Short course on Generalized Fiducial Inference

Parts of this short course are joint work with
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[a]NSF support acknowledged

Outline

- Introduction
- Definition
- Theoretical Results
- Applications
- Conclusions

Outline

Fiducial?

- Oxford English Dictionary
  - adjective technical (of a point or line) used as a fixed basis of comparison.
  - Origin from Latin fiducia ‘trust, confidence’
- Merriam-Webster dictionary
  1. taken as standard of reference *a fiducial mark*
  2. founded on faith or trust
  3. having the nature of a trust : fiduciary

Aims

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- My point of view is frequentist
  - Justified using asymptotic theorems and simulations.
  - GFI shows very good repeated sampling performance in applications.

Long, long, long time ago...

- Probabilistic uncertainty via Bayes Theorem:

$$P(\xi|X) = \frac{f(X|\xi)\pi(\xi)}{\int_\Xi f(X|\xi)\pi(\xi)d\xi}.$$

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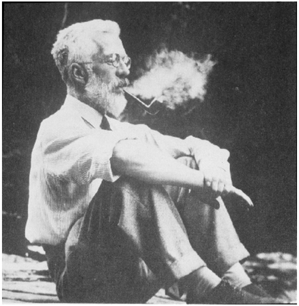
- Bayes-Laplace postulate:

  When nothing is known about the parameter in advance, let the prior be so that all values of the parameter are equally likely.

Long, long, time ago...



“Not knowing the chance of mutually exclusive events and knowing the chance to be equal are two quite different states of knowledge” R. A. Fisher

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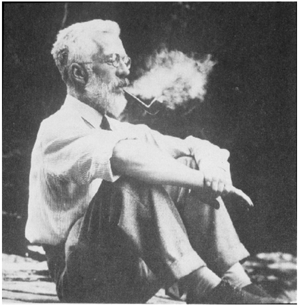

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It was a wild ride after that!

Brief history of fiducial inference

- Fisher (1922, 1930, 1935) no formal definition
- Lindley (1958) fiducial vs Bayes
- Fraser (1966) structural inference
- Dempster (1967) upper and lower probabilities
- Dawid and Stone (1982) theoretical results for simple cases.
- Barnard (1995) pivotal based methods.
- Weerahandi (1989, 1993), Krishnamoorthy generalized inference.

Fiducial Inspired Work in the New Millennium

        

- Dempster-Shafer calculus; Dempster (2008), Edlefsen, Liu & Dempster (2009)
- Inferential Models; Liu & Martin (2015)
- Confidence Distributions; Xie, Singh & Strawderman (2011), Schweder & Hjort (2016)
- Higher order likelihood, tangent exponential family, $r^\star$, Reid & Fraser (2010)
- Objective Bayesian inference, e.g., reference prior Berger, Bernardo & Sun (2009, 2012).
- Fiducial Inference H, Iyer & Patterson (2006), H (2009, 2013), H & Lee (2009), Taraldsen & Lindqvist (2013), Veronese & Melilli (2015), H, Iyer, Lai & Lee (2016)...

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- Common: quantify uncertainty using adequate data generating mechanism
- Difference: math details, interpretation, **replication**
  - My subjective opinion: If the underlying optimization problem is the same, the methods are the same.

Frequentist

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- **Modeling:** collection of distributions $\mathcal{P} = \{P_\xi\}_{\xi \in \Xi}$.

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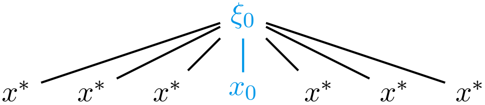

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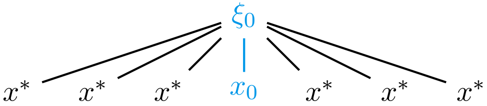

- **Issues:**
  - Quality judged by averaging over unobserved data $\boldsymbol{x}^*$ (SLLN + Cournot's principle)

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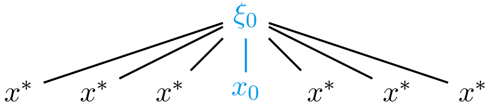

- **Issues:**
  - Quality judged by averaging over unobserved data $\boldsymbol{x}^*$ (SLLN + Cournot's principle)
  - Each problem requires its own solution

Bayesian

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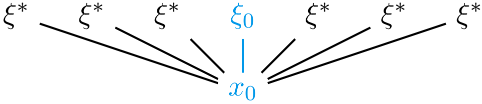

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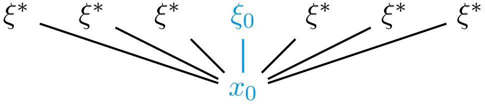

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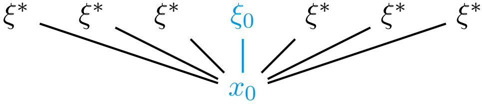

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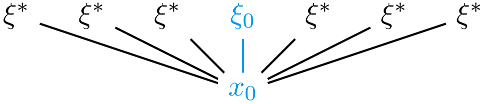

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  - Averaging over unused parameters ξ^* needs prior
  - Unique solution using Bayes theorem (conditional probability)
  - Axiomatic system for all of inference, subjective interpretation (de Finetti, Savage).

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$$
\begin{array}{cccccccc}
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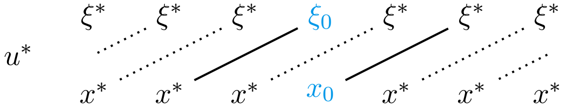

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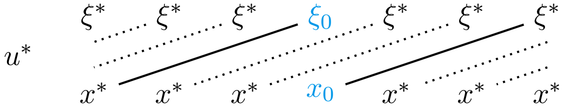

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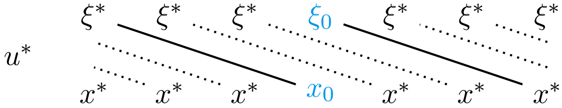

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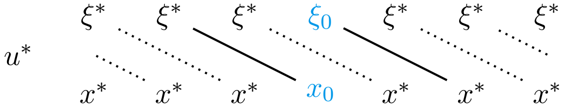

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  - Does not satisfy likelihood principle. Philosophical interpretation subject to argument

Outline

Comparison to likelihood

- Density is the function $f(\mathbf{x}, \xi)$, where ξ is fixed and $\mathbf{x}$ is variable.

