Inference under discrepancy

Richard Wilkinson

University of Sheffield

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Data generating process

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If $G = F_{\theta_0} \in \mathcal{F}$ then we know what to do[1].

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Interest lies in inference of θ not calibrated prediction.

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An appealing idea

Kennedy an O'Hagan 2001

Lets acknowledge that most models are imperfect.

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Can we expand the class of models by adding a Gaussian process (GP) to our simulator?

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This greatly expands $\mathcal{F}$ into a non-parametric world.

An appealing, but flawed, idea

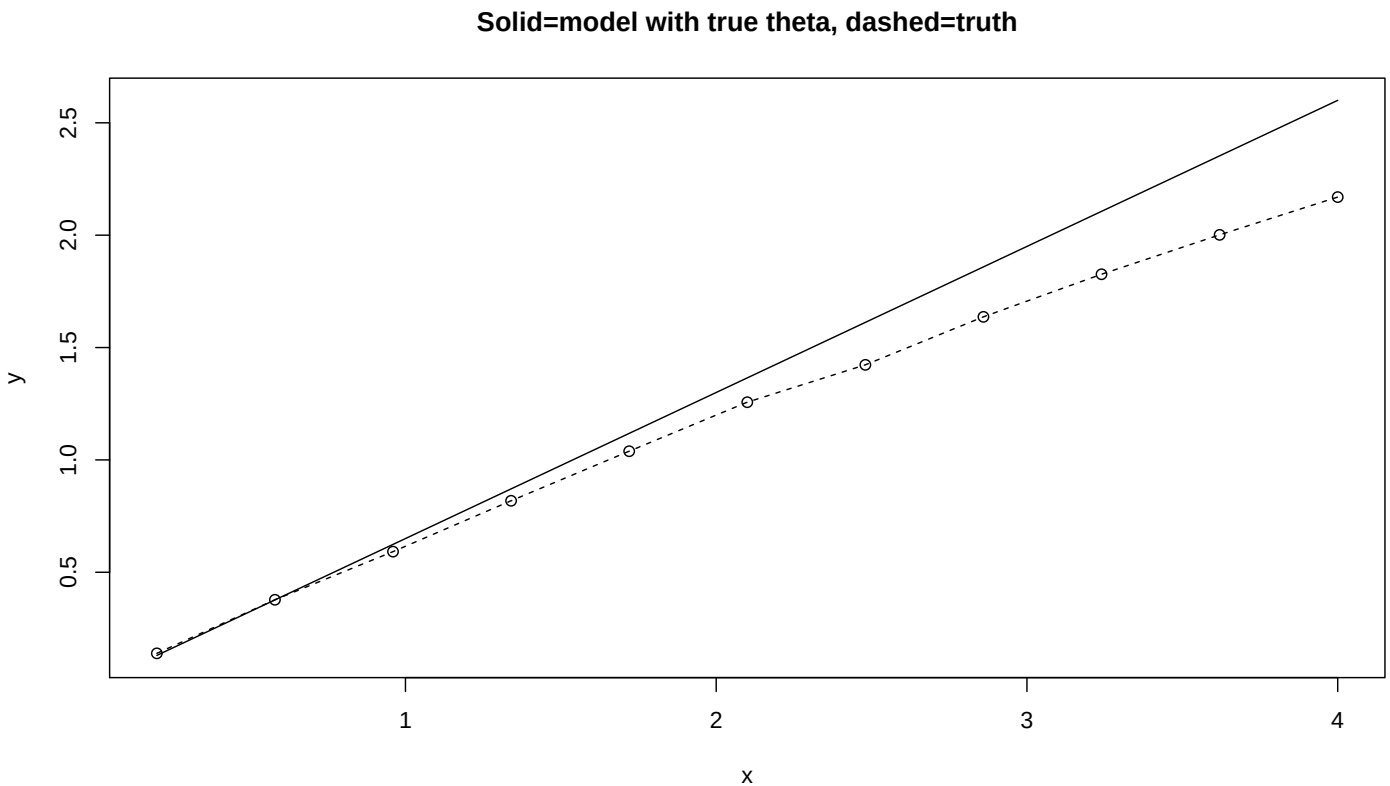
Kennedy and O'Hagan 2001, Brynjarsdottir and O'Hagan 2014

Simulator

$$f_\theta(x) = \theta x$$

Reality

$$g(x) = \frac{\theta x}{1 + \frac{x}{a}} \quad \theta = 0.65, a = 20$$



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An appealing, but flawed, idea

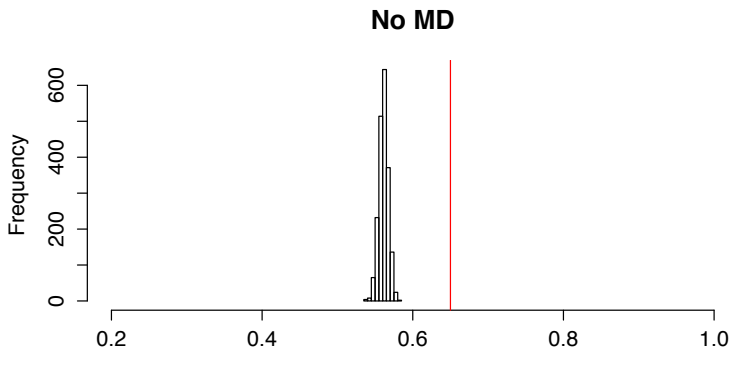
Bolting on a GP can correct your predictions, but won't necessarily fix your inference,e.g.

