, 1)$
- Uniform prior on θ_1, θ_2

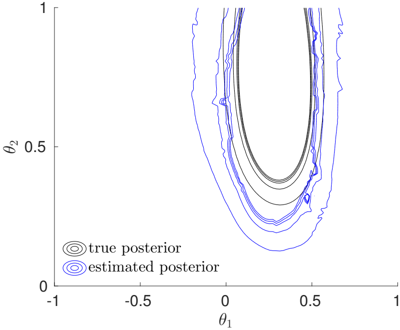
Application to ARCH model

- Summary statistics:
  - auto-correlations with lag one to five
  - all (unique) pairwise combinations of them
  - a constant
- To check robustness: 50% irrelevant summary statistics (drawn from standard normal)
- Comparison with synthetic likelihood with equivalent set of summary statistics (relevant sum. stats. only)

Example posterior

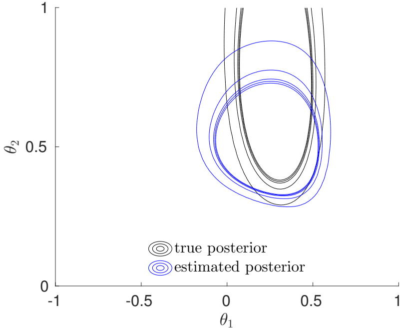


(a) synthetic likelihood

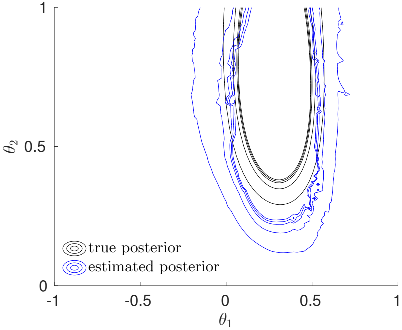


(b) proposed method

Example posterior



(c) synthetic likelihood

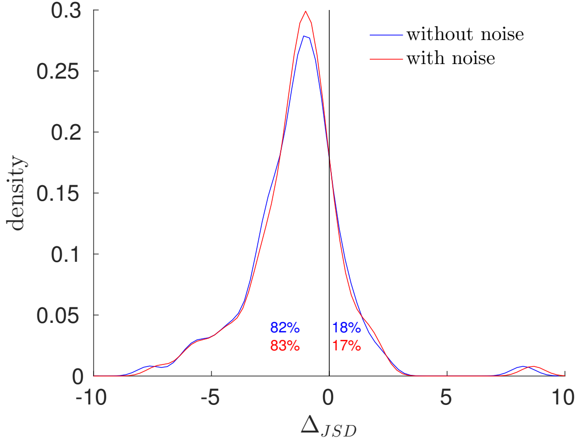


(d) proposed method subject to noise

Systematic analysis

- Jensen-Shannon div between estimated and true posterior
- Point-wise comparison with synthetic likelihood (100 data sets)

$$\Delta_{\text{JSD}} = \text{JSD for proposed method} - \text{JSD for synthetic likelihood}$$



Application to Ricker model

- Model

$$x^{(t)}|N^{(t)}, \phi \sim \mathrm{Poisson}(\phi N^{(t)}) \tag{17}$$

$$\log N^{(t)} = \log r + \log N^{(t-1)} - N^{(t-1)} + \sigma e^{(t)} \tag{18}$$

$$t = 1, \ldots, 50, \qquad N^{(0)} = 0 \tag{19}$$

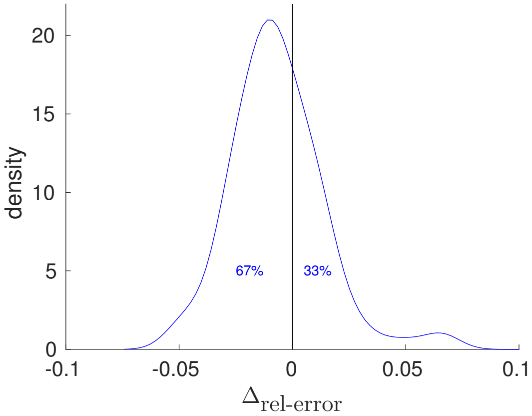
- Parameters and priors
  - log growth rate $\log r \sim \mathcal{U}(3, 5)$
  - scaling parameter $\phi \sim \mathcal{U}(5, 15)$
  - standard deviation $\sigma \sim \mathcal{U}(0, 0.6)$

Application to Ricker model

- Summary statistics: same as Simon Wood (Nature, 2010)
- 100 inference problems
- For each problem, relative errors in posterior means were computed
- Point-wise comparison with synthetic likelihood

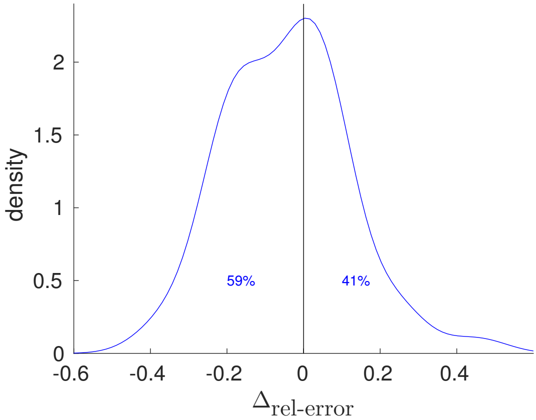
Results for log r

$$\Delta_{\text{rel error}} = \text{rel error proposed method} - \text{rel error synth likelihood}$$



Results for σ

$$\Delta_{\text{rel error}} = \text{rel error proposed method} - \text{rel error synth likelihood}$$



Results for ϕ

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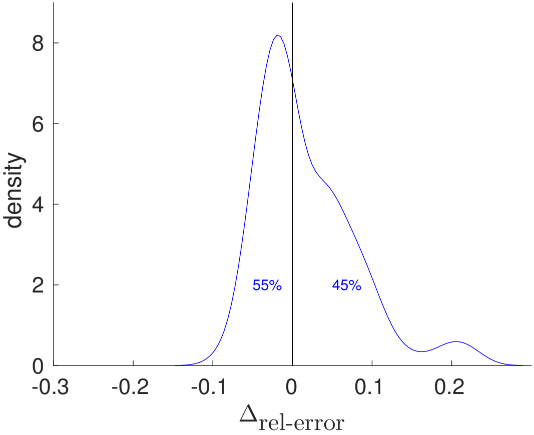

Observations

- Compared two auxiliary models: exponential vs Gaussian family
- For same summary statistics , typically more accurate inferences for the richer exponential family model
- Robustness to irrelevant summary statistics thanks to L_1 regularisation

Conclusions

- Background and previous work on inference with simulator-based / implicit statistical models
- Our work on:
  - Framing the posterior estimation problem as a density ratio estimation problem
  - Estimating the ratio with logistic regression
  - Using regularisation to automatically select summary statistics
- Multitude of research possibilities:
  - Choice of the auxiliary model
  - Choice of the loss function used to estimate the density ratio
  - Combine with Bayesian optimisation framework to reduce computational cost

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More results and details in arXiv:1611.10242v1