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- Likelihood is the function $f(\mathbf{x}, \xi)$, where ξ is variable and $\mathbf{x}$ is fixed.
  - Likelihood as a distribution?

Data generating algorithm

- Data generating algorithm (DGA)

$$\mathbf{X} = \mathbf{G}(\mathbf{U}, \xi),$$

  - U is a random with known distribution (iid $U(0,1)$)
  - Parameter ξ is fixed.
  - Generate $\mathbf{X}$s by generating $\mathbf{U}$s and DGA.
    - This determines sampling distribution

Data generating algorithm

- Data generating equation (DGA)

$$\mathbf{x} = \mathbf{G}(\mathbf{U}^\star, \xi^\star),$$

  - U is a random with known distribution (iid $U(0,1)$)
  - Data $\mathbf{x}$ is fixed
  - Generate ξ^* by generating $\mathbf{U}^\star$s and inverting DGA.
    - This determines fiducial distribution
    - Denote the inverse $Q_{\boldsymbol{x}}(\boldsymbol{U}^*)$.

Example -- Bernoulli trials

- Data generating algorithm

$$X_i = 1\{U_i \leq p\},\ U_i \sim \text{Uniform}(0,1)$$

Generating U_i samples Bernoulli(p).

Example -- Bernoulli trials

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Estimating U_i by $U_i^\star$ defines fiducial distribution

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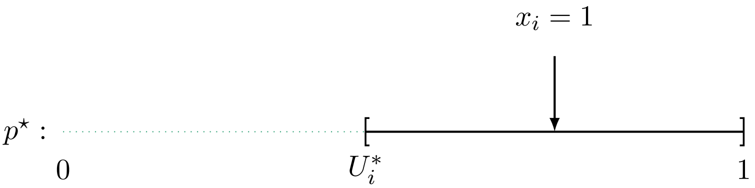
- If $x_i = 1$, then $p^\star \in [U_i^\star, 1]$



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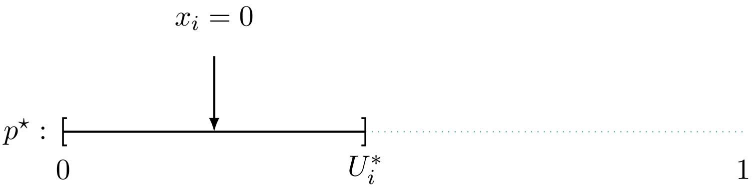
- If $x_i = 0$, then $p^\star \in [0, U_i^\star]$



Example -- Binomial

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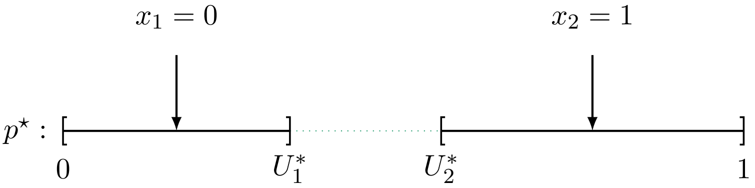
  $X_1 = 1\{U_1 \le p\},\ X_2 = 1\{U_2 \le p\}$ $\quad U_1, U_2$ i.i.d. Uniform(0,1)

- If $X_1 = 0, X_2 = 1$ and $U_1^\star < U_2^\star$



- No solution! Remove $(U_1^\star, U_2^\star)$ inconsistent with data.

Example -- Binomial

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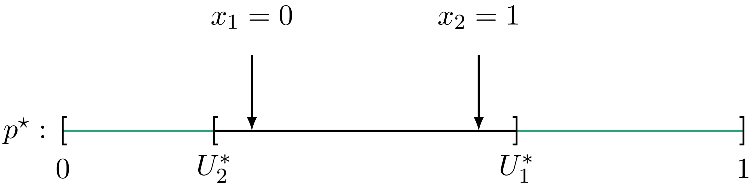

- $(U_1^\star, U_2^\star)$ uniform on $\{U_1^\star > U_2^\star\}$

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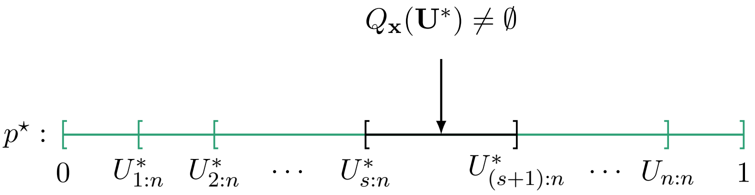
- $(X_1, \ldots X_n) \overset{iid}{\sim}$ Bernoulli(p), $S = \sum_{i=1}^{n} X_i \sim$ Binomial(n, p)
- Condition $\mathbf{U}^*$ on having a solution for p



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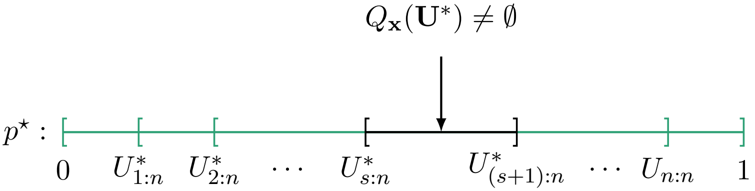

- Select a point in the interval.
  - A particular choice results in Beta$(s + 1/2, n - s + 1/2)$

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- Estimate $\boldsymbol{u}$ by

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  - Location problem – same as posterior computed using Jeffreys prior

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$$\xi(\mathbf{x}, \mathbf{U}^\star) = \arg\min_{\xi} \|\mathbf{x} - \boldsymbol{G}(\mathbf{U}^\star, \xi)\| \tag{1}$$

where $\boldsymbol{U}^\star$ is truncated to

$$\{\boldsymbol{U}^\star : \ \|\mathbf{x} - \boldsymbol{G}(\mathbf{U}^\star, \xi(\mathbf{x}, \mathbf{U}^\star))\| \leq \varepsilon\}$$

Take a limit as $\varepsilon \downarrow 0$.