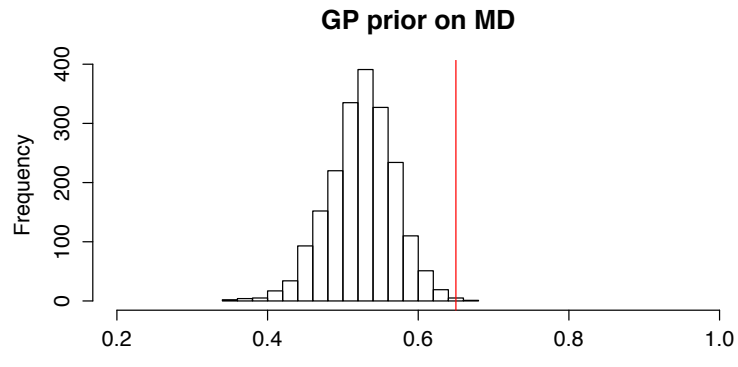
- No discrepancy:

$$y = f_\theta(x) + N(0, \sigma^2),$$
$$\theta \sim N(0{,}100), \sigma^2 \sim \Gamma^{-1}(0.001, 0.001)$$

- GP discrepancy:

$$y = f_\theta(x) + \delta(x) + N(0, \sigma^2),$$
$$\delta(\cdot) \sim GP(\cdot, \cdot)$$





Dangers of non-parametric model extensions

There are (at least) two problems with this approach:

- We may still find $G \notin \mathcal{F}$
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  - A GP is an incredibly complex infinite dimensional model, which is not necessarily identified even asymptotically. The posterior can concentrate not on a point, but on some sub manifold of parameter space, and the projection of the prior on this space continues to impact the posterior even as more and more data are collected.

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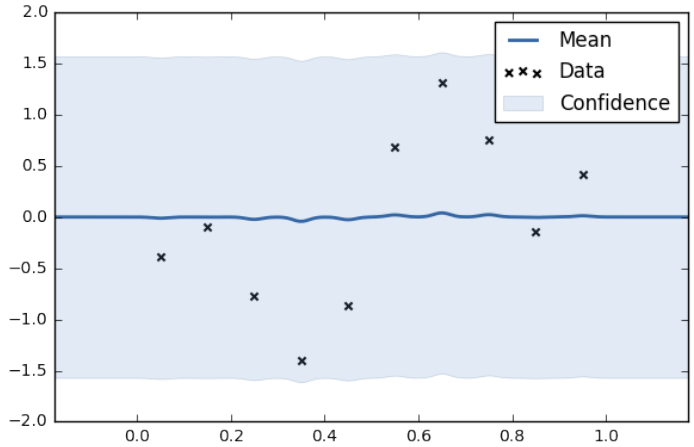
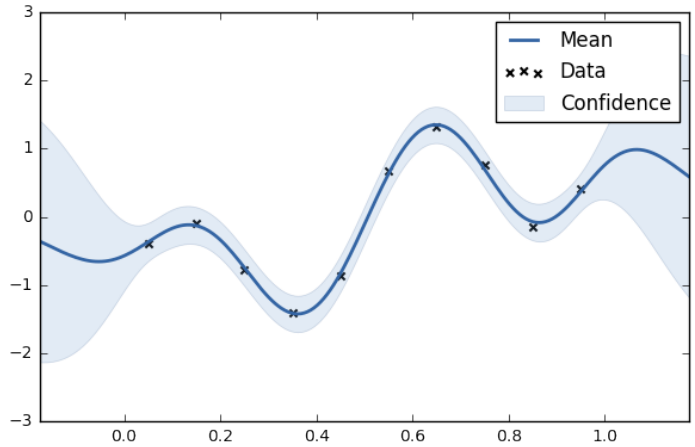
  - Brynjarsdottir and O'Hagan 2014 try to model their way out of trouble with prior information - which is great if you have it.

- We can also have problems finding the true optima for the hyperparameters, even in 1d problems:





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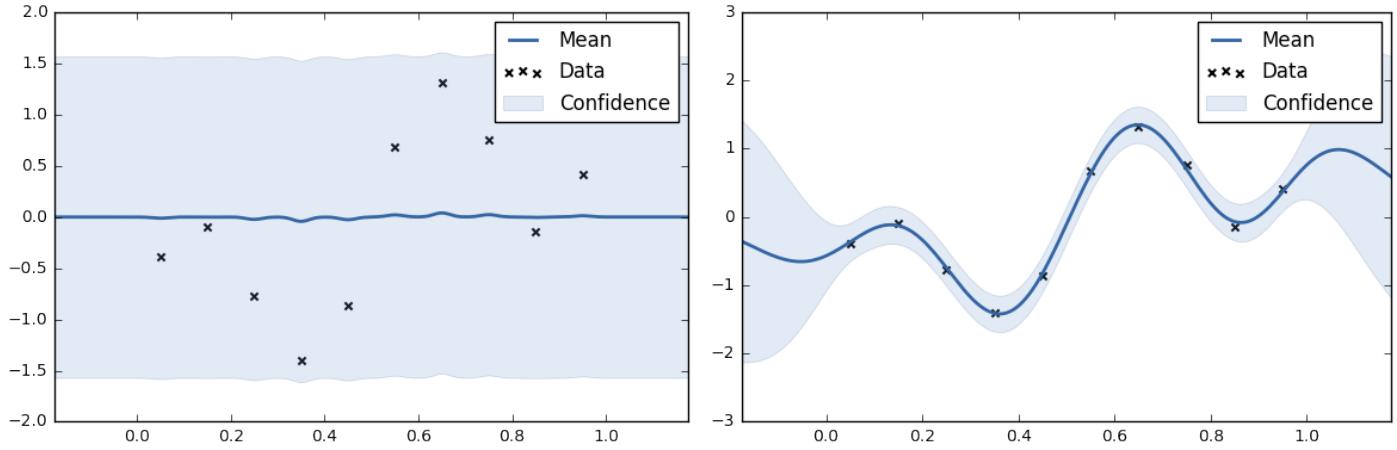

- Wong et al 2017 impose identifiability (for δ and θ) by giving up and identifying

$$\theta^* = \arg\min_{\theta} \int (\zeta(x) - f_\theta(x))^2 d\pi(x)$$

ROYAL STATISTICAL SOCIETY
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A frequentist approach to computer model calibration

Inferential approaches

- Maximum likelihood/minimum-distance
- Bayes(ish)
- History matching (HM)/ABC type methods (thresholding)

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We'll consider how they behave for well-specified and mis-specified models.

Try to understand why (at least anecdotally) HM and ABC seem to work well in mis-specified cases.

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Big question[2] is what properties would we like our inferential approach to possess.

[2] To which I have no answer

Maximum likelihood

Maximum likelihood estimator

$$\hat{\theta}_n = \arg\max_{\theta} l(y|\theta)$$

If $G = F_{\theta_0} \in \mathcal{F}$, then (under some conditions)

$$\hat{\theta}_n \to \theta_0 \text{ almost surely as } \quad n \to \infty$$

$$\sqrt{n}(\hat{\theta}_n - \theta_0) \overset{d}{\Rightarrow} N(0, \mathcal{I}^{-1}(\theta_0))$$

Asymptotic consistency, efficiency, normality.

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Asymptotic consistency, efficiency, normality.
If $G \notin \mathcal{F}$

$$\hat{\theta}_n \to \theta^* = \arg\min_{\theta} D_{KL}(G, F_\theta) \text{ almost surely}$$

$$= \arg\min_{\theta} \int \log \frac{dG}{dF_\theta} dG$$

$$\sqrt{n}(\hat{\theta}_n - \theta_0) \overset{d}{\Rightarrow} N(0, V^{-1})$$

Bayes

Bayesian posterior

$$\pi(\theta|y) \propto \pi(y|\theta)\pi(\theta)$$

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Often with non-parametric models (eg GPs), we don't even get this convergence to the pseudo-true value due to lack of identifiability.

ABC (Approximate Bayesian computation)

Rejection Algorithm

- Draw θ from prior $\pi(\cdot)$
- Accept θ with probability $\propto \pi(y \mid \theta)$

Accepted θ are independent draws from the posterior distribution, $\pi(\theta \mid D)$.

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Accepted θ are independent draws from the posterior distribution, $\pi(\theta \mid D)$.
If the likelihood, $\pi(D|\theta)$, is unknown:

'Mechanical' Rejection Algorithm

- Draw θ from $\pi(\cdot)$
- Simulate $y' \sim \pi(y|\theta)$ from the computer model
- Accept θ if $y = y'$, i.e., if computer output equals observation

Rejection ABC

If $\mathbb{P}(D)$ is small (or D continuous), we will rarely accept any θ. Instead, there is an approximate version:

Uniform Rejection Algorithm

- Draw θ from $\pi(\theta)$
- Simulate $y' \sim \pi(y|\theta)$
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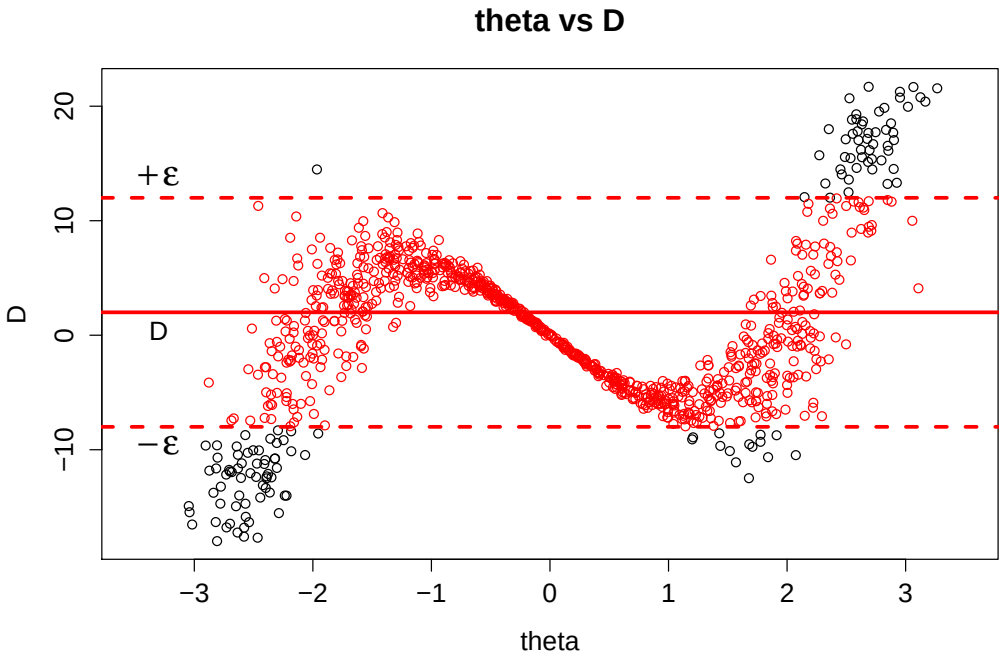
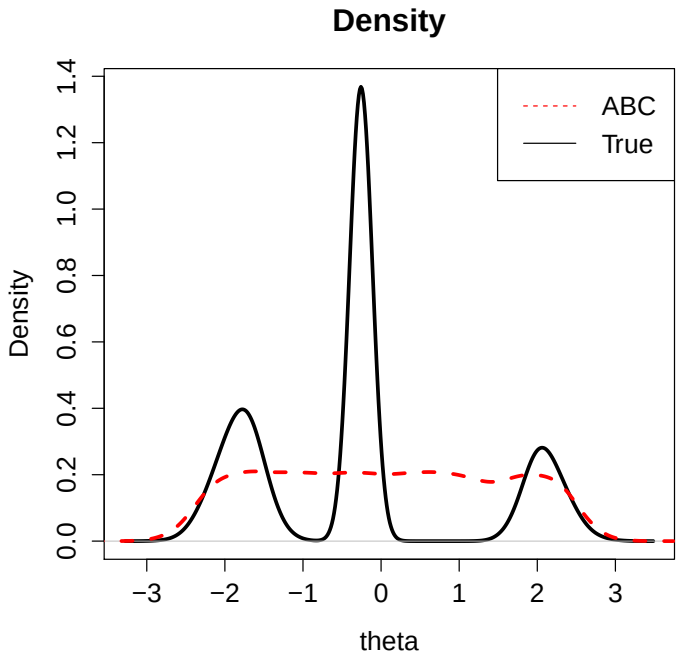
ϵ reflects the tension between computability and accuracy.

- As $\epsilon \to \infty$, we get observations from the prior, $\pi(\theta)$.
- If $\epsilon = 0$, we generate observations from $\pi(\theta \mid y)$.

$\epsilon = 10$

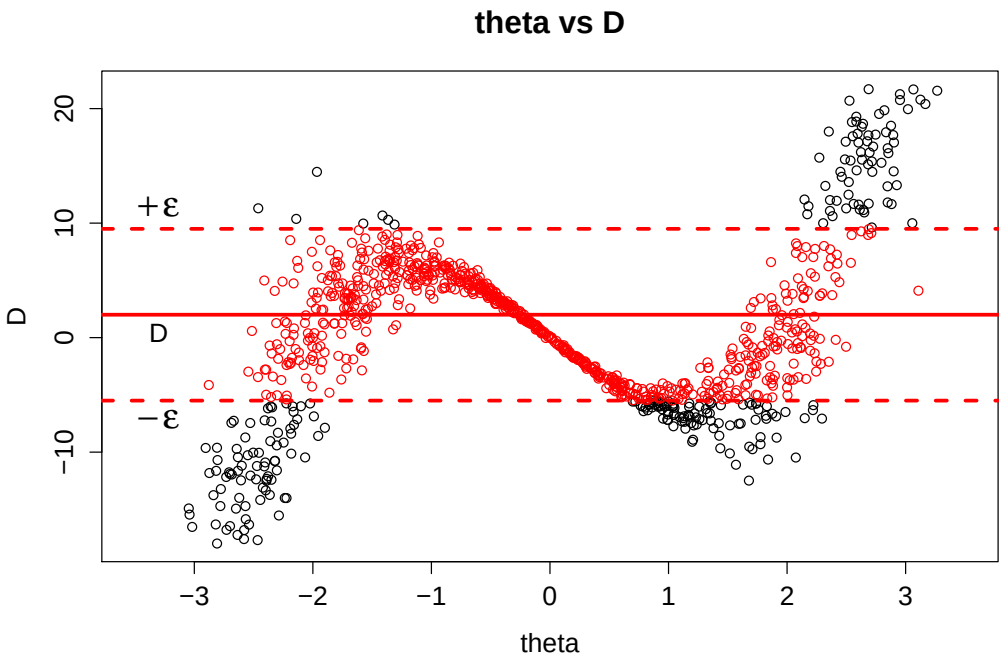




$$\theta \sim U[-10, 10], \qquad y \sim N(2(\theta + 2)\theta(\theta - 2), 0.1 + \theta^2)$$

