Approximate Bayesian Computation with Domain Expert in the Loop

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Outline

Inference from data

Setting:

- Let data $\mathbf{y}_{\mathrm{obs}} = \{y_{\mathrm{obs},i}\}_{i=1}^{n}$ be denoted by empirical distribution $\mathbb{Q}^n$.
- Model $\mathcal{M}_\Theta = \{\mathbb{P}_\theta : \theta \in \Theta \subset \mathbb{R}^q\}$ is a parametric family of distributions.

Estimation problem: Given data $\mathbf{y}_{\mathrm{obs}}$, estimate θ s.t. $\mathbb{Q}^n$ is “closest" to $\mathbb{P}_\theta$.

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Estimation problem: Given data $\mathbf{y}_{\text{obs}}$, estimate θ s.t. $\mathbb{Q}^n$ is “closest" to $\mathbb{P}_\theta$.

Classical estimation techniques such as

$$\text{Bayesian inference:} \quad p(\theta|\mathbf{y}_{\text{obs}}) \propto p(\mathbf{y}_{\text{obs}}|\theta)p(\theta)$$

$$\text{Maximum Likelihood (ML):} \quad \hat{\theta}_{\text{ML}} = \underset{\theta}{\operatorname{argmax}}\, p(\mathbf{y}_{\text{obs}}|\theta)$$

require access to the likelihood function.

Problem: Many models have intractable likelihoods

The likelihood function cannot be evaluated numerically, or approximated in reasonable computation time.

Therefore, standard estimation techniques are unrealizable.

Causes of intractable likelihood:

- The model is simply too complex.
- Variables that are important for model description are unobserved.
- The likelihood function has not been derived yet for a newly constructed model.

Such models are called:

- Simulators
- Implicit models
- Generative models

Simulators in the Sciences

Physical sciences and engineering:

- Population genetics [Pritchard et al., 1999]
- Ecology and evolution [Beaumont, 2010]
- Astrophysics [Akeret et al., 2015]
- Epidemiology [Kypraios et al., 2017]
- Radio communications [Bharti et al., 2021]
- Atmospheric science [Kopka et al., 2016]
- Economics [Dyer et al., 2022]

Solution: use likelihood-free inference methods based on simulating from the model

Outline

Approximate Bayesian Computation (ABC)

ABC is a likelihood-free inference method that permits sampling from the approximate posterior of a model, given that it is easy to simulate from.

Rejection ABC algorithm

- Sample $\theta^* \sim p(\theta)$
- Simulate data from model, $\mathbf{y}^* \sim \mathbb{P}_{\theta^*}$
- If $\rho(S(\mathbf{y}_{\text{obs}}), S(\mathbf{y}^*)) < \epsilon$, accept θ^*

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Here

- $\rho(\cdot\,,\,\cdot)$ is a distance metric (typical choice is Euclidean distance)
- $S(\cdot)$ is the summarizing function
- ϵ is a tolerance threshold
- Accepted samples $\theta_1, \ldots, \theta_N$ are iid from the approximate posterior:

$$p(\theta|\rho(S(\mathbf{y}_{\mathrm{obs}}), S(\mathbf{y}) < \epsilon) \approx p(\theta|\mathbf{y}_{\mathrm{obs}})$$

Approximate Bayesian Computation (ABC) — contd.

The “approximation" in Bayesian inference arises due to

- use of tolerance threshold in accepting parameter samples
- summarizing the data into a few statistics. If $S(\cdot)$ is a *sufficient statistic* of $\mathbf{y}$, then

$$p(\theta|\rho(S(\mathbf{y}^*), S(\mathbf{y}_{\text{obs}})) < \epsilon) = p(\theta|\rho(\mathbf{y}^*, \mathbf{y}_{\text{obs}}) < \epsilon)$$

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Ingredients required for implementing an ABC algorithm:

- distance metric $\rho(\cdot, \cdot)$
- summary statistics $S(\cdot)$
- tolerance threshold ϵ

$$\rho(S(\mathbf{y}_{\text{obs}}), S(\mathbf{y}^*)) < \epsilon$$

Approximate Bayesian Computation (ABC) — contd.