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- Computations?

Explicit limit (1)

- Assume $\mathbf{X} \in \mathbb{R}^n$ is continuous; parameter $\xi \in \mathbb{R}^p$
- The limit in (1) has density (H, Iyer, Lai & Lee, 2016)

$$r_{\mathbf{x}}(\xi) = \frac{f_{\mathbf{X}}(\mathbf{x}|\xi) J(\mathbf{x}, \xi)}{\int_{\Xi} f_{\mathbf{X}}(\mathbf{x}|\xi') J(\mathbf{x}, \xi') \, d\xi'},$$

where $J(\mathbf{x}, \xi) = D\left(\nabla_\xi \mathbf{G}(\mathbf{u}, \xi)|_{\mathbf{u}=\mathbf{G}^{-1}(\mathbf{x},\xi)} \right)$

- $n = p$ gives $D(A) = |\det A|$

Explicit limit (1)

- Assume $\mathbf{X} \in \mathbb{R}^n$ is continuous; parameter $\xi \in \mathbb{R}^p$
- The limit in (1) has density (H, Iyer, Lai & Lee, 2016)

$$r_{\mathbf{x}}(\xi) = \frac{f_{\mathbf{X}}(\mathbf{x}|\xi) J(\mathbf{x}, \xi)}{\int_{\Xi} f_{\mathbf{X}}(\mathbf{x}|\xi') J(\mathbf{x}, \xi')\, d\xi'},$$

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- $\|\cdot\|_\infty$ gives $D(A) = \sum_{\mathbf{i}=(i_1,\dots,i_p)} |\det(A)_{\mathbf{i}}|$
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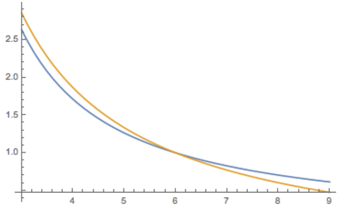

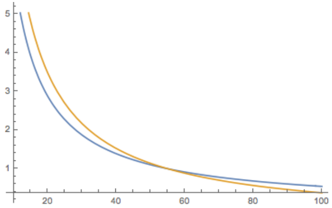

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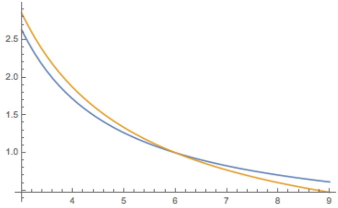

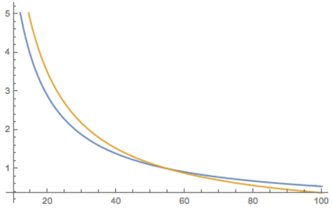

- In simulations fiducial was marginally better than reference prior which was much better than flat prior.

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Open problem:

- Derive Jacobian formula on manifolds

Outline

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  - Adding a multiple of a column to another column does not alter $D(A)$. Row operations not allowed!

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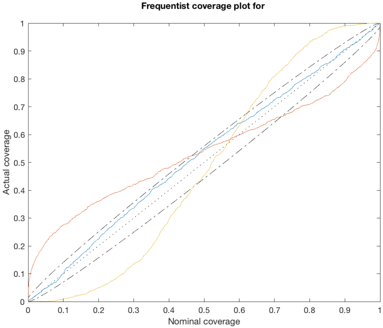
- This is general: simulate m fiducial p-values



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  - Reverse: Map $C(S)$ of fiducial probability $1 - \alpha$ to $\mathcal{U}$.
    If invariant in $\boldsymbol{X}$ then exact coverage.

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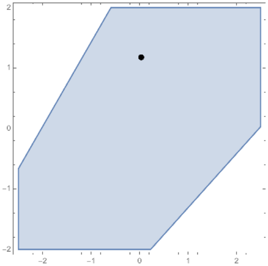

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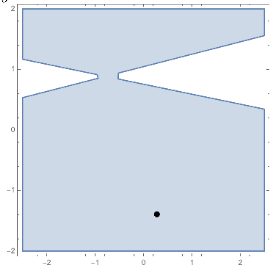

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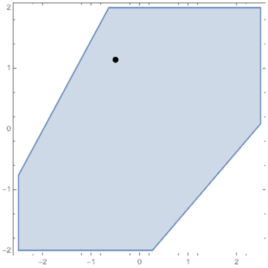

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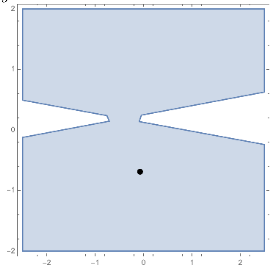

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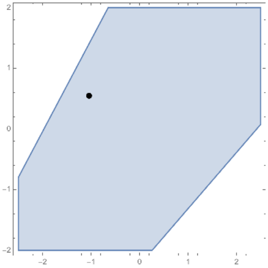

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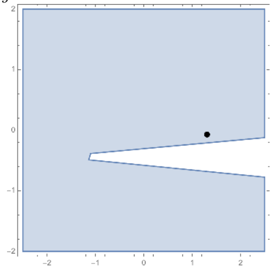

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  - Cons: The shape of the sets is strange (interval, complement of interval, whole real line)
- GFD1 $\approx$ GFD2 if $|y| >> 0$.

Ancillary Representation $(n > 1, p = 1)$

4. Let $(S(\mathbf{X}), \mathbf{A}(\mathbf{X}))$ be a smooth 1-1 transformation of $\boldsymbol{X} = \boldsymbol{G}(\boldsymbol{U}, \xi)$.
   - $S(\mathbf{X})$ is one dimensional satisfying 1, 2, 3.
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- Same argument works for $p > 1$.

