

# Achieving Accuracy and Correctness in Parametric Frequentist Inference

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Acknowledgements: Tom DiCiccio (Cornell), Todd Kuffner (Washington University in St. Louis).

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BUT, among key desiderata of such inference are **high accuracy** and **inferential correctness**:

- ▶ Low error (e.g. high levels of coverage accuracy of CIs), particularly with small sample sizes  $n$ ;
- ▶ Inferential correctness, in relation to key principles of inference, especially those involving appropriate conditioning and parameterization invariance.

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- ▶ Discuss relationships between analytic and bootstrap methodologies;
- ▶ Special consideration to high-dimensional nuisance parameter problems;
- ▶ Discuss computational issues [computational intensiveness versus analytic requirements].

# Structure of Tutorial

- ▶ Background, key ideas.
- ▶ Detailed theoretical analysis.
- ▶ Further illustrations.

# I: Background, key ideas

# The inferential problem

Let  $Y = \{Y_1, \dots, Y_n\}$  be random sample from underlying distribution  $F(y; \theta)$ , indexed by  $d$ -dimensional parameter  $\theta = (\theta^1, \dots, \theta^d) = (\psi, \phi)$ ,  $\psi$   $p$ -dimensional interest parameter,  $\phi$   $q$ -dimensional nuisance parameter,  $p + q = d$ . May have  $\phi$  **high-dimensional**.

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Wish to test  $H_0 : \psi = \psi_0$ , or (duality) construct confidence set for  $\psi$ .

If  $p = 1$ ,  $\psi = \theta^1$ , want one-sided inference e.g. test  $H_0$  against (one-sided) alternative  $\psi > \psi_0$  or  $\psi < \psi_0$ , or one-sided confidence limit.

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Typically,  $p = 1$ .

# Inference

Let  $L(\theta) \equiv L(\theta; Y)$  be log-likelihood,  $\hat{\theta} = (\hat{\psi}, \hat{\phi})$  the overall MLE of  $\theta$ ,  $\hat{\phi}_{\psi}$  the constrained MLE of  $\phi$ , for fixed value of  $\psi$ . Write  $\tilde{\theta} \equiv \tilde{\theta}(\psi) = (\psi, \hat{\phi}_{\psi})$ .

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Likelihood ratio statistic is  $W(\psi) = 2\{M(\hat{\psi}) - M(\psi)\}$ .

In case of **scalar**  $\psi$ , use signed root likelihood ratio statistic:

$$R(\psi) = \text{sgn}(\hat{\psi} - \psi) W(\psi)^{1/2}.$$

# Notation

Arrays and summation are denoted by using the standard conventions, for which the indices  $r, s, t, \dots$  are assumed to range over  $1, \dots, d$ . Summation over the range is implied for any index appearing in an expression both as a subscript and as a superscript.

Differentiation is indicated by subscripts, so  $L_r(\theta) = \partial L(\theta) / \partial \theta^r$ ,  $L_{rs}(\theta) = \partial^2 L(\theta) / \partial \theta^r \partial \theta^s$ , etc. Then  $E\{L_r(\theta)\} = 0$ ; let  $\lambda_{rs} = E\{L_{rs}(\theta)\}$ ,  $\lambda_{rst} = E\{L_{rst}(\theta)\}$ , etc.

The constants  $\lambda_{rs}$ ,  $\lambda_{rst}$ ,  $\dots$ , are assumed to be of order  $O(n)$ . These assumptions are usually satisfied in situations involving independent observations, structured (e.g. time series) dependent data problems.

Let  $\lambda_{r,s} = E(L_r L_s)$ ,  $\lambda_{rs,t} = E(L_{rs} L_t)$ , etc.

Let  $(\lambda^{rs})$  be the  $d \times d$  matrix inverse of  $(\lambda_{rs})$ , and let  $\eta = -1/\lambda^{11}$ ,  $\tau^{rs} = \eta \lambda^{1r} \lambda^{1s}$ , and  $\nu^{rs} = \lambda^{rs} + \tau^{rs}$ . Thus,  $\lambda^{rs}$ ,  $\tau^{rs}$ , and  $\nu^{rs}$  are of order  $O(n^{-1})$ , while  $\eta$  is of order  $O(n)$ .

## A comment

Calculation of quantities just defined requires (at most) evaluation of expectations of log-likelihood derivatives.

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Wald statistic,

$$T_W(\psi) = (\hat{\psi} - \psi)\{-\lambda^{11}(\hat{\theta})\}^{-1/2}.$$

Score statistic,

$$T_S(\psi) = L_1\{\tilde{\theta}(\psi)\}\{\lambda^{11}(\hat{\theta})\}^{1/2}.$$

Constructed using **expected** (inverse) information matrix  $[\lambda^{rs}]$ , evaluated at global MLE. Alternatively: use **observed** (inverse) information matrix  $[L^{rs}]$ ; evaluate at constrained MLE  $\tilde{\theta}(\psi), \dots$

## Running Example (RE): Inverse Gaussian distribution

$Y_1, \dots, Y_n$  IID inverse Gaussian,  $IG(\mu, \psi)$ , with density

$$f(y; \mu, \psi) = \left( \frac{\psi}{2\pi y^3} \right)^{1/2} \exp \left( -\frac{\psi}{2\mu^2 y} (y - \mu)^2 \right), \quad y > 0,$$

interest parameter is shape  $\psi > 0$ , mean  $\mu > 0$  as nuisance.

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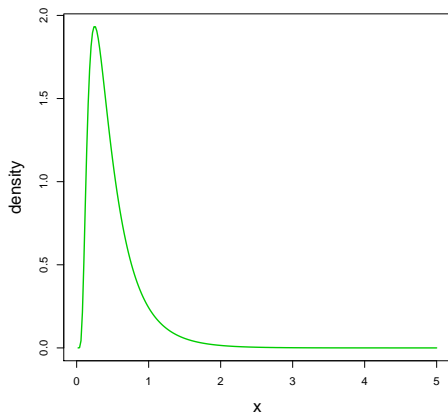
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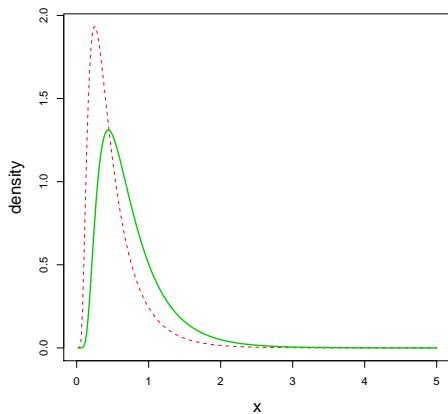
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First passage time of Brownian motion, widely used to model phenomena in biosciences/reliability/survival/....

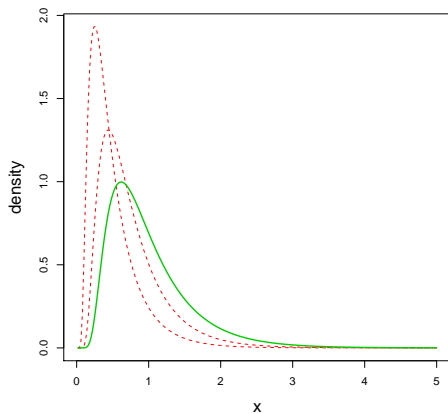
Density:  $\psi = 1, \mu = 0.5$



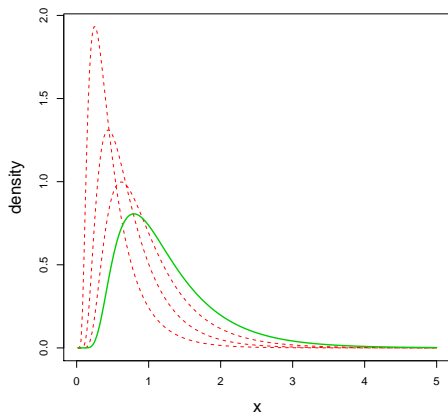
Density:  $\psi = 2, \mu = 0.75$



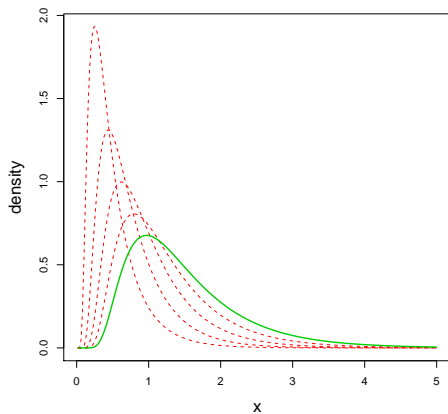
Density:  $\psi = 3, \mu = 1.0$



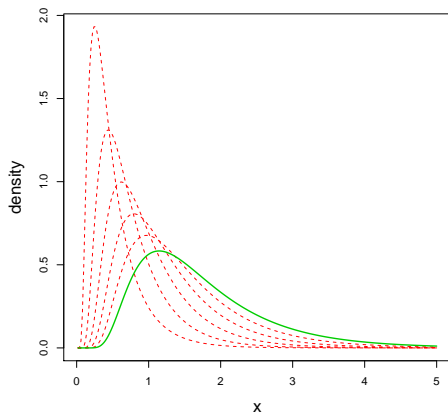
Density:  $\psi = 4, \mu = 1.25$



Density:  $\psi = 5, \mu = 1.5$



Density:  $\psi = 6, \mu = 1.75$



MLES are:

$$\hat{\psi} = n/V, \quad \hat{\mu} = \hat{\mu}_{\psi} = \bar{Y},$$

$$V = \sum_{i=1}^n (Y_i^{-1} - \bar{Y}^{-1}), \quad \bar{Y} = n^{-1} \sum_{i=1}^n Y_i.$$