$$\rho(y, y') = |y - y'|, \qquad y = 2$$

$\epsilon = 7.5$


theta vs D
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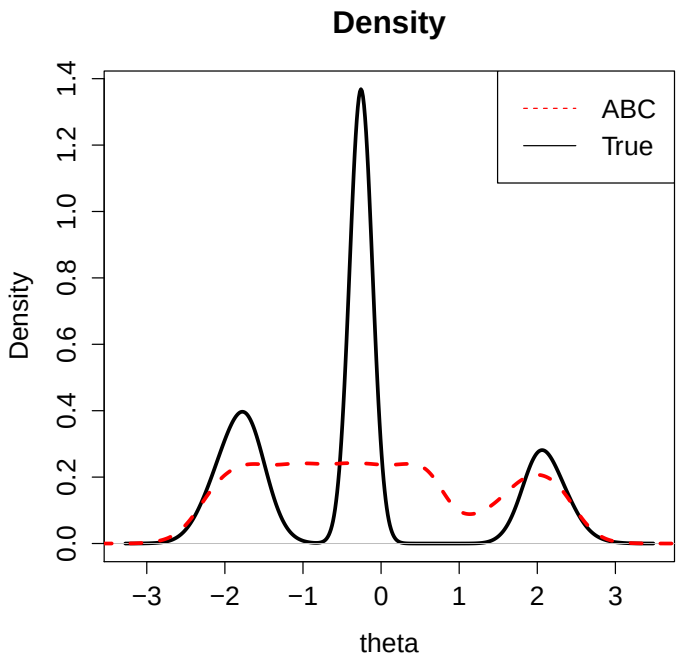
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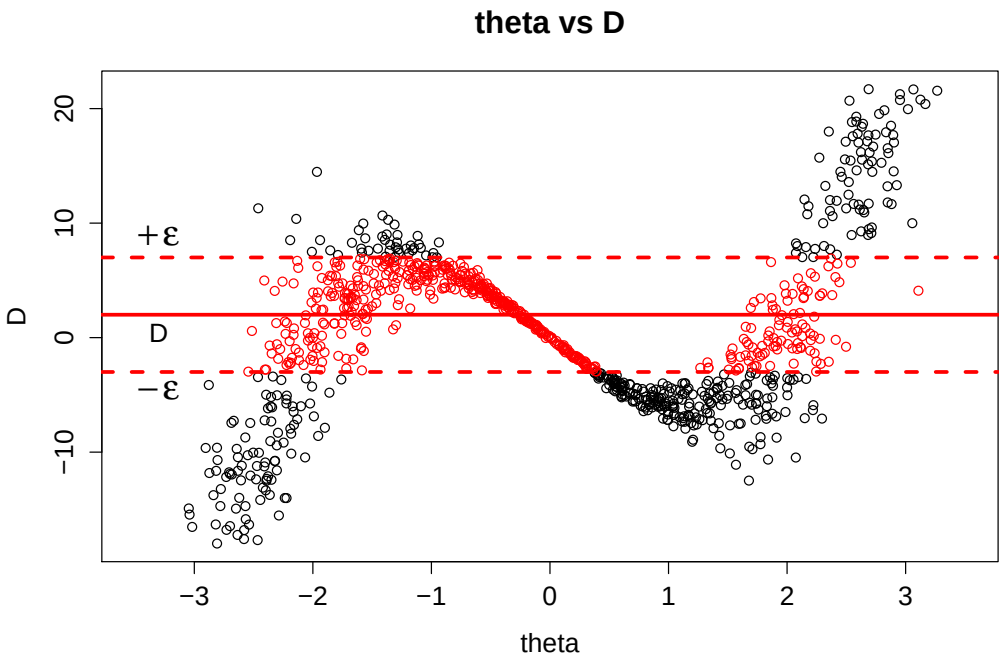
$\epsilon = 5$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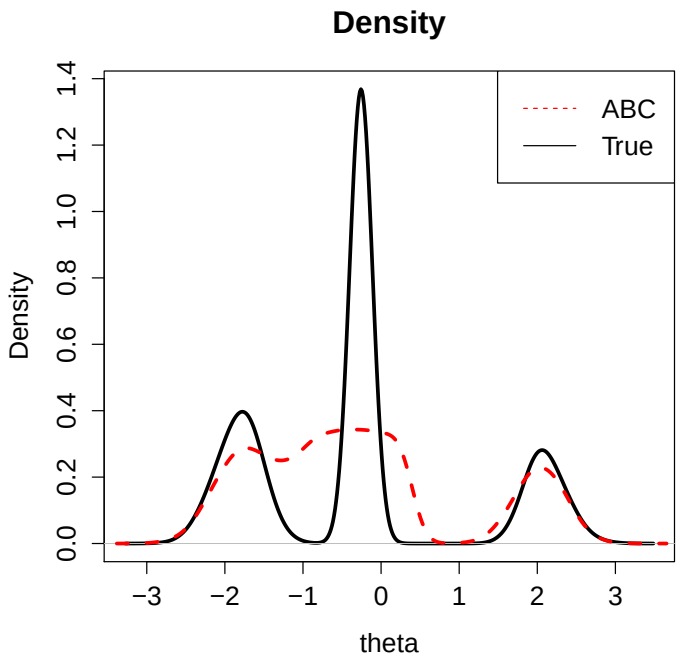
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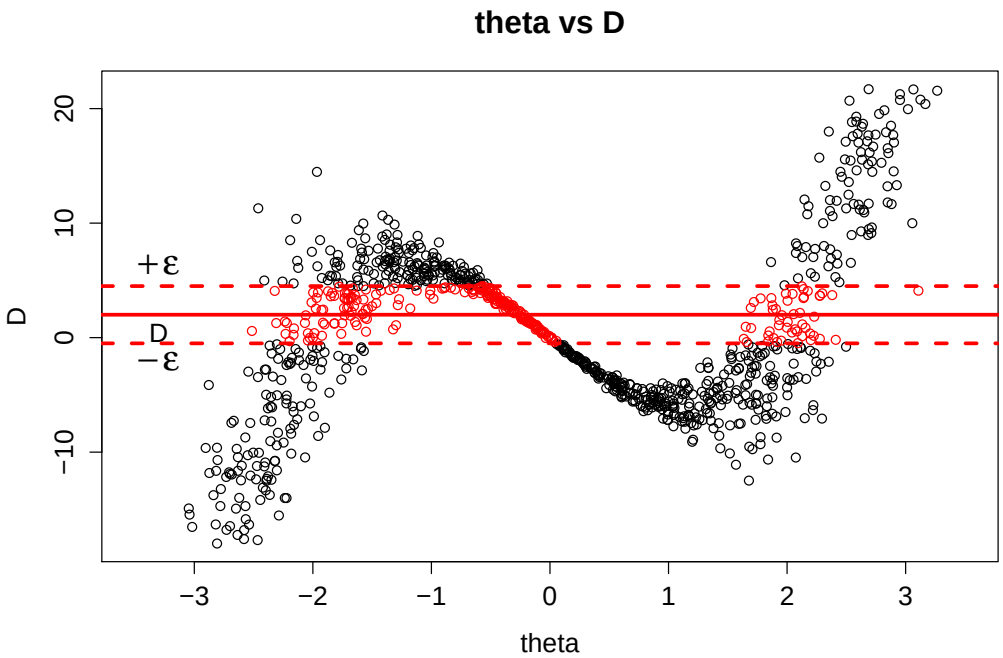