Take home

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- Confidence Curves provide both confidence distribution and confidence sets

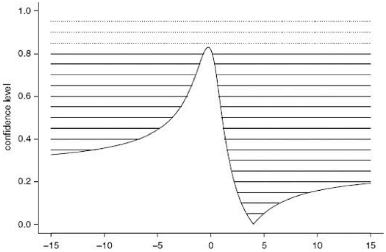

Figure 4.11 from Schweder & Hjort (2017) $x = 1.333, y = 0.333$

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- What is needed about asymptoticly correct coverage?
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  - Linkage of credible sets across all potential data (one sided CI)

Various Asymptotic Results (Frequentist)

$r_{\boldsymbol{x}}(\xi) \propto f_{\mathbf{X}}(\mathbf{x}|\xi) J(\mathbf{x}, \xi)$ where $J(\mathbf{x}, \xi) = D\left(\nabla_\xi \mathbf{G}(\mathbf{u}, \xi)|_{\mathbf{u}=\mathbf{G}^{-1}(\mathbf{x}, \xi)} \right)$

- Most start with $C_n^{-1} J(\mathbf{x}, \xi) \to J(\xi_0, \xi)$
- Bernstein-von Mises theorem for fiducial distributions provides asymptotic correctness of fiducial CIs H (2009, 2013), Sonderegger & H (2013) .
- Consistency of model selection H & Lee (2009), Lai, H & Lee (2015), H, Iyer, Lai & Lee (2016).
- Fiducial non-parametrics Cui & H (2019, 2020+, 2021+)

Outline

- Introduction
- Definition
- Theoretical Results
- Applications
  - High D Regression
  - Distributed Data
  - Fiducial Autoencoder
  - Likelihood ratio in Forensic Science
- Conclusions

Outline

Model Selection

- $\boldsymbol{Y} = \boldsymbol{G}(M, \boldsymbol{\xi}_M, \boldsymbol{U}), \qquad M \in \mathcal{M},\ \boldsymbol{\xi}_M \in \boldsymbol{\xi}_M$

Theorem: (H, Iyer, Lai, Lee 2016) Under assumptions

$$r_{\boldsymbol{y}}(M) \propto q^{|M|} \int_{\boldsymbol{\xi}_M} f_M(\boldsymbol{y}, \boldsymbol{\xi}_M) J_M(\boldsymbol{y}, \boldsymbol{\xi}_M)\, d\boldsymbol{\xi}_M$$

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  - Default value $q = n^{-1/2}$ (motivated by MDL)

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- Motivated by non-local priors of Johnson & Rossell (2009)

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where b_{min} solves

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  - Call this: ε-admissible subset

GFD

$$r_{\boldsymbol{y}}(M) \propto \pi^{\frac{|M|}{2}} \Gamma\Big(\frac{n-|M|}{2}\Big) RSS_M^{-(\frac{n-|M|-1}{2})} E[h_M^{\varepsilon}(\beta_M^{\star})]$$

Observations:

- Expectation with respect to within model GFD (usual T)

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- Implemented using Grouped Independence Metropolis Hastings (Andrieu & Roberts, 2009).

Main Result

Theorem Williams & H (2017+)
Suppose the true model is given by M_T. *Then under certain conditions, for a fixed positive constant* $\alpha < 1$,

$$r_{\boldsymbol{y}}(M_T) = \frac{r_{\boldsymbol{y}}(M_T)}{\sum_{j=1}^{n^\alpha} \sum_{M:|M|=j} r_{\boldsymbol{y}}(M)} \xrightarrow{P} 1 \text{ as } n, p \to \infty.$$

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- For a large model $|M| > p_T$ and large enough n or p,

$$\frac{9}{2}\|X^T(H_M - H_{M(-1)})\mu_T\|_2^2 < \varepsilon_M,$$

where H_M and $H_{M(-1)}$ are the projection matrix for M and M with a covariate removed respectively.

Default ε

$$\varepsilon = \Lambda_M \widehat{\sigma}^2_M \left(\frac{n^{0.51}}{9} + |M| \frac{\log(p\pi)^{1.1}}{9} - p_T \right)_+,$$

- $\Lambda_M := \mathrm{tr}\left((H_M X)' H_M X\right)$ with $H_M := X_M (X_M' X_M)^{-1} X_M'$
- $\widehat{\sigma}^2_M := \mathsf{RSS}_M / (n - |M|)$

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- $\widehat{\sigma}^2_M :=$ RSS$_M/(n - |M|)$
- Tuning parameter p_T represents belief about true $|M_T|$.

Simulation setup 1

- Generate 1000 data vectors y from linear model with $\beta^0_{M_o} = (-1.5, -1, -.8, -.6, .6, .8, 1, 1.5)'$, and $\sigma^0_{M_o} = 1$.

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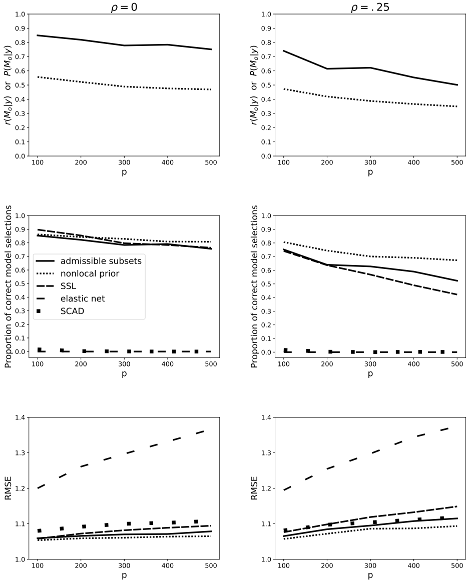
- Implement 10-fold cross-validation scheme for choosing the tuning parameter p_o (prior to starting the algorithm).
- Set $n = 100$, and consider $p = 100, 200, 300, 400, 500$.