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Distribution of  $\psi V$  is  $\chi_{n-1}^2$ , distribution of  $\hat{\mu}$  is  $IG(\mu, \psi)$ .

$$R(\psi) = \operatorname{sgn}(\hat{\psi} - \psi) \{n(\log \hat{\psi} - 1 - \log \psi + \psi/\hat{\psi})\}^{1/2},$$

$$T_W(\psi) = \sqrt{\frac{n}{2}} \left(1 - \frac{\psi}{\hat{\psi}}\right),$$

$$T_S(\psi) = \sqrt{\frac{n}{2}} \left(\frac{\hat{\psi}}{\psi} - 1\right)$$

## A data sample

Data sample size  $n = 10$ , generated with  $\mu = 1, \psi = 2$ :

0.435, 0.466, 1.624, 0.304, 2.165

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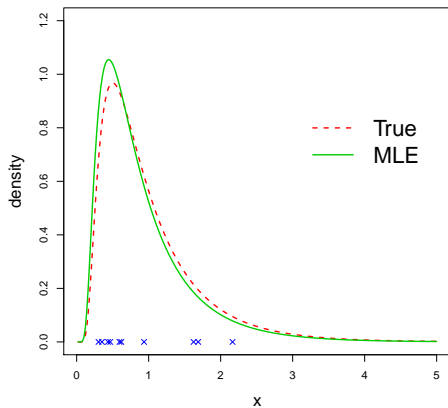
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Have:  $\hat{\psi} = 1.745, \hat{\mu} = 0.918$ .

## RE: True and estimated densities



## Comment

Concentrate here on inference based on  $R$ ,  $W$ , for simplicity. Most results true also for Wald and score statistics.

# Parameterization invariance

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If  $\theta$  and  $\zeta$  are two alternative parameterizations and  $\mathcal{P}(\cdot)$  is an inference procedure, with  $C_\theta$  and  $C_\zeta$  the conclusions that  $\mathcal{P}(\cdot)$  leads to, expressed in the two parameterizations, then the same conclusion  $C_\zeta$  should be reached by **both** application of  $\mathcal{P}(\cdot)$  in the  $\zeta$  parameterization **and** translation into the  $\zeta$  parameterization of the conclusion  $C_\theta$ .

# Nuisance parameter

With nuisance parameters, parameterization invariance is restricted to mean invariance under **interest respecting reparameterization**.

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Suppose  $\theta = (\psi, \phi)$ , with  $\psi$  interest parameter and  $\phi$  nuisance parameter. An interest respecting reparameterization is of the form  $v = v(\theta) = v(\psi, \phi)$  with  $v = (\varphi, \chi)$ , such that

$$\varphi = \varphi(\psi), \chi = \chi(\psi, \phi).$$

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Inference based on  $T_W(\psi)$  **does not**.

# Adjusted likelihood

Broadly, properties to be discussed hold also for versions of statistics based on **adjusted** forms of profile likelihood.

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Intractable likelihood? Composite/pseudo-likelihood. Analysis of inference for these incomplete, **predictable**.

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Latter true also for  $T_W(\psi)$  and  $T_S(\psi)$ , and variants.

## Inference: illustration, $p = 1$

A confidence set of asymptotic coverage  $1 - \alpha$  for  $\psi$  is

$$\mathcal{I}(Y) \equiv \mathcal{I}_{1-\alpha}(Y) = \{\psi : u(Y, \psi) \leq 1 - \alpha\},$$

with  $u(Y, \psi) = \Phi\{R(\psi)\}$ , in terms of the  $N(0, 1)$  distribution function  $\Phi(\cdot)$ . Call  $u(Y, \psi)$  the ‘significance function’.

Equivalently, the confidence set is

$$\mathcal{I}(Y) = \{\psi : R(\psi) \leq \Phi^{-1}(1 - \alpha)\}.$$

The coverage error of the confidence set is  $O(n^{-1/2})$ : first-order accuracy.

Have that  $u(Y, \psi)$  is monotonic in  $\psi$ , so confidence set is semi-infinite interval of form  $(\hat{\psi}_l(Y), \infty)$ . Lower confidence limit.

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If two-sided inference is required, an equi-tailed two-sided confidence interval  $\mathcal{J}(Y)$  of nominal coverage  $1 - \alpha$  may be obtained by taking the set difference of two one-sided sets:

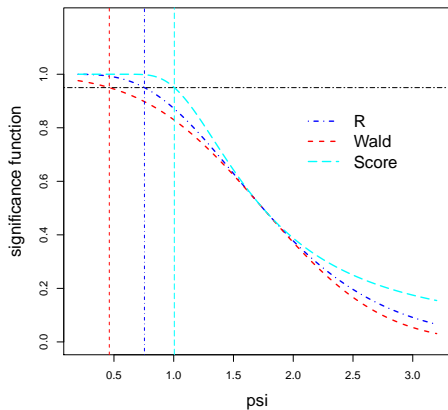
$$\mathcal{J}(Y) \equiv \mathcal{J}_{1-\alpha}(Y) = \mathcal{I}_{1-\alpha/2}(Y) \setminus \mathcal{I}_{\alpha/2}(Y).$$

Similar statements about coverage error of confidence sets true for other asymptotically  $N(0, 1)$  pivots.

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In case  $p > 1$ , confidence set of coverage error  $O(n^{-1})$  (**second-order** accuracy) from  $\chi_p^2$  approximation to sampling distribution of  $W(\psi)$ .

# RE, data sample: significance functions



## RE, data example: 95% confidence limits

- ▶  $R(\psi)$ : interval is  $(0.755, \infty)$ .
- ▶  $T_W(\psi)$ : interval is  $(0.461, \infty)$ .
- ▶  $T_S(\psi)$ : interval is  $(1.005, \infty)$ .

# Motivations for refinements

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- ▶ To accommodate appropriate conditioning: **multi-parameter exponential families** (conditioning dictated by theory of optimal tests etc.); **ancillary statistic models** (relevance, by conditioning on component of minimal sufficient statistic that is approximately distribution constant).

# Exponential family context

Suppose that the log-likelihood is of the form

$$L(\theta) = \psi s_1(Y) + \phi s_2(Y) - k(\psi, \phi) - d(Y),$$

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The conditional distribution of  $s_1$  given  $s_2$  depends only on  $\psi$ : conditioning on  $s_2$  eliminates the nuisance parameter.

Appropriate inference on  $\psi$  is based on the distribution of  $s_1$ , given the observed value of  $s_2$ . This is, in principle, known, since it is completely specified, once  $\psi$  fixed.

In fact, this conditional inference has unconditional (repeated sampling) **optimality properties** of being uniformly most powerful unbiased etc etc.

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In practice, the exact inference may be difficult to construct: the relevant conditional distribution typically requires awkward analytic calculations, numerical integrations etc.

# Ancillary statistic context

Fisherian proposition: inference about  $\psi$  should be based not on the original specified model  $F(y; \theta)$ , but instead on derived model obtained by **conditioning on an ancillary statistic, when this exists**.

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Suppose minimal sufficient statistic for  $\theta$  can be written as

$$(\hat{\theta}, A),$$

with  $A$  (approximately) distribution constant.

Then,  $A$  is **ancillary**, and the **Conditionality Principle** (CP) dictates that to be relevant inference on  $\psi$  should be made conditional on the observed value  $a$  of  $A$ . CP automatically respected by Bayesian inference.

