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Decoding the H-likelihood

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Decoding the H-likelihood

Xiao-Li Meng

Key words and phrases: Ancillary statistics, Bartlett identities, Fisher information, Hessian information, likelihood principle, missing data, pivotal predictive distribution, prediction, posterior predictive distribution, random effect.

1. PROLOGUE

The invitation for this discussion contribution came at the busiest time in my (professional) life with four courses and many more meetings attempting to compensate, psychologically, for the lost endowment at Harvard. I could not possibly, however, decline David Madigan's kind invitation. The topic is dear to my heart, as it should be to any statistician's, for without "unobservables," we would be unemployable. And I always wanted to know what "h-likelihood" is! I first heard the term from my academic twin brother, Andrew Gelman, who sent me his discussion of Lee and Nelder (1996). Gelman's conclusion was that "To the extent that the methods in this paper give different answers from the full Bayesian treatment, I would trust the latter." This of course did not entice me to read the paper. Indeed, I still did not know its definition when I started to type this Prologue, nor have I had any professional or personal contact with either author. I surmise this qualifies me as an *objective* discussant, though I hope in this case the phrase *objective* is not exchangeable with *noninformative* or *ignorant*!

But surely, one may quibble, Gelman's comment must have influenced me. True, but I'm not the kind of Bayesian who is unwilling to change his/her prior. My pure interest is to decode the h-likelihood. If my brother is right, I'll be more proud of him. If he is wrong, I'll be wiser by learning something new. (But I do ask Professors Lee and Nelder for their tolerance as I try to follow my brother's critical style, in the name of good discussion!) So here I am, setting aside the 72-hour Memorial Day weekend, after persuading my teenagers that their father's H-bomb mystery is more

urgent to solve than his colleague Dr. Langdon's prevention of the antimatter explosion in 24 hours, which actually repeats every weekend.

2. PREPARING FOR A BAYESIAN INFERENCE OF H-LIKELIHOOD

2.1 Prior Formulation

Naturally I will adopt a Bayesian approach to infer what is the real "H" in the h-likelihood. What could it actually stand for? (I) Heuristic argument? (II) Handy approximation? (III) Hybrid method? Or even (IV) Hidden treasure? Of course, a priori I would not be a good Bayesian if I exclude "(V) Hype?" no matter how small my prior belief in it. Gelman's comment led me to assign the highest prior probability to (III), 60%. Since the events here are clearly not mutually exclusive, (I) and (II) also deserve some nontrivial prior probabilities which are 40% each for reasons I can only explain to myself. But for reasons everyone can explain, the prior probabilities for categories such as (IV) or (V) are best kept confidential, other than that they of course depend on one's knowledge of the author(s) and the journal.

2.2 Data Collection

Immediately, I ran into the usual problem of any real-life data collection—there are never enough time or resources! It is already 2:31 pm Saturday as I am typing this sentence, and I yet need to read the paper plus four reference papers I was able to download from JSTOR: two discussion papers by the same authors (Lee and Nelder, 1996, 2005) and the two papers in *Biometrika* that illustrate the use of h-likelihood (Ha, Lee and Song, 2001, Lee and Nelder, 2001). Lee, Nelder and Pawitan's (2006) book of course would be invaluable which, unfortunately, turns out to be literally true in this case because apparently no Harvard library can afford it.

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So I settle with these four papers as background, knowing well the potential bias due to my haphazard selection and all the “unobservables” to me at this moment. Hence my apologies to the authors—and readers—in advance. To compensate for my hastiness, I’ll actually read all five papers, and the discussions, before forming my likelihood, with or without “H”!

2.3 Data Processing

Another grand challenge in real-life statistical analysis is *data processing*, something that unfortunately has not received nearly enough systematic treatment in the literature but which typically can have a substantial, if not detrimental, impact on the final conclusions. One key component in data processing is to sort out contradictions in the data, some obvious and some subtle.