$\epsilon = 2.5$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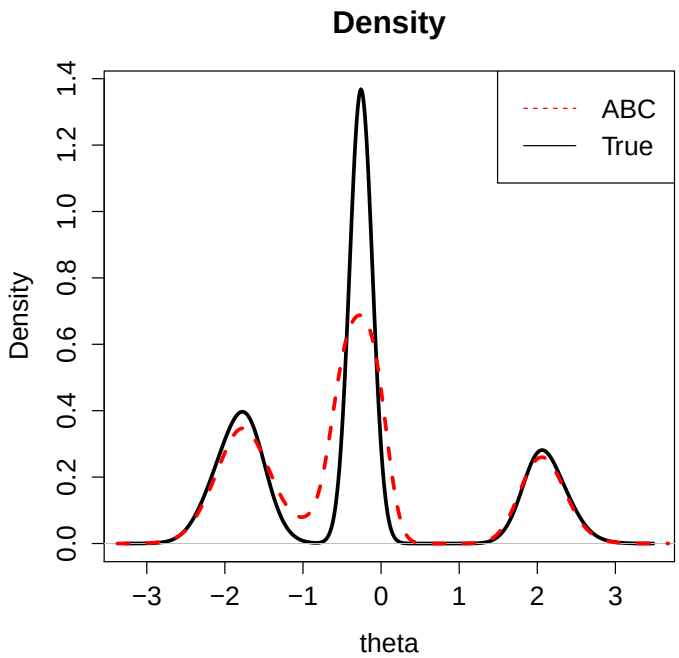
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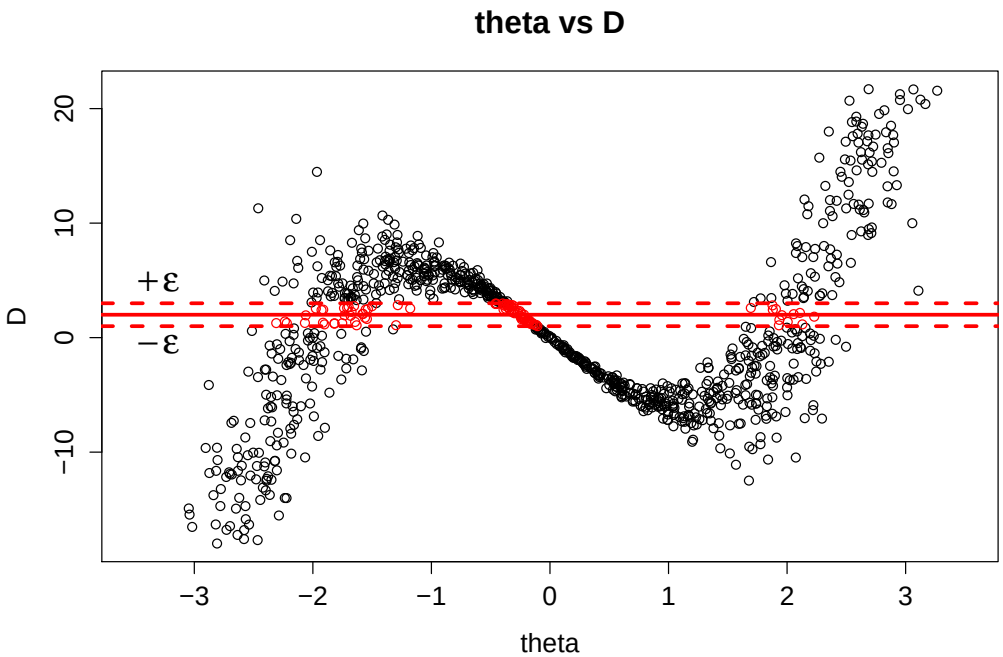
$\epsilon = 1$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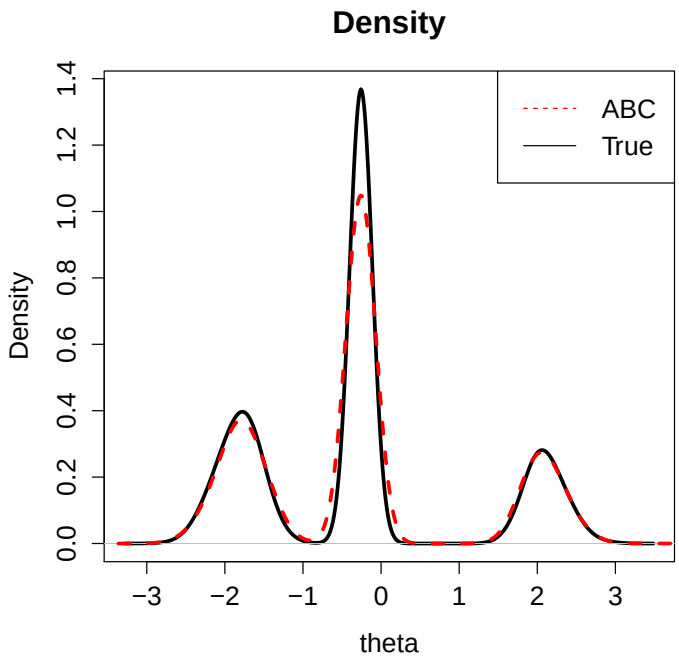
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History matching and ABC