# Refinements: approaches

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Bayes with prior explicitly specified so (marginal) posterior for  $\psi$  yields confidence limits with correct frequentist interpretation, to high-order: 'probability matching prior'.

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- ▶ conceptually simple;
- ▶ typically awkward with high-dimensional nuisance parameter, as need to find marginal posterior of  $\psi$ ;
- ▶ route not always open, higher-order (conditional) accuracy **not** necessarily obtainable.

## Detail

Require prior  $\pi(\psi, \phi)$  so that

$$Pr_{\theta}\{\psi \leq \psi^{(1-\alpha)}(\pi, Y)\} = 1 - \alpha + O(n^{-r/2}),$$

for  $r = 2$  or  $3$ , each  $0 < \alpha < 1$ .

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- ▶  $Pr_{\theta}$  denotes frequentist probability, under repeated sampling of  $Y$ , under parameter  $\theta$ .

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If condition holds with  $r = 3$ , speak of  $\pi(\psi, \phi)$  as **second-order probability matching prior**.

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Want the posterior  $1 - \alpha$  quantile to match the  $1 - \alpha$  **conditional frequentist confidence limit** for  $\psi$ .

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- ▶ Analytically modified forms of  $R(\psi)$ , **specifically designed** to offer conditional validity, to high (asymptotic) order, in both contexts. 'Barndorff-Nielsen's  $R^*$ '.

# Bartlett correction

Have

$$E_{\theta}\{W(\psi)\} = p \left( 1 + \frac{b(\theta)}{n} + O(n^{-2}) \right),$$

so modify  $W(\psi)$  to

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or

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Then  $W_c(\psi)$  and  $\bar{W}_c(\psi)$  are distributed as  $\chi_p^2$ , to error of order  $O(n^{-2})$ . Confidence sets constructed by  $\chi_p^2$  approximation have coverage error  $O(n^{-2})$ .

$E_{(\psi, \hat{\phi}_\psi)}\{W(\psi)\}$  constructed by (bootstrap) simulation. Estimation of expectation requires smaller MC simulation than estimation of whole sampling distribution.

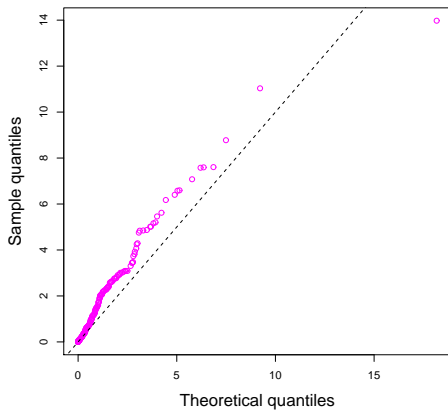
Inference by  $\chi_p^2$  approximation to distribution of  $\bar{W}_c(\psi)$ : 'Empirical Bartlett correction'.

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Inference by  $\chi_p^2$  approximation to distribution of  $\bar{W}_c(\psi)$ : 'Empirical Bartlett correction'.

Could replace  $\chi_p^2$  approximation to sampling distribution of  $W(\psi)$  by bootstrap distribution: sampling distribution under sampling with parameter fixed as  $\theta = (\psi, \hat{\phi}_\psi)$ . Confidence set will also have coverage error  $O(n^{-2})$ .

RE:  $n = 5, \psi = 2, \mu = 1.0, \chi_1^2$  QQ plot,  $W(\psi)$



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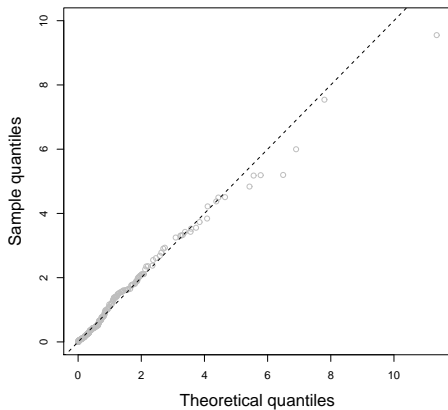
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**Big** simulation shows,  $E_{\theta}\{W(\psi)\} = 1.4632$ .

RE:  $n = 5, \psi = 2, \mu = 1.0, \chi_1^2$  QQ plot,  $\bar{W}_c(\psi)$



# Adjusted signed root statistic $R^*$

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- ▶ explicit specification of ancillary  $A$  in ancillary statistic (e.g. transformation) context;
- ▶ potentially awkward analytic calculations, in both ancillary/exponential family situations.

## Other formulations

Other formulations of  $\nu(\psi)$ , due to Fraser and co-workers,  
possible: use of 'tangent exponential model' avoids need to specify  
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Still analytically fiddly.

## RE: adjustment function

In inverse Gaussian example,

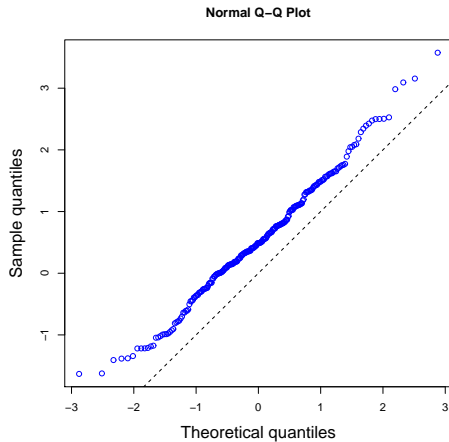
$$v(\psi) = \sqrt{\frac{n\psi}{2\hat{\psi}}} \left(1 - \frac{\psi}{\hat{\psi}}\right).$$

Sampling distribution of  $R^*(\psi)$  is  $N(0, 1)$ , to error of order  $O(n^{-3/2})$ , conditional on ancillary, hence unconditionally. Normal approximation to distribution of  $R^*(\psi)$  yields third-order (relative) conditional accuracy in ancillary statistic setting, and confidence sets with third-order repeated sampling coverage accuracy.

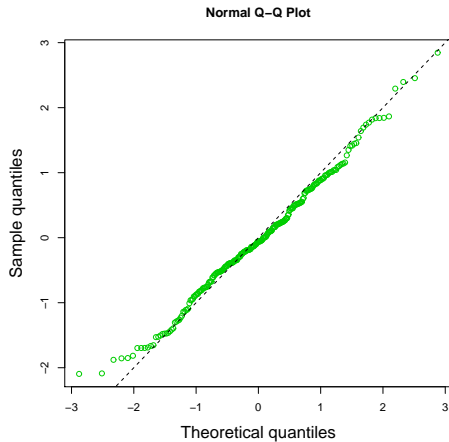
Sampling distribution of  $R^*(\psi)$  is  $N(0, 1)$ , to error of order  $O(n^{-3/2})$ , **conditional on ancillary**, hence unconditionally. Normal approximation to distribution of  $R^*(\psi)$  yields **third-order (relative) conditional accuracy** in ancillary statistic setting, and confidence sets with third-order repeated sampling coverage accuracy.

Inference which respects that of exact conditional inference in exponential family setting to same **third-order**.

RE:  $n = 5$ ,  $\psi = 2$ ,  $\mu = 1.0$ , QQ plot,  $R(\psi)$



RE:  $n = 5$ ,  $\psi = 2$ ,  $\mu = 1.0$ , QQ plot,  $R^*(\psi)$



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- ▶ Successfully packaged (Davison et al.) for certain classes of model, e.g. nonlinear heteroscedastic regression models.
- ▶ Also, relatively unexplored is idea of using simulation to replace analytic calculations, specifically to calculate Bartlett correction.
- ▶ Versions of  $R^*$  for vector interest parameters possible, seen as less effective than in case  $p = 1$ , or than Bartlett correction.

# (Constrained) Bootstrap

**Bootstrap Principle:** estimate sampling distribution of interest by that under a fitted model.

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**Bootstrap Principle:** estimate sampling distribution of interest by that under a fitted model.

**Key:** appropriate handling of nuisance parameter. Repeated sampling properties of bootstrap are [modulo Monte Carlo error from using finite simulation] **entirely** determined by nuisance parameter effects.

# The key recommendation

Use as basis of bootstrap calculation  $F(y; (\psi, \hat{\phi}_\psi))$ , fitted model with nuisance parameter taken as **constrained MLE**, for given value of interest parameter.

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- ▶ Estimate true sampling distribution of  $R(\psi)$  to error of order  $O(n^{-1})$ .

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- ▶ Estimate true sampling distribution of  $R(\psi)$  to error of order  $O(n^{-1})$ .
- ▶ But, confidence sets constructed from bootstrap distribution of  $R(\psi)$  have third-order coverage accuracy: coverage error of order  $O(n^{-3/2})$ .