Choosing ϵ

- In practice, select ϵ as a small percentile of the simulated distances, i.e. given $\{(\boldsymbol{\theta}_i^*, S(\mathbf{y}_i^*))\}_{i=1}^M$, accept the ϵM samples of $\boldsymbol{\theta}_i^*$ with the least $\rho(S(\mathbf{y}), S(\mathbf{y}_i^*))$

Choose $\rho(\cdot, \cdot)$

- Euclidean distance for summary-based ABC
- Integral probability metrics such as maximum mean discrepancy, Wasserstein distance

Approximate Bayesian Computation (ABC) — contd.

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Choosing $S(\cdot)$

- The choice of statistics is non-trivial as it involves trade-off between
    1. information loss due to summarization
    2. curse of dimensionality
- Fundamental unsolved problem in ABC

Choosing Summary Statistics

In practice, domain experts manually handcraft and select statistics:

- laborious and time-consuming
- involves multiple trial-and-error steps
- takes up majority of the time of likelihood-free inference projects

Hence, domain knowledge is vital for constructing summaries.

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Hence, domain knowledge is vital for constructing summaries.

Existing methods given a pool of candidate statistics:

- Subset selection (Joyce & Marjoram, 2008)
- Projection techniques (Fearnhead & Prangle, 2012)
- Regression adjustment (Beaumont et al., 2010)

However, performance of these methods degrade when

- number of available model simulations is limited (low-simulation regime)
- model is misspecified, i.e., $\mathbb{Q}^n \notin \mathcal{M}_\Theta$

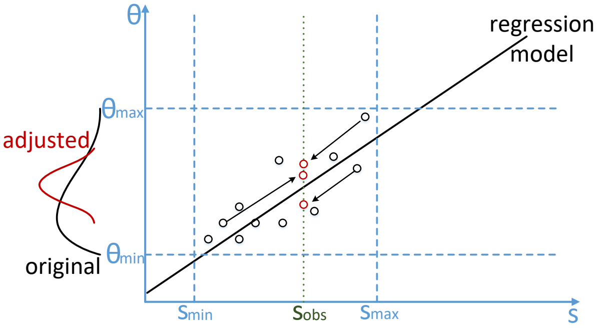
Outline

Case study: Regression-ABC methods

Given accepted samples $(\theta_i, \mathbf{s}_i)_{i=1}^{n_\epsilon}$, regression-ABC methods account for the difference between the simulated and observed statistic by adjusting the parameter values using model

$$\theta_i = \varphi(\mathbf{s}_i) + \varepsilon_i, \quad i = 1, \ldots, n_\epsilon.$$

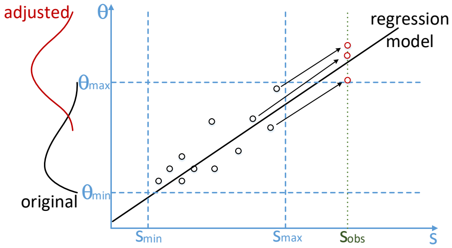
- $\mathbf{s}$: statistics vector
- $\varphi(\cdot)$: conditional expectation $\mathbb{E}[\theta|\mathbf{s}]$
- ε_i: the residuals
- Adjusted samples: $\tilde{\theta}_i = \hat{\varphi}(\mathbf{s}_{\text{obs}}) + \hat{\varepsilon}_i$



Failure of regression-ABC methods

Model misspecification

- Regression-ABC can yield erroneous results under misspecification.
- Approx. posterior can lie beyond prior range.