History matching seeks to find a NROY set

$$\mathcal{P}_\theta = \{\theta : S_{HM}(\hat{F}_\theta, y) \leq 3\}$$

where

$$S_{HM}(F_\theta, y) = \frac{|\mathbb{E}_{F_\theta}(Y) - y|}{\sqrt{\mathbb{V}\text{ar}_{F_\theta}(Y)}}$$

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They have thresholding of a score in common and are algorithmically comparable.

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- Ease of specification?

Generalized scores

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$$G = \arg\min_F \mathbb{E}_{Y \sim G} S(F, Y)$$

i.e. predicting G gives the best possibly score.

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Examples:

- Log-likelihood $S(F, y) = -\log f(y)$
- Tsallis-score $(\gamma - 1) \int f(x)^\alpha dx - \gamma f(y)^{\alpha - 1}$

Minimum scoring rule estimation (Dawid *et al.* 2014 etc) uses

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For proper scores

$$\begin{aligned}\mathbb{E}_{\theta_0}\left(\frac{\partial}{\partial\theta}S(F_\theta, y)\Big|_{\theta=\theta_0}\right) &= \frac{\partial}{\partial\theta}\mathbb{E}_{\theta_0}S(F_\theta, y)\Big|_{\theta=\theta_0} \\ &= 0\end{aligned}$$

so we have an unbiased estimating equation, and hence get asymptotic consistency for well-specified models. We also get asymptotic normality.

Dawid *et al.* 2014 show that if

- $\nabla_\theta f_\theta(x)$ is bounded in x for all θ
- Bregman gauge of scoring rule is locally bounded

then the minimum scoring rule estimator $\hat{\theta}$ is B-robust

- i.e. it has bounded influence function

$$IF(x; \hat{\theta}, F_\theta) = \lim_{\epsilon \to 0} \frac{\hat{\theta}(\epsilon \delta_x + (1-\epsilon)F_\theta) - \hat{\theta}(F_\theta)}{\epsilon}$$

  i.e. if F_θ is infected by outlier at x, this doesn't unduly affect the inference.

Note both ABC and HM are B-robust in this sense, but using the log-likelihood is not.

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  i.e. if F_θ is infected by outlier at x, this doesn't unduly affect the inference.

Note both ABC and HM are B-robust in this sense, but using the log-likelihood is not.

What type of robustness do we want here?

Dawid *et al.* 2014 show that if

- $\nabla_\theta f_\theta(x)$ is bounded in x for all θ
- Bregman gauge of scoring rule is locally bounded

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J. R. Statist. Soc. B (2016)
78, *Part* 5, *pp.* 1103–1130

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They argue the update must be of the form

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via coherency arguments.
Note using log-likelihood as the loss function ($L(\theta, x) = -\log f_\theta(x)$) recovers Bayes.