The confidence set is

$$\{\psi : R(\psi) \leq \tilde{G}^{-1}(1 - \alpha)\},$$

where  $\tilde{G}$  denotes the sampling distribution of  $R(\psi)$  under  $F(y; \tilde{\theta})$ , the distribution with parameter value fixed as  $\tilde{\theta} = (\psi, \hat{\phi}_\psi)$ .

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Corresponds to a significance function  $u(Y, \psi) = \tilde{G}(R(\psi))$ .

Note: a **different** bootstrap calculation required for each  $\psi$ . The significance function may not be monotonic.

Other schemes, e.g. substituting **global MLE** of nuisance parameter, less effective, in general. If  $\hat{G}$  denotes the distribution of  $R(\psi)$  under sampling from  $F(y; \hat{\theta})$ , the confidence set

$$\{\psi : R(\psi) \leq \hat{G}^{-1}(1 - \alpha)\},$$

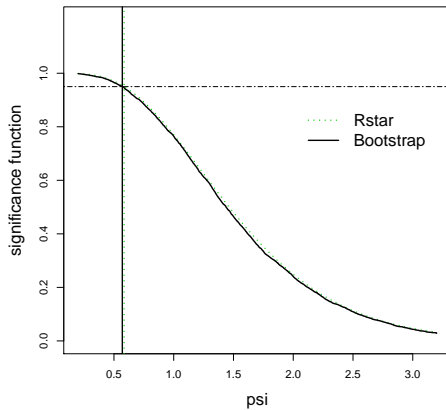
has coverage error of order  $O(n^{-1})$ .

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So does making normal approximation to sampling distribution of  $R^*(\psi)$ .

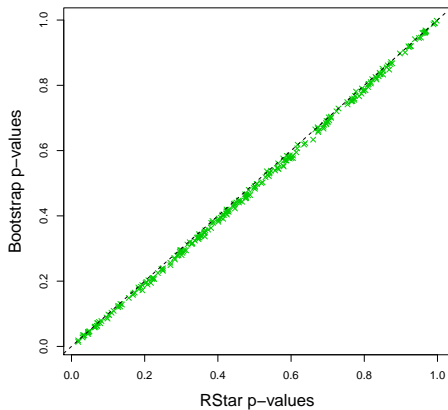
# RE, data sample: significance functions



## RE, data example: 95% confidence limits

- ▶  $R^*(\psi)$ : interval is  $(0.585, \infty)$ .
- ▶ Bootstrap  $R(\psi)$ : interval is  $(0.570, \infty)$ .

RE:  $n = 5$ , bootstrap  $p$ -values vs  $R^*$   $p$ -values



# A practical example: signal detection

LHC: detection of signal in presence of background noise.

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Set confidence limits on underlying signal, based on data from observation channel.

Observation is number of times a particular event is observed. Supposed to have Poisson distribution with mean  $\psi\gamma + \beta$ , where interest parameter  $\psi$  represents signal,  $\beta$  and  $\gamma$  represent respectively a background rate at which event occurs and efficiency of the measurement device.

# Precise formulation

Available data is  $y_1, y_2, y_3$ . Realizations of independent Poisson random variables with means  $\psi\gamma + \beta$ ,  $\beta t$  and  $\gamma u$  respectively, where  $t$  and  $u$  are **known** and parameters  $\psi, \beta, \gamma$  are **unknown**.

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In principle,  $\psi \geq 0$ , and nuisance parameters  $\beta, \gamma$  are positive.

Consider  $y_1 = 1, y_2 = 8, y_3 = 14$ , with  $t = 27, u = 80$ .

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$R(\psi)$ :  $p$ -value is  $1 - \Phi\{R(0)\} = 0.163$ .

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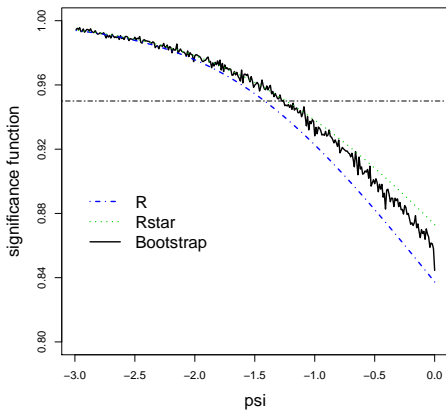
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Weak evidence of positive signal.

# Significance functions



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- ▶ Even though large simulation is carried out, bootstrap significance function here is not smooth. Smoothing required?
- ▶ **Discrete** distribution. Does not effect essential inferential issues, but introduces (mainly computational) complications. Not all theoretical results about rates of error etc. necessarily apply to such cases. **Good practical performance.**

## Example: $p = 1$ , $q = 20$ , 'Behrens-Fisher'

Let  $Y_{ij}$ ,  $i = 1, \dots, n_g$ ,  $j = 1, \dots, n_i$  be independent normal rvs,  
 $Y_{ij} \sim N(\mu, \sigma_i^2)$ .

Interest parameter is  $\mu$ , nuisance parameter  $(\sigma_1^2, \dots, \sigma_{n_g}^2)$ .

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Take case  $n_g = 20$ ,  $n_i \equiv n$ ,  $\sigma_i^2 = i$ , varying  $n$ .

Compare coverages of one-sided (upper) confidence limits for true  $\mu = 0$ , obtained by  $N(0, 1)$  approximation to distributions of  $R$ ,  $R^*$ , and by (constrained) bootstrap estimation of distribution of  $R$  (based on drawing 10,000 bootstrap samples). Figures based on 50,000 MC replications.

Nominal (%)		1.0	5.0	10.0	90.0	95.0	99.0
$n = 3$	$R$	7.6	16.3	22.5	77.6	83.7	92.4
	$R^*$	3.3	9.9	15.9	83.3	89.4	96.1
	boot	1.1	5.1	10.2	89.9	94.8	99.0
$n = 5$	$R$	3.3	9.9	15.7	84.3	90.2	96.7
	$R^*$	1.9	7.2	12.8	87.3	92.7	98.0
	boot	1.0	5.0	10.0	90.1	95.0	99.0
$n = 10$	$R$	1.8	7.0	12.5	87.6	92.9	98.1
	$R^*$	1.3	5.9	11.1	88.9	93.9	98.6
	boot	1.0	5.1	10.0	90.0	94.8	98.9

Example:  $p = 2$ ,  $q = 10$

Let  $Y_{1ij}, Y_{2ij}$ ,  $i = 1, \dots, n_g$ ,  $j = 1, \dots, n_i$  be independent normal rvs,  $Y_{1ij} \sim N(\mu_1, \sigma_i^2)$ ,  $Y_{2ij} \sim N(\mu_2, \sigma_i^2)$ .

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Example:  $p = 2, q = 10$

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Interest parameter is  $(\mu_1, \mu_2)$ , nuisance parameter  $(\sigma_1^2, \dots, \sigma_{n_g}^2)$ .

Take case  $n_g = 10, n_i \equiv n, \sigma_i^2 = i$ , varying  $n$ .

Compare coverages of confidence regions for true  $(\mu_1, \mu_2) = (1, 2)$ , obtained by  $\chi^2_2$  approximation to distribution of LRS  $W$ , (empirical) Bartlett correction of  $W$  and by bootstrap estimation of sampling distribution of  $W$  (based on drawing 10,000 bootstrap samples). Figures based on 50,000 MC replications.

Nominal (%)		1.0	5.0	10.0	90.0	95.0	99.0
$n = 5$	$W$	0.8	4.1	8.0	83.9	90.7	97.5
	$\bar{W}_c$	1.1	5.1	10.1	90.0	95.0	99.1
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- ▶ Multi-parameter exponential family context: inference agreeing with exact **conditional** inference to **relative** error third-order,  $O(n^{-3/2})$ . Same conditional accuracy as  $R^*$ . DiCiccio & Young (2008).
- ▶ Same context, automatically reproduces appropriate objective ('conditional second-order probability matching') Bayesian inference to order  $O(n^{-3/2})$ , in many circumstances.

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- ▶ Compare with third-order conditional accuracy of  $R^*$ .
- ▶ Third-order conditional accuracy unwarranted? Ancillary statistics typically not unique, different conditional inferences will typically only agree to second-order.

## Vector interest parameter ( $p > 1$ )

Repeated sampling perspective: simulating the distribution of  $W(\psi)$ , at **either** global MLE **or** constrained MLE, produces  $p$ -values uniformly distributed under  $H_0$ , to error of order  $O(n^{-2})$ .