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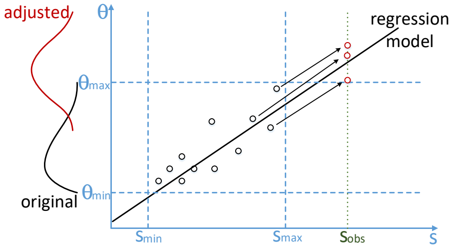
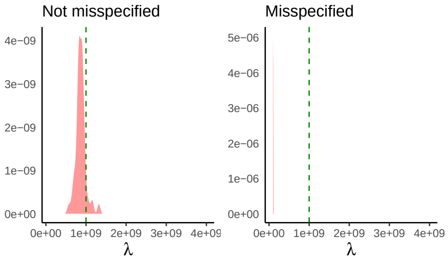
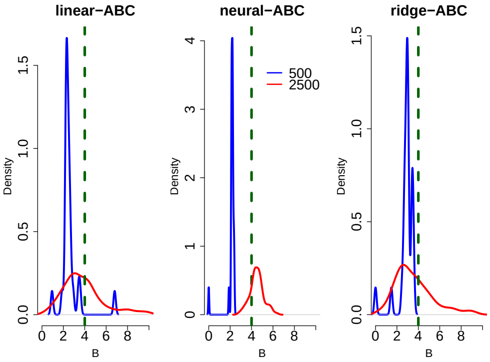




Failure of regression-ABC methods

Low-simulation regime

- When model is expensive, number of simulations are limited.
- Regression is susceptible to overfitting.
- ABC posteriors can be concentrated far from the true value.



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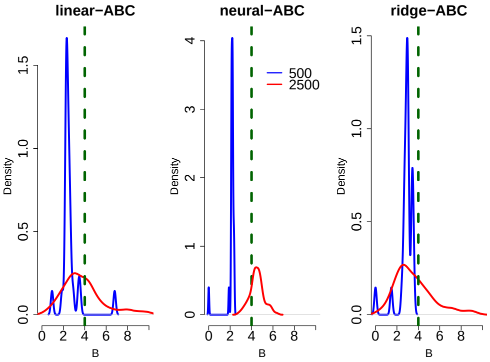
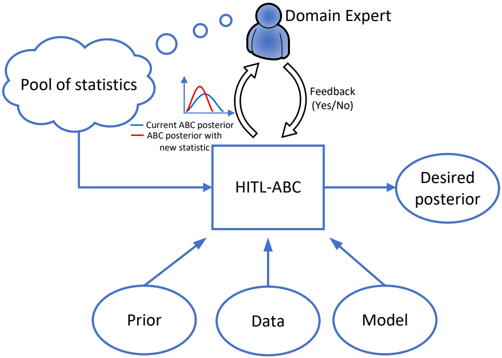


Can we mitigate these issues by leveraging domain expertise?

Outline

Human-in-the-loop (HITL) ABC

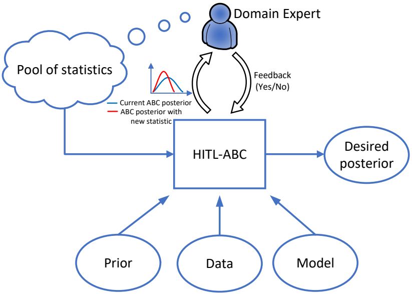
- Involve the expert in the inference procedure
- Elicit domain knowledge about statistics
- Assumptions:
  - Expert knowledge is tacit
  - Querying the expert is costly



Problem setting

Human-in-the-loop (HITL) ABC

- Pool of statistics: $\mathcal{S} = \{s_1, s_2, \ldots, s_w\}$
- Indicator of inclusion or exclusion of s_j: $\gamma_j \in \{0, 1\}$
- With each vector **s**, we have associated $\gamma = [\gamma_1, \ldots, \gamma_w]^\top$
- ABC posterior: $p^{\epsilon}_{\mathrm{ABC}}(\theta|\mathbf{y}_{\mathrm{obs}}, \gamma)$
- Let γ^* represent the “desired" statistics vector
- **Goal:** converge towards γ^* by querying expert about $\mathcal{S}$