Simulation results 1



Simulation setup 2

To illustrate the difference from the nonlocal prior approach, for $n = 30$, generate data from the following model.

$$Y \sim \mathsf{N}_n\Big(1 \cdot x^{(1)} + 1 \cdot x^{(2)} + \cdots + 1 \cdot x^{(9)}, I_n\Big),$$

where $x^{(1)}, x^{(2)}, x^{(3)} \overset{\text{iid}}{\sim} \mathsf{N}_n(0, I_n)$, and

$$\begin{array}{ccllllll}
x^{(4)} & \sim & \mathsf{N}_n\Big(& .25 \cdot x^{(1)} & & & & , .1^2 I_n\Big) \\
x^{(5)} & \sim & \mathsf{N}_n\Big(& & & .5 \cdot x^{(2)} & & , .1^2 I_n\Big) \\
x^{(6)} & \sim & \mathsf{N}_n\Big(& & & & - \; .75 \cdot x^{(3)} & , .1^2 I_n\Big) \\
x^{(7)} & \sim & \mathsf{N}_n\Big(& x^{(1)} & & & + \; x^{(3)} & , .1^2 I_n\Big) \\
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\end{array}$$

Simulation results 2

	MAP size	RMSE	$P(M_{\text{MAP}}\|y)$
ε-*admissible* subsets	3.476	1.138	.365
nonlocal prior	8.997	1.197	.333

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- Nonlocal prior procedure typically includes all 9 covariates even though the y can be mostly explained by 3.

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  - merge results from different nodes

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- $r_{\boldsymbol{x}}(\boldsymbol{\xi})$ – the generalized fiducial density of $\boldsymbol{x}$
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- On each worker sample from $q_k(\boldsymbol{\xi})$

$$r_{\boldsymbol{x}}(\boldsymbol{\xi}) \propto \sum_k \text{'importance weight'} \times q_k(\boldsymbol{\xi})$$

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  - Target of order $n^{-1/2}$
  - Fiducial sample on each worker of order $n_k^{-1/2}$.
  - Most realizations get extremely small weights.

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- Weight $w_k(\boldsymbol{\xi}) \approx \prod_{j \neq k} \frac{f(\mathbf{x}_k, \boldsymbol{\xi})}{g(\boldsymbol{\xi} | \theta_j, I_j)}$
  (Computed and thinned in parallel.)

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- Each worker simulates a sample from $q(\mathbf{x}_k) \propto r_{\boldsymbol{x}_k}(\boldsymbol{\xi}) \times \prod_{j \neq k} g(\boldsymbol{\xi}|\hat{\theta}_j, \hat{I}_j)$
  - Practical choice $g \sim$ Normal$(\hat{\theta}_j, \gamma \hat{I}_k^{-1})$.
- Weight $w_k(\boldsymbol{\xi}) \approx \prod_{j \neq k} \frac{f(\mathbf{x}_k, \boldsymbol{\xi})}{g(\boldsymbol{\xi}|\theta_j, I_j)}$
  (Computed and thinned in parallel.)

- We have shown consistency and asymptotic normality of the error of our importance sampling scheme.

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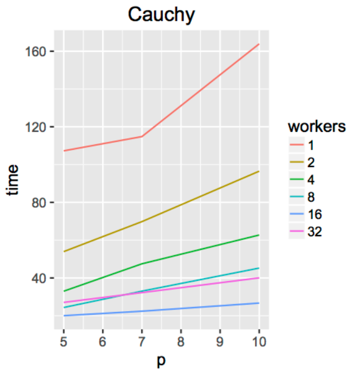
  - Generalized pareto, prediction of out of sample quantiles ($n = 10^6$, $K = 10$, $N_{\text{rep}} = 100$)

Computational time



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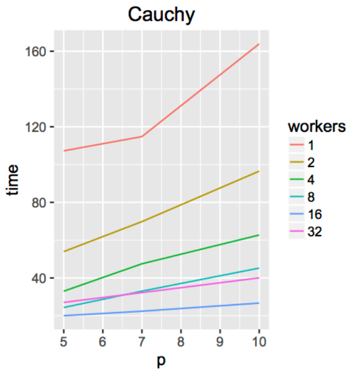
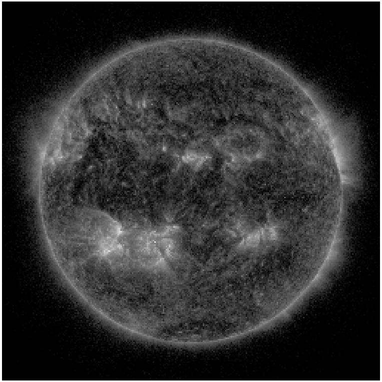
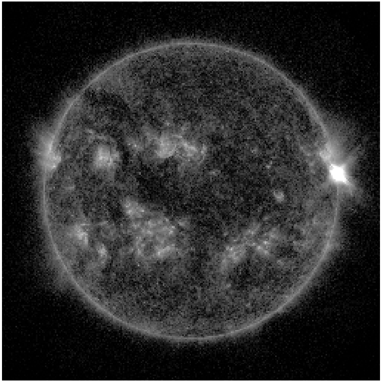


- Speed improves until $K = 16$ then deteriorates.
  (Cheng & Shang, 2015)

Sun Spots



low activity



high activity

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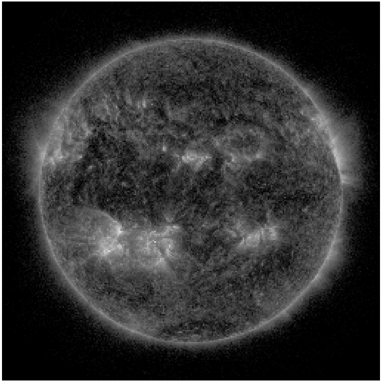

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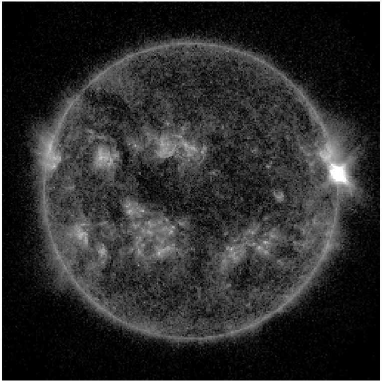

high activity

- The bright flare on the right has value 253. Is this high?