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- ▶ Ancillary statistics models: unconditional higher-order probability matching priors give conditional frequentist accuracy to  $O(n^{-3/2})$  under some further conditions (DiCiccio, Kuffner & Young, 2012). But now, in key cases exact conditional matching priors exist and are unique. **In these cases, objective Bayes is preferred route to conditional frequentist accuracy?**

## II: Detailed theoretical analysis

# A detailed analysis of $R^*(\psi)$

The  $R^*$  statistic is defined by

$$R^*(\psi) = R(\psi) + R(\psi)^{-1} \log(v(\psi)/R(\psi)),$$

where  $v(\psi)$  is given by

$$v(\psi) = \left| \frac{L_{;\hat{\theta}}(\hat{\theta}) - L_{;\hat{\theta}}(\tilde{\theta})}{L_{\phi;\hat{\theta}}(\tilde{\theta})} \right| / \{|j_{\phi\phi}(\tilde{\theta})|^{1/2} |j(\hat{\theta})|^{1/2}\}.$$

Here, the log-likelihood function has been written as  $L(\theta; \hat{\theta}, a)$ , with  $(\hat{\theta}, a)$  minimal sufficient and  $a$  ancillary, and

$$L_{;\hat{\theta}}(\theta) \equiv L_{;\hat{\theta}}(\theta; \hat{\theta}, a) = \frac{\partial}{\partial \hat{\theta}} L(\theta; \hat{\theta}, a),$$

$$L_{\phi;\hat{\theta}}(\theta) \equiv L_{\phi;\hat{\theta}}(\theta; \hat{\theta}, a) = \frac{\partial^2}{\partial \phi \partial \hat{\theta}} L(\theta; \hat{\theta}, a).$$

Also,  $j$  denotes the observed information matrix,  $j(\theta) = (-L_{rs}(\theta))$ , with  $L_{rs}(\theta) = \partial^2 L(\theta) / \partial \theta^r \partial \theta^s$ , and  $j_{\phi\phi}$  denotes its  $(\phi, \phi)$  component.

# A decomposition

We may decompose  $R^*(\psi)$  as

$$R^*(\psi) = R(\psi) + \text{NP}(\psi) + \text{INF}(\psi),$$

for quantities  $\text{NP}(\psi)$  and  $\text{INF}(\psi)$ , both of order  $O_p(n^{-1/2})$ .

# Definitions

Explicitly, we have

$$\text{NP}(\psi) = -\frac{1}{R(\psi)} \log C(\psi),$$

where

$$C(\psi) = \frac{\{|j_{\phi\phi}(\hat{\theta})||j_{\phi\phi}(\tilde{\theta})|\}^{1/2}}{|L_{\phi;\hat{\phi}}(\tilde{\theta})|},$$

with  $L_{\phi;\hat{\phi}}(\theta) \equiv L_{\phi;\hat{\phi}}(\theta; \hat{\theta}, a) = \partial^2 L(\theta; \hat{\theta}, a) / \partial \phi \partial \hat{\phi}$  and  $j_{\phi\phi}$  denoting, as before, the  $(\phi, \phi)$  component of the observed information  $j$ .

Also,

$$\text{INF}(\psi) = \frac{1}{R(\psi)} \log\{u(\psi)/R(\psi)\},$$

where

$$u(\psi) = j_p(\hat{\psi})^{-1/2} \frac{\partial}{\partial \hat{\psi}} \{M(\hat{\psi}) - M(\psi)\}.$$

Here  $j_p$  is the profile observed information,

$j_p(\psi) = -\partial^2 M(\psi)/\partial \psi^2$ , and the derivative with respect to  $\hat{\psi}$  is calculated with  $M(\hat{\psi}) - M(\psi)$  considered as a function of  $\psi, \hat{\psi}, \hat{\phi}_\psi$  and  $a$ .

# Interpretations

$\text{NP}(\psi)$  and  $\text{INF}(\psi)$  are **interpreted** as correcting respectively for presence of the nuisance parameter  $\phi$  and deviation from standard normality of  $R(\psi)$  itself.

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So, broadly speaking,  $\text{INF}(\psi)$  represents what we can eliminate by bootstrapping to replace asymptotic approximation,  $\text{NP}(\psi)$  represents intrinsic difficulty of the inference.

# Quantitative analysis

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- ▶ Explicit approximation of  $E\{\text{NP}(\psi)\}$  and  $E\{\text{INF}(\psi)\}$  provides statistical insight, in particular to effects of high-dimensional nuisance parameter on inference and to impact of nuisance parameter on parametric bootstrap.

# Expectations

We have:

$$E\{\text{INF}(\psi)\} = \eta^{1/2} \lambda^{1r} \tau^{st} \left( \frac{1}{2} \lambda_{rs,t} + \frac{1}{6} \lambda_{rst} \right) + O(n^{-1});$$

$$E\{\text{NP}(\psi)\} = -\eta^{1/2} \lambda^{1r} \nu^{st} \left( \lambda_{rs,t} + \frac{1}{2} \lambda_{rst} \right) + O(n^{-1}).$$

# Interpretation

If there is no nuisance parameter, then  $\lambda^{11} = (\lambda_{11})^{-1}$ ,  $\eta = -\lambda_{11}$ ,  $\tau^{11} = (-\lambda_{11})^{-1}$ , and  $\nu^{11} = 0$ , and it follows that

$$E\{R(\psi)\} = (-\lambda_{11})^{-3/2}(\frac{1}{2}\lambda_{11,1} + \frac{1}{6}\lambda_{111}) + O(n^{-1}).$$

Suppose there is a vector nuisance parameter  $\phi$ , but assume that the interest parameter  $\psi$  and  $\phi$  are **orthogonal** [always achievable in principle]; then  $\lambda^{11} = (\lambda_{11})^{-1}$ ,  $\eta = -\lambda_{11}$ ,  $\lambda^{1a} = 0$  ( $a = 2, \dots, d$ ),  $\tau^{rs} = 0$  except when  $r = s = 1$ , in which case  $\tau^{11} = (-\lambda_{11})^{-1}$ , and

$$E\{\text{INF}(\psi)\} = -(-\lambda_{11})^{-3/2}(\tfrac{1}{2}\lambda_{11,1} + \tfrac{1}{6}\lambda_{111}) + O(n^{-1}).$$

Therefore, to error of order  $O(n^{-1})$ ,  $E\{\text{INF}(\psi)\}$  corresponds to a mean adjustment for the signed root statistic  $R(\psi)$  in the problem where the orthogonal nuisance parameter  $\phi$  is **known**.

The  $N(0, 1)$  approximation to the distribution of  $R(\psi)$  is typically rather accurate in scalar parameter problems, so the mean adjustment should be generally small, so we can anticipate that  $\text{INF}(\psi)$  is in some generality **small**.

## Further analysis

In principle, we can always reparameterize so that  $\psi$  and the nuisance parameter  $\phi$  are orthogonal.

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In principle, we can always reparameterize so that  $\psi$  and the nuisance parameter  $\phi$  are orthogonal.

Invariance of adjustments to reparameterization allows nuisance parameter effects to be quantified by

$$E\{\text{NP}(\psi)\} = -\frac{1}{2}(-\lambda_{11})^{-1/2}\lambda^{ab}\lambda_{ab1} + O(n^{-1}).$$

**Multiple sum** over nuisance parameter, in accordance with intuition that  $\text{NP}(\psi)$  can be anticipated to be large when dimensionality of nuisance parameter is large. How large?

# Explicit approximations

We may explicitly approximate  $E\{\text{INF}(\psi)\}$  to  $O(n^{-1})$  by

$$g_{\text{INF}}(\theta) = \eta^{1/2} \lambda^{1r} \tau^{st} \left( \frac{1}{2} \lambda_{rs,t} + \frac{1}{6} \lambda_{rst} \right)$$

and  $E\{\text{NP}(\psi)\}$  to the same order by

$$g_{\text{NP}}(\theta) = -\eta^{1/2} \lambda^{1r} \nu^{st} (\lambda_{rs,t} + \frac{1}{2} \lambda_{rst}).$$

## Remarks 1

Quantities  $g_{\text{INF}}(\theta)$  and  $g_{\text{NP}}(\theta)$  are related to asymptotic quantities detailed by Efron (1987, JASA) in description of the 'bias corrected accelerated',  $BC_a$ , method of construction of bootstrap confidence intervals.

# Remarks 1

Quantities  $g_{\text{INF}}(\theta)$  and  $g_{\text{NP}}(\theta)$  are related to asymptotic quantities detailed by Efron (1987, JASA) in description of the 'bias corrected accelerated',  $BC_a$ , method of construction of bootstrap confidence intervals.

