Inference under discrepancy

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Model (complex simulator, finite dimensional parameter)

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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

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

An appealing, but flawed, idea

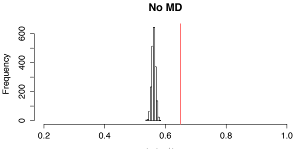
Kennedy and O'Hagan 2001, Brynjarsdottir and O'Hagan 2014

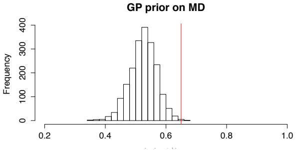
Simulator

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

Reality

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





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

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

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

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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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If $G \notin \mathcal{F}$

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

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

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Bayes

Bayesian posterior

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

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This also requires (a long list of) identifiability conditions to hold.

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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.

History matching and ABC

History matching seeks to find a NROY set

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

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

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These methods (anecdotally) seem to work better in mis-specified situations.

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They differ from likelihood based approaches in that

- They only use some aspect of the simulator output
  - Typically we hand pick which simulator outputs to compare, and weight them on a case by case basis.
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- Robustness to small mis-specifications?

Generalized scores

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S is a proper score if

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

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

- Encourages honest reporting

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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

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

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

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

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A general framework for updating belief distributions

Bissiri et al. 2016 consider updating prior beliefs when parameter θ is connected to observations via a loss function $L(\theta, y)$.

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via coherency arguments.
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- Allows focus solely on the quantities of interest.
  - Full Bayesian inference requires us to model the complete data distribution even when we're only interested in a low-dimensional summary statistic of the population.
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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

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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

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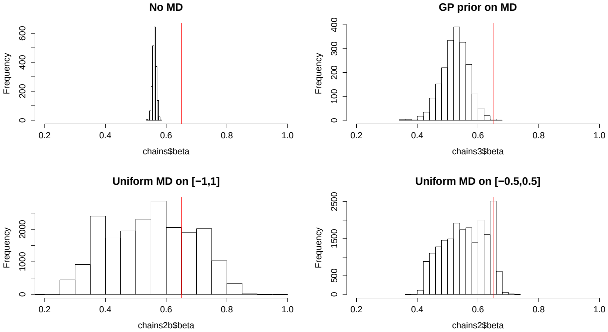

Recent work in ABC

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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!