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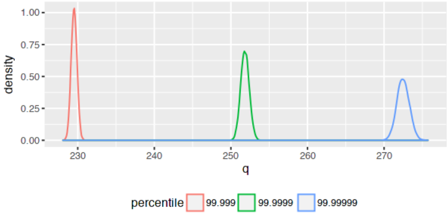
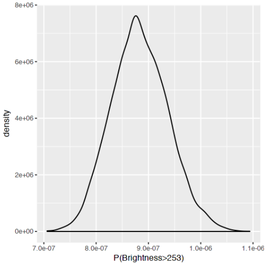
- Tool: GFD for Generalized Pareto (Wandler & H, 2012)

GFD for extreme quantiles



Large Quantiles



Fiducial probability of exceeding 253

Outline

Deep Neural Network (DNN)

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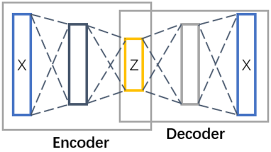
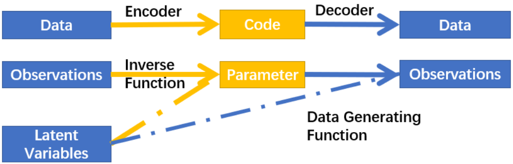
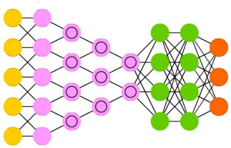
  - Idea: Use Auto-encoder to approximate fiducial inverse





Challenges



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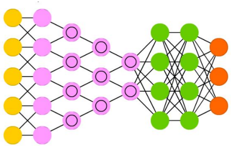

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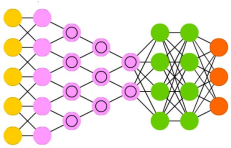

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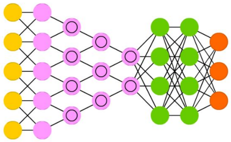

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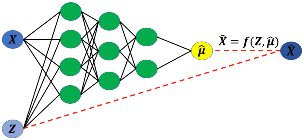
  - Host of other sensitivities (data generation, stopping rules, anti-over fitting measures,...)

Fiducial Auto Encoder



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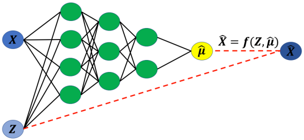

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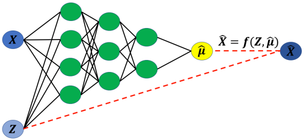

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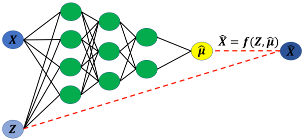

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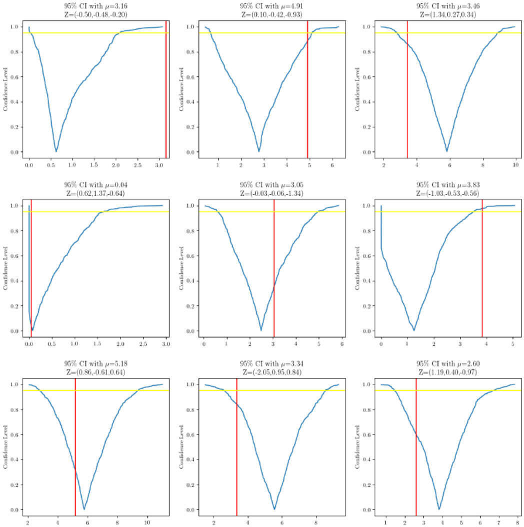
- Trained encoder used for inference

Inference

- Model: $\boldsymbol{X} = \mu + \mu^{q/2}\boldsymbol{Z}$
- Use encoder repeatedly
- Inputs: Observed $\boldsymbol{X}$, multiple independent $\boldsymbol{Z}^*$
- Output: Approximate fiducial sample μ^*



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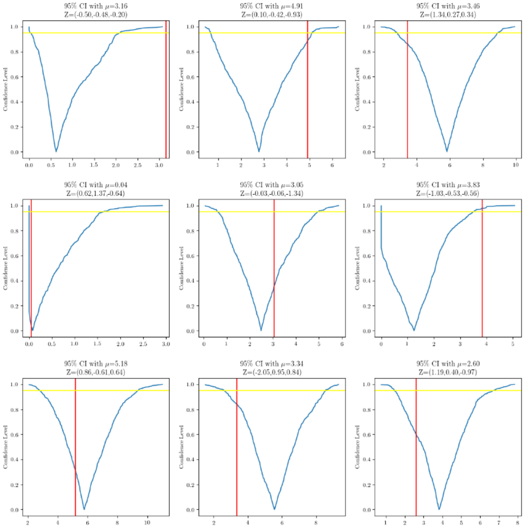

Approximate Fiducial Calculations

- Following AE: $\boldsymbol{X}^\star = \boldsymbol{G}(\boldsymbol{Z}^\star, \mu^\star)$ needs to replicate $\boldsymbol{X}$.
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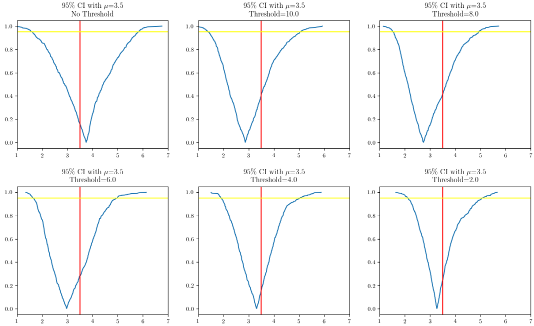