Specifically, we have  $g_{\text{INF}}(\theta) = a_c$  and  $g_{\text{NP}}(\theta) = z_0 - a_c$ , where  $a_c$  and  $z_0$  are respectively acceleration and bias-correction quantities.

The quantity  $a_c$  satisfies

$$a_c = -\frac{1}{6}\{\text{skew}(U) + \text{skew}(T)\} + O(n^{-1}),$$

where  $U = (\hat{\psi} - \psi)/\sigma$ , with  $\sigma^2$  the asymptotic variance of  $\hat{\psi}$ , so that  $\sigma^2 \equiv \sigma^2(\theta) = \lambda^{1,1} + O(n^{-2})$ , and  $T = (\hat{\psi} - \psi)/\hat{\sigma}$ , with  $\hat{\sigma}^2 = \sigma^2(\hat{\theta})$ .

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Also,  $z_0$  is interpreted by

$$\Phi(z_0) = \Pr(\hat{\psi} \leq \psi) + O(n^{-1}),$$

where  $\Phi$  is the standard normal distribution function.

## Remarks 2

Quantities  $g_{\text{NP}}(\theta)$  and  $g_{\text{INF}}(\theta)$  are both of order  $O(n^{-1/2})$ .

Calculation of the individual values provides valuable statistical insight to importance of nuisance parameter effects **and** likely operational performance of bootstrap (which is completely determined by nuisance parameter).

## Remarks 3

In general,  $g_{\text{NP}}(\theta)$  and  $g_{\text{INF}}(\theta)$  depend on the **unknown** parameter  $\theta$ .

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A simple adjustment of the signed root statistic  $R(\psi)$ , is given by  $R_a(\psi) = R(\psi) + g_{\text{NP}}(\tilde{\theta}) + g_{\text{INF}}(\tilde{\theta})$ .

Since  $g_{\text{NP}}(\tilde{\theta}) - g_{\text{NP}}(\theta) = O_p(n^{-1})$ , we have that  $R_a(\psi) = R^*(\psi) + O_p(n^{-1})$ , and therefore that  $R_a(\psi)$  is  $N(0, 1)$  to error of order  $O(n^{-1})$ .

# Methodological Issues

- ▶ 'Uniqueness of inference'.
- ▶ Computational considerations.
- ▶ Relationship between analytic and bootstrap approaches.
- ▶ Choice of a 'good pivot'.

# When do inferences agree?

In general,  $p$ -values from different asymptotically  $N(0, 1)$  pivots will agree only to first-order,  $O(n^{-1/2})$ .

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However, establish simple sufficient conditions, under which  $p$ -values from two statistics will agree to second-order,  $O(n^{-1})$ , provided approximations to distributions accurate to  $O(n^{-1})$  are employed. Such accurate approximation obtained quite generally by bootstrap.

# Consequences

- ▶  $T_W(\psi)$  and  $T_S(\psi)$  in general **do not** provide  $p$ -values that agree with those from  $R(\psi)$  to order  $O_p(n^{-1})$ .

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- ▶ But, versions of Wald and score statistics constructed using **observed** information **will** yield  $p$ -values agreeing with those from  $R(\psi)$  to  $O_p(n^{-1})$ .

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- ▶ But, versions of Wald and score statistics constructed using **observed** information **will** yield  $p$ -values agreeing with those from  $R(\psi)$  to  $O_p(n^{-1})$ .
- ▶ Etc., etc.

# Computational considerations

Use of  $W(\psi)$  and  $R(\psi)$  requires calculation of both global and constrained MLEs. Potentially unattractive compared to Wald statistic,  $T_W(\psi)$  [or multivariate version]. Latter routinely employed in statistical packages etc., but not stable or parameterization invariant.

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**Bootstrap**: must recalculate for a series of  $B$  bootstrap samples. General guideline:  $B$  of order of few 1000's to reduce Monte Carlo variability to acceptable levels, to 'capture' good theoretical properties. In small samples or with high-dimensional nuisance parameter solution of likelihood equations **can** be a worry.

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$R^*(\psi)$ : computationally simple, potentially awkward analytic calculations/coding. (Highly) stable, parameterization invariant.

# General pivot

For general, asymptotically  $N(0, 1)$  pivot  $T(\psi)$ , producing same  $p$ -values as  $R(\psi)$  to  $O_p(n^{-1})$ , normalized (Cornish-Fisher) version of  $T(\psi)$ ,  $N(0, 1)$  to error of order  $O(n^{-1})$ , is:

$$T(\psi) - \frac{1}{6}\kappa_3\{T(\psi)\}^2 + NP(\psi) + INF(\psi),$$

in terms of third cumulant  $\kappa_3$  of  $T(\psi)$ .

# When does bootstrap work?

Normalizing transformation is automatically incorporated by bootstrap refinement of the asymptotic  $N(0, 1)$  approximation.

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Normalizing transformation is automatically incorporated by bootstrap refinement of the asymptotic  $N(0, 1)$  approximation.

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- ▶ 'Primary effect of bootstrap is to estimate skewness'. Key requirement for bootstrap to perform well is that third cumulant of  $T(\psi)$  can be estimated accurately. Difficult if  $n$  is small, or number of nuisance parameters is large.
- ▶ If skewness is small, as with  $R(\psi)$ , where it is of order  $O(n^{-1})$ , estimation of skewness less crucial, explaining why bootstrap works extraordinarily well with  $R(\psi)$ .

- ▶ If skewness is constant with respect to nuisance parameter, bootstrap should work well, inaccuracy in estimating nuisance parameter does not translate into inaccuracy in estimating skewness.

- ▶ If skewness is constant with respect to nuisance parameter, bootstrap should work well, inaccuracy in estimating nuisance parameter does not translate into inaccuracy in estimating skewness.
- ▶ Previous focus on variance-stabilizing transformations to improve bootstrap accuracy: variance stabilizing transformations typically reduce skewness of parameterization dependent pivot  $T(\psi)$ . DiCiccio, Monti & Young (2006).

# Relationship between Bootstrap and $R^*(\psi)$

Conceptually related, **not** distinct methodologies.

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Specifically:

- ▶  $p$ -values calculated from  $N(0, 1)$  approximation to distribution of  $R^*(\psi)$  will **quite generally** agree with those from bootstrap to order  $O_p(n^{-1})$ .
- ▶ Multi-parameter exponential family models: (unconditional) bootstrap  $p$ -values agree with those from  $R^*(\psi)$  to  $O_p(n^{-3/2})$ .

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- ▶ Multi-parameter exponential family models: (unconditional) bootstrap  $p$ -values agree with those from  $R^*(\psi)$  to  $O_p(n^{-3/2})$ .
- ▶ Ancillary statistic models: normal approximation to  $R^*(\psi)$  is an  $O(n^{-3/2})$  (saddlepoint) approximation to conditional bootstrap [which could use if we could simulate the conditional distribution of  $R(\psi)$  given  $A = a$ ].

# The bottom line

If likelihood equations can be reliably solved, analytic simplicity indicates bootstrapping of  $R(\psi)$  or  $W(\psi)$  as a highly effective methodology.

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- ▶ Unlikely to be computationally prohibitive [moderate  $B$  adequate to ensure MC variability does not impair good theoretical properties].
- ▶ Stable (respects CP to high-order) and parameterization invariant: ‘inferentially correctness is OK’.
- ▶ Vector  $\psi$ : use bootstrap calculation to estimate mean of  $W(\psi)$ , then base inference on  $\chi^2$  approximation to empirically Bartlett-corrected statistic  $\bar{W}_c(\psi)$ .

### III: Further illustrations

## Further Illustration 1: resampling accuracy, RE (ctd)

$Y_1, \dots, Y_n$  IID inverse Gaussian, with density

$$f(y; \mu, \psi) = \left( \frac{\psi}{2\pi y^3} \right)^{1/2} \exp \left( -\frac{\psi}{2\mu^2 y} (y - \mu)^2 \right), \quad y > 0,$$

interest parameter is shape  $\psi$ , mean  $\mu$  as nuisance.

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interest parameter is shape  $\psi$ , mean  $\mu$  as nuisance.

20,000 replications,  $n = 5$ , true  $\mu = 1, \psi = 2$ . Compare coverages of confidence limits of different nominal coverages obtained by: normal approximation to  $R(\psi)$ ; normal approximation to  $R^*(\psi)$ ; bootstrap of  $R(\psi)$ ; three objective Bayes priors (*OB1*, *OB2* and *OB3*). Each replication: 5,000 bootstrap samples, MC construction of Bayes posterior quantile.