Expert feedback model

Human-in-the-loop (HITL) ABC

Formulate expert feedback as a probabilistic model

- Expert provides binary feedback $f_j \in \{0, 1\}$ about s_j
- Model f_j as a noisy version of γ_j:

$$\gamma_j \sim \text{Bernoulli}(\rho_j),$$
$$f_j|\gamma_j \sim \gamma_j \text{Bernoulli}(\pi) + (1 - \gamma_j)\text{Bernoulli}(1 - \pi).$$

- $\pi \in [0, 1]$: the level of noise
- ρ_j: prior probability of selecting s_j
- Let $\mathcal{F}$ be the set of feedback obtained
- $p(\boldsymbol{\gamma}|\mathcal{F})$ available in closed-form

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ABC posterior based on $\mathcal{F}$:

$$p^{\epsilon}_{\text{ABC}}(\theta|\mathbf{y}_{\text{obs}}, \mathcal{F}) := \sum_{\boldsymbol{\gamma} \in \{0,1\}^w} p^{\epsilon}_{\text{ABC}}(\theta|\mathbf{y}_{\text{obs}}, \boldsymbol{\gamma}) p(\boldsymbol{\gamma}|\mathcal{F})$$

Sequential experimental design

Human-in-the-loop (HITL) ABC

We design a sequential Bayesian experiment to select next statistic to query.

At iteration $k+1$, we select s_{j^*}, where

$$j^* = \underset{j \notin \mathcal{J}_k}{\arg\max} \quad \mathrm{KL}[p^{\epsilon}_{\mathrm{ABC}}(\theta|\mathbf{y}_{\mathrm{obs}}, \mathcal{F}_k, \tilde{\mathcal{F}}_j) \,||\, p^{\epsilon}_{\mathrm{ABC}}(\theta|\mathbf{y}_{\mathrm{obs}}, \mathcal{F}_k)]$$

- $\mathcal{J}_k$: set of indices of statistics queried after k iterations
- Estimate KL from samples as per [Perez-Cruz, 2008]

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- $\mathcal{J}_k$: set of indices of statistics queried after k iterations
- Estimate KL from samples as per [Perez-Cruz, 2008]
- **Stopping criterion:** when utility of next statistic < δ
- **Output:** ABC posterior $p^{\epsilon}_{\text{ABC}}(\theta|\mathbf{y}_{\text{obs}}, \hat{\gamma})$, where

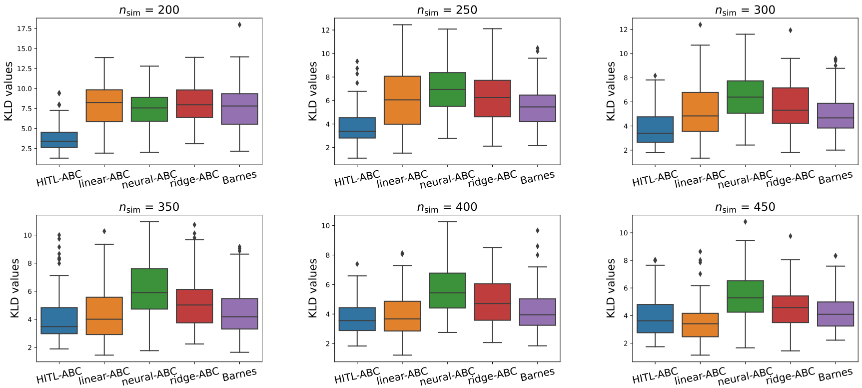
$$\hat{\gamma}_{k,j} = \begin{cases} \underset{\gamma_j \in \{0,1\}}{\arg\max}\, p(\gamma_j|f_j), & \text{if } j \in \mathcal{J}_k \\ 0, & \text{otherwise.} \end{cases}$$

Outline

Results

Low-simulation regime

- Model: g-and-k distribution (4 parameters)
- Total 15 statistics in the pool (4 informative, 6 correlated, 5 noisy)
- HITL-ABC outperforms other methods for $n_{\mathrm{sim}} \leq 350$, otherwise at par.
- Lack of simulations is compensated by expert's feedback.