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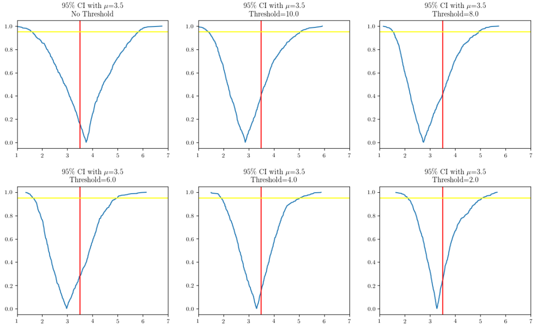
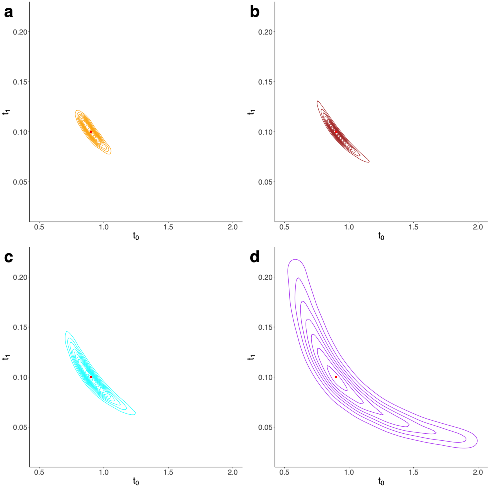
- Future work: GAN improve efficiency?



Biological Oxygen Demand

- $\boldsymbol{Y} = \xi_1(1 - e^{-\xi_2 \boldsymbol{X}}) + \boldsymbol{Z}$
- $\boldsymbol{x} = (2, 4, 6, 8, 10)$, $\boldsymbol{y} = (0.15, 0.30, 0.41, 0.48, 0.57)$, $\boldsymbol{Z} \sim N(0, 0.015I)$
- Methods:
  - a FAE
  - b GFD-HMC
  - c bootstrap
  - d Bayes ROT (Bardsley et al, 2014)



Outline

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- Reliable = Can be trusted

Examples of data

Likelihood ratio	Hotelling T^2/univariate kernel, equations (6)/(7)	Normal, equations (11)/(12)	MVK kernel, equations (14)/(15)
$>10^7$	0	1	0
10^7–10^6	0	3	0
10^6–10^5	0	8	0
10^5–10^4	0	9	0
10^4–10^3	22	11	16
10^3–10^2	10	17	19
10^2–10^1	12	5	13
10^1–1	5	8	5
1–10^{-1}	3	10	10
10^{-1}–10^{-2}	5	7	9
10^{-2}–10^{-3}	3	3	8
10^{-3}–10^{-4}	6	6	6
10^{-4}–10^{-5}	4	6	3
$<10^{-5}$	1821	1797	1802
Total	1891	1891	1891

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10^2–10^3	18	8	13
10^3–10^4	35	17	48
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10^5–10^6	0	11	0
10^6–10^7	0	5	0
10^7–10^8	0	0	0
10^8–10^9	0	1	0
10^9–10^{10}	0	1	0
$>10^{10}$	0	3	0
Total	62	62	62

Figure: Glass evidence from Aitken & Lucy (2004)

not mated

mated

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not mated | mated

- Our mathematical abstraction:
  - Two streams of data (mated/non mated). Algorithms produce LR-like measure.

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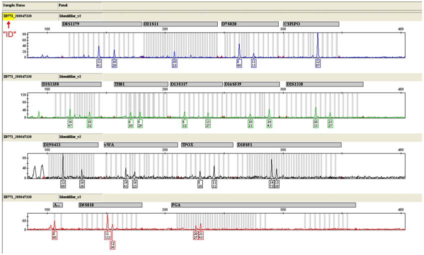
- When is $1,000,000 : 1$ more like $100 : 1$? Does it matter?

Well-calibrated?

- When is $1,000,000 : 1$ more like $100 : 1$? Does it matter?
- The LR value may have an effect on verdict
  - Barrie et al (2018) report LR values across different labs of 172 to 3.2×10^{14} starting from the same EPG!



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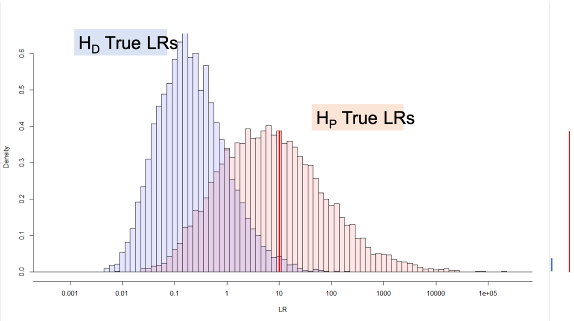

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- Integrating (2)

$$G(b) - G(a) = bF(b) - aF(a) - \int_a^b F(l)dl, \quad 0 < a < b < \infty.$$

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- Estimation and uncertainty quantification via GFD

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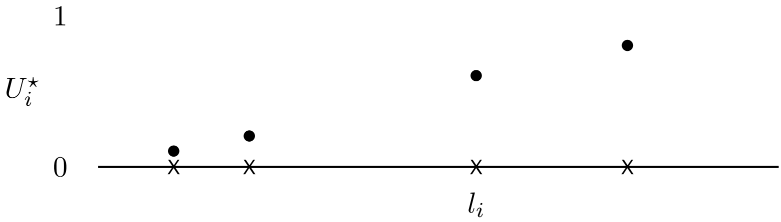

U_i^* ordered uniforms

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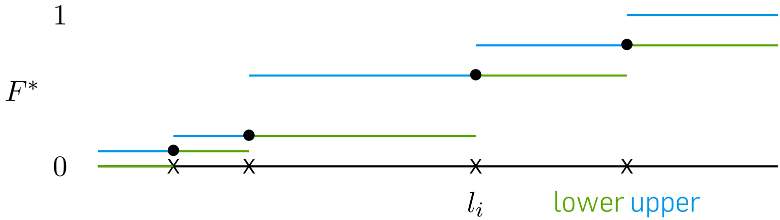

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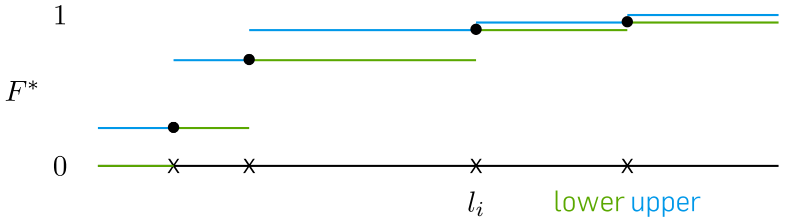