*OB1* has  $\pi(\psi, \mu) \propto \psi^{-1} \mu^{-2}$ , *OB2* has  $\pi(\psi, \mu) \propto \psi^{-1/2} \mu^{-3/2}$  and *OB3* has  $\psi(\psi, \mu) \propto \psi^{-1} \mu^{-3/2}$ .

In theory, *OB1* and *OB3* should give  $O(n^{-3/2})$  coverage accuracy, but not *OB2*. Typical of non-uniqueness of second-order ( $O(n^{-3/2})$ ) matching prior.

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In theory, *OB1* and *OB3* should give  $O(n^{-3/2})$  coverage accuracy, but not *OB2*. Typical of non-uniqueness of second-order ( $O(n^{-3/2})$ ) matching prior.

Actually exponential family, appropriate frequentist inference is conditional, but provides instructive example where repeated sampling properties should, in principle, be very similar.

Nominal (%)	1.0	5.0	10.0	90.0	95.0	99.0
$\Phi(R)$	0.3	1.7	3.8	74.6	84.4	95.0
Bootstrap $R$	1.1	5.1	10.1	90.1	95.1	99.0
$\Phi(R^*)$	1.0	4.8	9.6	89.4	94.8	98.9
$OB1$	1.0	4.9	10.0	90.3	95.1	99.0
$OB2$	3.0	10.6	18.4	94.1	97.2	99.5
$OB3$	1.0	4.7	9.3	89.6	94.7	98.9

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- ▶ Bootstrap and normal approximation to  $R^*(\psi)$  both highly accurate.
- ▶ Objective Bayes yields good repeated sampling accuracy, with OB1 or OB3.

## Conditional inference: detail

With  $S = n^{-1} \sum_i Y_i^{-1}$ ,  $C = n^{-1} \sum_i Y_i$ , correct inference is **conditional**, based on conditional distribution of  $S$ , given  $C = c$ .

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Equivalent to inference based on the marginal distribution of  $V = \sum_i (Y_i^{-1} - \bar{Y}^{-1})$ . Distribution of  $\psi V$  is  $\chi_{n-1}^2$ .

Have

$$R(\psi) = \text{sgn}(\hat{\psi} - \psi) \{n(\log \hat{\psi} - 1 - \log \psi + \psi/\hat{\psi})\}^{1/2},$$

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Distribution of  $R(\psi)$  is **free** of nuisance parameter  $\mu$ : infinite simulation bootstrap will approximate sampling distribution **exactly**, no coverage error.

Also, since  $R(\psi)$  is a monotonic function of  $V$ , bootstrap inference will actually replicate the appropriate **exact conditional inference** without error.

## Further Illustration 2: RE (ctd), extended

Let  $Y_{ij}$ , for  $i = 1, \dots, n$  and  $j = 1, \dots, q$  be independent, inverse Gaussian random variables, with  $Y_{ij}$  having probability density

$$f(y; \psi, \phi_j) = \{\psi/(2\pi)\}^{1/2} y^{-3/2} \exp\{-\frac{1}{2}(\psi y^{-1} + \phi_j y) + (\psi\phi_j)^{1/2}\},$$

$y > 0$ ,  $\psi, \phi_j > 0$ , so that  $\theta = (\psi, \phi_1, \dots, \phi_q)$ . Here  $\psi$  and  $(\phi_1, \dots, \phi_q)$  are **non-orthogonal**.

Here, irrespective of the parameter value  $\theta$ ,

$$n^{1/2}g_{\text{INF}}(\theta) \equiv -1/\{3(2q)^{1/2}/2\},$$

and

$$n^{1/2}g_{\text{NP}}(\theta) \equiv -(q/2)^{1/2},$$

so that

$$g_{\text{NP}}(\theta)/g_{\text{INF}}(\theta) \equiv 3q/2.$$

The adjusted statistic  $R_a(\psi)$  may be constructed in this example without the need to estimate the nuisance parameters  $\phi_1, \dots, \phi_q$ .

# Implications for bootstrap

To order  $O(n^{-1})$  expectations of adjustments do not depend on **values** of nuisance parameters, only **dimension**.

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To order  $O(n^{-1})$  expectations of adjustments do not depend on **values** of nuisance parameters, only **dimension**.

Parametric bootstrap ought to be accurate? Inference, at least to order  $O(n^{-1})$ , not governed by nuisance parameter values: bootstrap substitution should be OK.

In fact, here  $R(\psi)$  readily seen to be exactly '**pivotal**': its sampling distribution **is completely free of nuisance parameter**. (Infinite simulation) bootstrap gives **exact** inference. In practice, finite Monte Carlo simulation: exactness is compromised by finiteness of simulation.

# Numerical results

Consider sample size  $n = 5$ , and two values of  $q$ ,  $q = 5, 20$ . For parameter settings  $\psi = 2, \phi_i = i, i = 1, \dots, q$ , 100,000 datasets were generated.

Accuracy of inference based on  $N(0, 1)$  approximation to the distributions of the three statistics  $R(\psi)$ ,  $R^*(\psi)$  and  $R_a(\psi)$  expressed in terms of observed coverages over the 100,000 samples of confidence sets for  $\psi$ , obtained by the normal approximation, for different nominal coverages.

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Also, coverages when bootstrapping used to approximate sampling distribution of  $R(\psi)$ , using 5000 bootstrap samples.

Nominal (%)	1.0	2.5	5.0	10.0	90.0	95.0	97.5	99.0
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$q = 5$

$R(\psi)$	0.1	0.3	0.8	1.9	65.4	77.2	85.3	91.9
$R^*(\psi)$	0.9	2.3	4.7	9.5	89.4	94.7	97.4	98.9
$R_a(\psi)$	1.1	2.6	5.0	9.7	87.8	93.6	96.6	98.5
Boot	1.0	2.5	5.0	10.0	90.2	95.1	97.6	99.0

$q = 20$

$R(\psi)$	0.0	0.0	0.0	0.0	38.8	52.6	64.4	76.5
$R^*(\psi)$	0.8	2.2	4.4	8.8	88.8	94.3	97.2	98.8
$R_a(\psi)$	0.9	2.3	4.4	8.7	86.8	92.9	96.2	98.3
Boot	1.0	2.5	4.9	9.8	90.0	95.0	97.6	99.0

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- ▶ Normal approximation to the distribution of  $R(\psi)$  itself is highly inaccurate, and the nuisance parameter effect is substantial.
- ▶ Coverage figures for the simple adjusted statistic  $R_a(\psi)$  are decent.

# Discussion

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- ▶ Normal approximation to the distribution of  $R(\psi)$  itself is highly inaccurate, and the nuisance parameter effect is substantial.
- ▶ Coverage figures for the simple adjusted statistic  $R_a(\psi)$  are decent.
- ▶ Bootstrap is, however, highly accurate.

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- ▶ Coverage figures for the simple adjusted statistic  $R_a(\psi)$  are decent.
- ▶ Bootstrap is, however, highly accurate.
- ▶ Simulation allows estimation of  $E\{\text{NP}(\psi)\}$  and  $E\{\text{INF}(\psi)\}$ : we have,  $q = 5$ ,  $E\{\text{NP}(\psi)\}/g_{\text{NP}}(\theta) = 1.05$ , with  $E\{\text{INF}(\psi)\}/g_{\text{INF}}(\theta) = 1.02$ , so that the approximations to the means of the two adjustments are highly accurate even for  $n = 5$ .

## Further Illustration 3: Curved exponential family model

Let  $Y_{ij}$ , for  $i = 1, \dots, n$  and  $j = 1, \dots, q$  be independent normal random variables with means  $\mu_j > 0$  and variances  $\psi\mu_j^\zeta$ , with  $\zeta$  a known constant.

If  $\zeta = 0$  or  $\zeta = 1$  the model is a full exponential family, otherwise it is **curved**. The parameter of interest is  $\psi$ , with  $\mu_1, \dots, \mu_q$  as nuisance parameters,  $\theta = (\psi, \mu_1, \dots, \mu_q)$ . Fix  $\zeta = 1/2$ . Again,  $\psi$  and  $(\mu_1, \dots, \mu_q)$  are **non-orthogonal**.

Calculation of  $R^*(\psi)$  is **intractable**. Construction of  $R_a(\psi)$  is no more complex than in Further Illustration 2.

Now the ratio  $g_{\text{NP}}(\theta)/g_{\text{INF}}(\theta)$  **does** depend (weakly?) on the value of the parameter  $\theta$ . Illustrative values are given below, for two cases: case (a) has  $\psi = 1, \mu_i = i, i = 1, \dots, q$ , while case (b) has  $\psi = 2, \mu_i = i, i = 1, \dots, q$ .