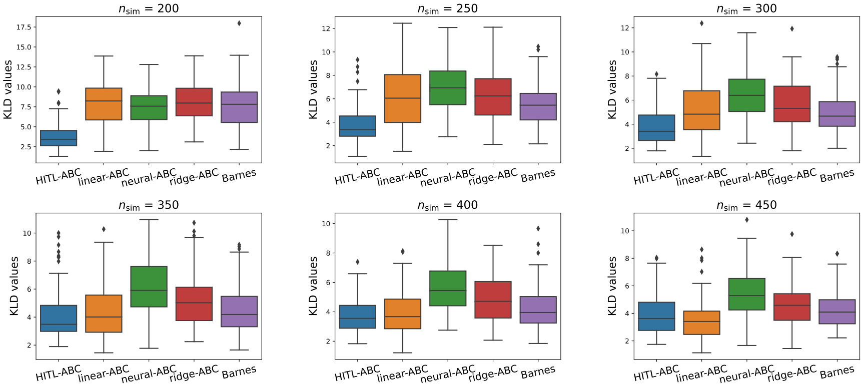


Results

Low-simulation regime

Table: Average number of expert feedback required.

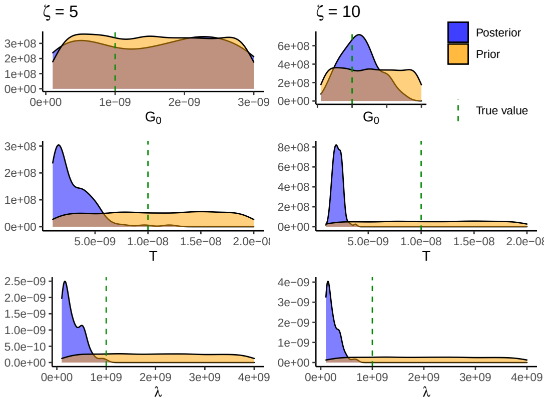
n_{sim}	200	250	300	350	400	450
HITL-ABC	**10.1**	**8.5**	**8.3**	**6.3**	**6.0**	**6.3**
Random	13.8	13.6	13.4	13.3	13.1	13.4



Results

Model misspecification

- Radio propagation model (high-dimensional, complex-valued time series)
- Expert is shown inference results, and can detect misspecified statistics
- Parameters $[G_0, T, \lambda]$, 6 statistics (one mismatch)
- ζ: misspecification level



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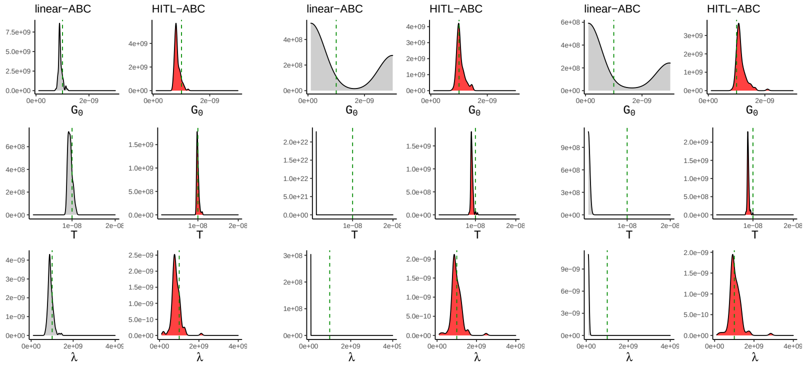

(a) $\zeta = 0$ (b) $\zeta = 5$ (c) $\zeta = 10$

- When $\zeta > 0$, performance of linear regression ABC seriously degrades
- Removing mismatched statistic improves performance

Conclusion

- We introduce the first ABC method that actively leverages domain knowledge from experts in order to select summary statistics.
- With fairly limited effort from the expert (answering yes/no when presented with a few statistics), we are able to outperform the regression-ABC methods in situations where the simulation budget is low.
- Involving the experts in the ABC method gives us the opportunity to handle misspecified models, something the existing methods fail in.

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