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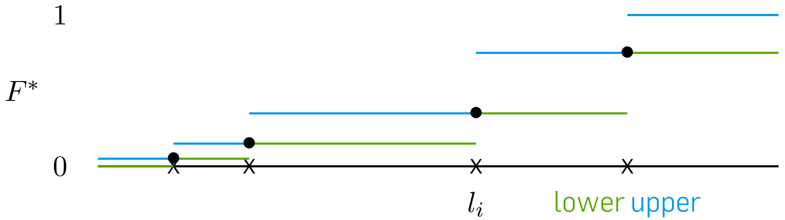

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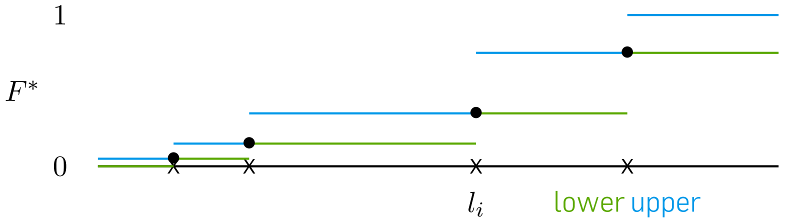

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- Facts (Cui & H, 2019)
  - $EF^\star_{lower}(l) < \hat{F}(l) < EF^\star_{upper}(l)$
  - Bernstein-von Mises theorem, good small sample properties

Calibration Confidence Intervals

- Recall

$$d(G,F) = \left(\log_{10}\left(\frac{G(a_i)-G(a_{i-1})}{a_iF(a_i)-a_{i-1}F(a_{i-1})-\int_{a_{i-1}}^{a_i}F(l)dl}\right), \quad i=2,\dots k\right)^\top$$

Theorem (H, Iyer, 2020+)

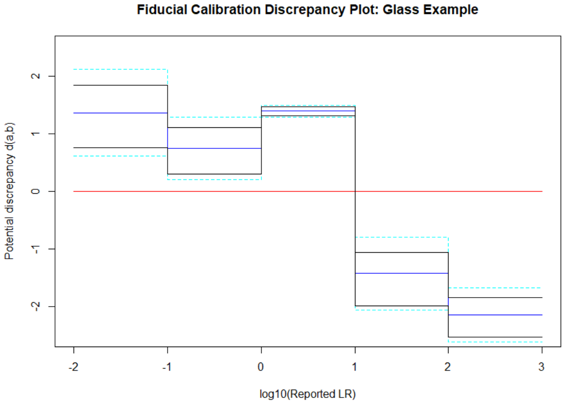
Assume obs LRs independent; $0 < F(a_1) < \cdots < F(a_k) < 1$, $0 < G(a_1) < \cdots < G(a_k) < 1$, $n = \min(n_g, n_f)$, $n/n_f \to p_f$, $n/n_g \to p_g$. *Then*

$$\sqrt{n}(d(\hat{G},\hat{F}) - d(G,F)) \xrightarrow{\mathcal{D}} N(0,\Sigma_{g,f}),$$

and conditionally on the observed LRs

$$\sqrt{n}(d(G^\star,F^\star) - d(\hat{G},\hat{F})) \xrightarrow{\mathcal{D}} N(0,\Sigma_{g,f}) \quad a.s.$$

Calibration -- glass LR



Glass (classical)

target
median
fiducial CI
fid cband

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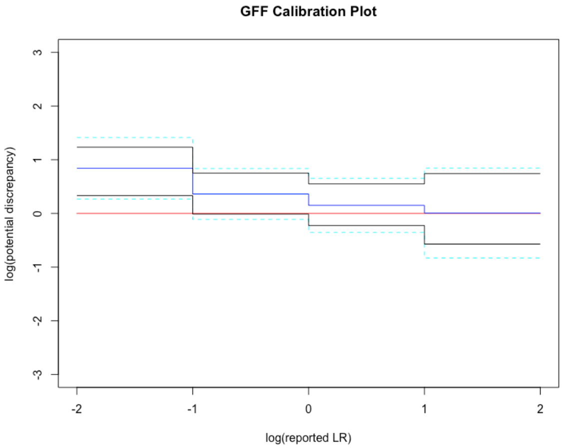

Glass (Williams, H., Omen)

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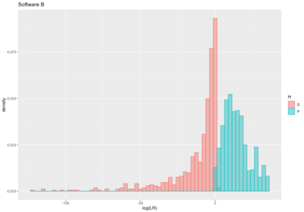
Extrapolation via Generalized Pareto Distribution (GPD)

- DNA: Little overlap between mated and non-mated LR



Extrapolation via Generalized Pareto Distribution (GPD)

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- Data above large threshold follow GPD
  - GPD interpolates bounded, exponential and Pareto tails

$$f(x) = \frac{1}{\sigma}\left(1 + \frac{kx}{\sigma}\right)^{-1-1/k}, \quad x > 0 \quad \text{and if } k < 0 \text{ then also } x < -\frac{\sigma}{k}$$

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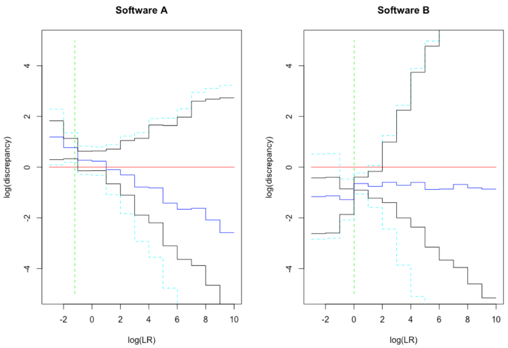
- Above threshold use GFD for GPD (Wandler & H, 2012)

DNA calibration



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Outline

BFF

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Can Bayesian, Fiducial and Frequentist become Best Friends Forever?

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Thank you!