$q$	1	2	5	10	20	50
(a)	1.11	2.45	6.77	14.17	29.09	74.01
(b)	0.82	2.04	6.19	13.49	28.33	73.19

# Numerical results

Obtain empirical estimates, based on 20,000 replications, for case (a), with sample size  $n = 15$ , of coverages of confidence sets obtained by normal approximation to the distributions of  $R(\psi)$  and  $R_a(\psi)$  in this problem, as before for two values of nuisance parameter dimension,  $q = 5, 20$ .

Again, compare with bootstrap using 5000 bootstrap samples for each estimation.

Nominal (%)	1.0	2.5	5.0	10.0	90.0	95.0	97.5	99.0
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$q = 5$

$R(\psi)$	4.0	8.2	14.2	23.4	96.5	98.5	99.3	99.8
$R_a(\psi)$	1.1	2.9	5.6	11.1	90.3	95.1	97.6	99.0
Boot	1.0	2.5	5.0	10.2	90.4	95.3	97.7	99.1

$q = 20$

$R(\psi)$	10.5	18.8	28.0	40.7	98.8	99.6	99.7	99.9
$R_a(\psi)$	1.4	3.1	6.0	11.4	90.4	94.9	97.5	99.0
Boot	1.1	2.6	5.2	10.2	90.2	94.8	97.5	99.0

The distribution of the unadjusted statistic  $R(\psi)$  is very far from  $N(0, 1)$ : the empirical adjustment leads to a statistic  $R_a(\psi)$  whose distribution is satisfactorily approximated as  $N(0, 1)$ .

Bootstrap is again best.

## Further Illustration 4: an example of conditional inference

$Y_1, \dots, Y_n$  IID gamma, mean  $\mu$ , shape parameter  $\nu$  and density

$$f(y; \mu, \nu) = \frac{\nu^\nu}{\Gamma(\nu)} \exp\left[-\nu\left\{\frac{y}{\mu} - \log\left(\frac{y}{\mu}\right)\right\}\right] \frac{1}{y}, \quad y > 0.$$

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Appropriate inference on  $\nu$ , with  $\mu$  as nuisance, is **conditional**, based on conditional distribution of  $Q = \prod Y_i$ , given observed value,  $c$ , of  $C = \sum Y_i$ .

Data configuration  $q = 1.0, c = 20.0$ , varying  $n$ .

Evaluate conditional frequentist confidence levels of bootstrap, analytic and specific objective Bayes limits, against **exact** conditional inference.

Bootstrap limits based on 5 million samples. MC construction of objective Bayes (OB) limits.

Model condition is **not** satisfied here, so objective Bayes here does not achieve theoretical  $O(n^{-3/2})$  accuracy.

$n$	Method	5%	(quantile)	95%	(quantile)
5	OB	5.18	(0.122)	95.03	(0.820)
	boot	5.07	(0.121)	95.01	(0.819)
	$R^*$	5.67	(0.126)	95.35	(0.832)
10	OB	5.11	(0.357)	95.01	(1.370)
	boot	5.00	(0.355)	95.00	(1.369)
	$R^*$	5.19	(0.358)	95.11	(1.374)
15	OB	5.05	(0.912)	95.01	(2.908)
	boot	4.98	(0.909)	95.00	(2.907)
	$R^*$	5.06	(0.913)	95.06	(2.912)

## Further Illustration 5: conditional inference, Weibull

Let  $\{T_1, \dots, T_n\}$  be random sample from the Weibull density

$$f(t; \nu, \lambda) = \lambda \nu (\lambda t)^{\nu-1} \exp\{-(\lambda t)^\nu\}, \quad t > 0,$$

interest parameter  $\nu$ .

Take  $Y_i = \log T_i$ : the  $Y_i$  are random sample from extreme value distribution  $EV(\mu, \psi)$ , location-scale family, with scale and location parameters  $\psi = \nu^{-1}$ ,  $\mu = -\log \lambda$ .

Exact conditional inference for  $\psi$  conditions on  $a = (a_1, \dots, a_n)$ , with  $a_i = (y_i - \hat{\mu})/\hat{\psi}$ .

5000 replications from  $\nu = \lambda = 1$ .

**One-sided inference:** test  $H_0 : \psi = 1$ , against  $\psi > 1$ . Inference based on:  $N(0, 1)$  approximation to distribution of  $R$ ;  $N(0, 1)$  approximation to distribution of  $R^*$ ; bootstrapping (marginal) distribution of  $R$ .

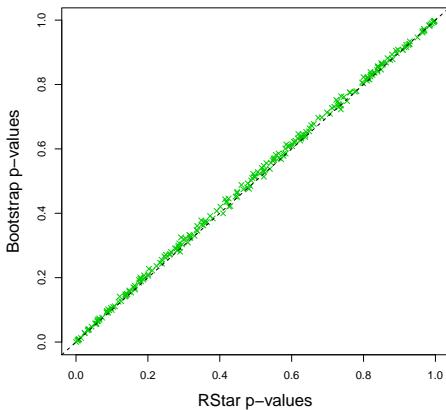
**Two-sided inference:** test  $H_0$  against  $\psi \neq 1$ . Inference based on:  $\chi^2_1$  approximation to distribution of  $W$ ; empirical (marginal) Bartlett correction; bootstrapping (marginal) distribution of  $W$ .

Compare the average absolute percentage relative error of different approximations to the **exact** conditional p-values over the 5000 replications.

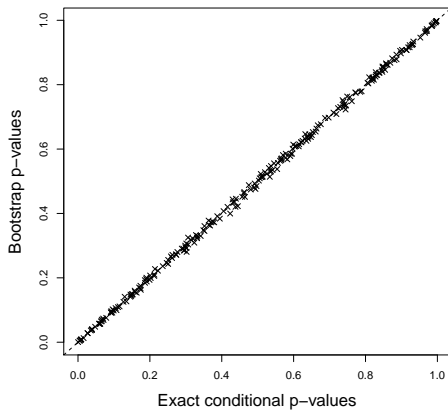
Bootstrap results are based on 5,000,000 samples, same simulation being used for empirical Bartlett correction.

$n$	One-sided			Two-sided		
	$R$	$R^*$	boot	$W$	$\bar{W}_c$	boot
10	37.387 (0.0%)	1.009 (17.1%)	0.674 (82.9%)	12.318 (0.0%)	0.666 (43.9%)	0.611 (56.1%)
20	25.473 (0.0%)	0.388 (46.2%)	0.397 (53.8%)	6.118 (0.0%)	0.185 (63.4%)	0.227 (36.6%)
30	20.040 (0.0%)	0.252 (60.9%)	0.307 (39.1%)	4.158 (0.0%)	0.131 (68.7%)	0.200 (31.3%)
40	17.865 (0.0%)	0.250 (70.1%)	0.273 (29.9%)	3.064 (0.0%)	0.117 (69.7%)	0.177 (30.3%)

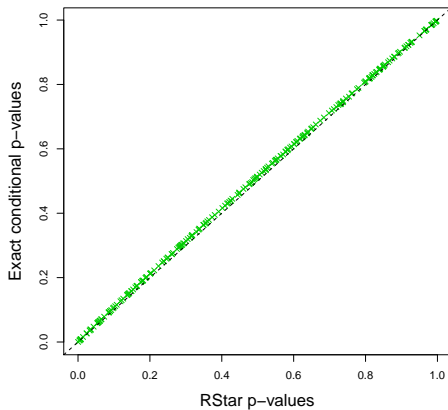
## Weibull: $n = 5$ , $R^*$ $p$ -values vs bootstrap $p$ -values



## Weibull: $n = 5$ , exact conditional $p$ -values vs bootstrap $p$ -values



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- ▶ Strong theoretical basis for use of **signed root statistic** (and likelihood ratio statistic).
- ▶ Discrete data problems. Broad operational conclusions OK, detail of theory less certain.
- ▶ Non-regular problems?

- **Robustness** to model (mis-)specification important. Lu & Young (2012): work with a robustified version of  $R(\psi)$  or  $W(\psi)$ . Bootstrapping the robust statistic is strikingly effective: simulation of the statistic under **wrong** distribution can nevertheless yield accurate inference with small  $n$ , even if theoretical order of error does not improve on normal approximation. By contrast, methods such as  $R^*(\psi)$  are highly non-robust.

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- ▶ Conclusions valid for common adjusted forms of likelihood. Intractable or complex likelihood: theory necessary for composite and pseudo-likelihood, but practical effectiveness striking.
- ▶ Stratification of a bootstrap simulation by values of appropriate conditioning statistic effective as means of reducing error, but awkward to implement.