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- Allows focus solely on the quantities of interest.
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Relates to the Bayes linear approach of Goldstein and Wooff which is also motivated by difficulties with specifying a complete model for the data.

HM and ABC thresholding

History matching was an approach designed for inference for mis-specified models.

$$S_{HM}(F_\theta) = \frac{|\mathbb{E}_{F_\theta}(Y) - y|}{\sqrt{\mathbb{V}\text{ar}_{F_\theta}(y)}}$$

Often applied in a Bayes linear type setting, with $\mathbb{V}\text{ar}_{F_\theta}(y)$ broken down into constituent parts

$$\mathbb{V}\text{ar}_{F_\theta}(y) = \mathbb{V}\text{ar}_{sim} + \mathbb{V}\text{ar}_{discrep} + \mathbb{V}\text{ar}_{emulator}$$

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Combined with the thresholding nature

$$\mathcal{P}_\theta = \{\theta : S_{HM}(\hat{F}_{\theta,y}) \leq 3\}$$

means we don't get asymptotic concentration.

- ABC shares similar properties if ϵ fixed at something reasonable.

$$\pi_\epsilon(\theta) \propto \pi(\theta)\mathbb{I}_{S(\hat{F}_\theta, y) \leq \epsilon}$$

  The indicator functions acts to add a ball of radius ϵ around the data, so that we only need to get within it.
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Also

- Allow for crude/simple discrepancy characterization.
- Some form of robustness arises from the scores used.

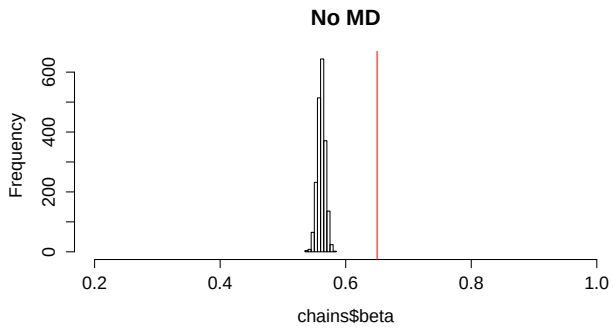
Brynjarsdottir *et al.* revisited

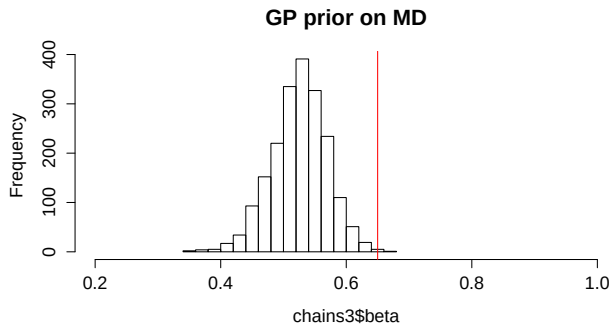
Simulator

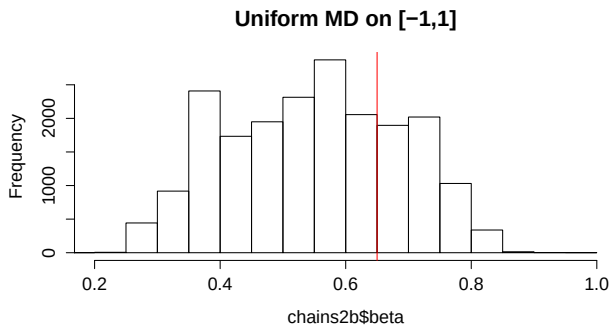
$$f_\theta(x) = \theta x$$

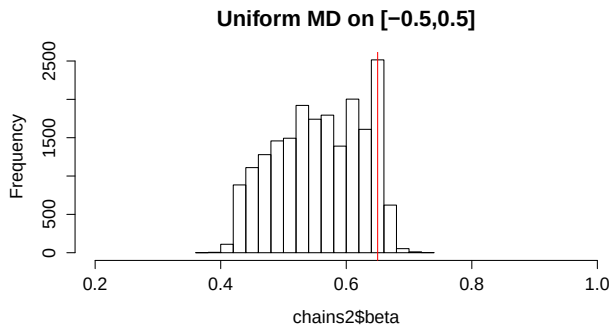
Reality

$$g(x) = \frac{\theta x}{1 + \frac{x}{a}} \quad \theta = 0.65, a = 20$$









Recent work in ABC

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- Bernton *et al.* 2017 look at Bayes like procedures based on the Wasserstein distance (get different pseudo-true value)
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Several papers (Frazier *et al.* 2017, Ridgeway 2017, ...) have studied asymptotic properties of ABC

- Consider version of ABC where we accept or reject according to

$$\rho(\eta(y), \eta(y'))$$

  where $y' \sim F_\theta(\cdot)$

Then if b_0 is limit of $\eta(y)$ and $b(\theta)$ the limit of $\eta(y')$, then they've studied convergence to

$$\theta^* = \arg\inf_\theta \rho(b_0, b(\theta))$$

as $\epsilon \to 0$.

This focus is again on prediction not inference.

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Thank you for listening!