A priori I did not expect this to be a part of the mystery that would await me. But that prior belief quickly shrank to ε after reading the first paragraph. The authors started by emphasizing Pearson’s (1920) point that Fisher’s likelihood is not useful for predicting future observations or unobservables. Regardless of whether Fisher ever had such an intention, this is an *inference/prediction* issue. The authors then immediately stated that existing efforts in generalizing Fisher’s likelihood inferences with unobservables run into the problem of not having “explicit forms” due to the difficulty in integration. But that is squarely a *computational/calculus* issue. Putting aside the vast literature on the EM algorithm and related computational methods that have successfully dealt with this very computational issue in many common applications (see the overview by van Dyk and Meng (2010) and other papers in the coming theme issue on EM in this journal), I am mystified by the logic and aims here—which issue do the authors intend to address? Both?

Of course this could actually be a sign of a great mystery novel, enticing the reader from the very beginning, with multiple seemingly related or unrelated lines to pursue, and a Holy Grail at the end—a gigantic H! (Clearly I am still in my Dan Brown mood, though hopefully this time the Holy Grail is more than a legend.)

The data processing indeed took much longer than I expected, mainly because the “unobservables” that I need to infer, from a number of mystic symbols whose meaning can only be surmised retrospectively to reasons that can explain the authors’ conviction that their h-likelihood methods have been misunderstood by almost all the discussants, since Lee and Nelder (1996).

It is already 6:39 pm, Sunday. So let me get to the three main storylines as I comprehend. The first two

lines are generally well understood, so I shall reflect on them briefly. The third line, which is the most controversial, namely, h-likelihood inference for unobservables, touches upon some fundamental issues about statistical inference and prediction, and turns out to have at least one unexpected intriguing property, at least to me. Therefore, the rest (three quarters of the) discussion attempts to provide an explanation of this controversy to a general audience, along with some ramifications and thoughts it generates. Indeed, if a reader is in a rush to catch *Angles and Demons*, as my teenagers were, the reader should just skip the following section, which contains no real enlightenment or entertainment, other than some shameless self-advertisements and academic quibbles.

3. TWO UNCONTROVERSIAL STORYLINES

3.1 Line One: Unobservables are Useful for Modeling

Much of the authors’ Section 1 and Section 2 were devoted to arguing and demonstrating the usefulness of unobservables for statistical modeling. Other than the authors’ preference for using *unobservables* as the all-encompassing term instead of the more common term *missing data* (though I agree that “unobservables” is semantically more appropriate), the same message has been repeatedly emphasized in the literature, and it is indeed worthy of repeating. As I wrote in “Missing Data: Dial M for ???”, a JASA Y2K vignette (Meng, 2000), “The topic of missing data is as old and as extensive as statistics itself—after all, statistics is about knowing the unknowns.” Unable to outshine the summary there, I ask readers’ indulgence for a more extensive self-quotation. Below is the opening paragraph of the same vignette, echoing well the authors’ key emphases, but with a more extended history (e.g., McKendrick’s missing-data modeling/formulation went back 1926; see Meng, 1997):

The question mark is common notation for the missing data that occur in most applied statistical analyses. Over the past century, statisticians and other scientists not only have invented numerous methods for handling missing/incomplete data, but also have invented many forms of missing data, including data augmentation, hidden states, latent variables, potential outcome, and auxiliary variables. Purposely constructing unobserved/unobservable variables offers an extraordinarily flexible and powerful framework for both scientific modeling and com-

putation and is one of the central statistical contributions to natural, engineering, and social sciences. In parallel, much research has been devoted to better understanding and modeling of real-life missing-data mechanisms; that is, the unintended data selection process that prevents us from observing our intended data. This article is a very brief and personal tour of these developments, and thus necessarily has much missing history and citations. The tour consists of a number of Ms, starting with a historic story of the mysterious method of McKendrick for analyzing an epidemic study and its link to the EM algorithm, the most popular and powerful method of the twentieth century for fitting models involving missing data and latent variables. The remaining Ms touch on theoretical, methodological and practical aspects of missing-data problems, highlighted with some common applications in social, computational, biological, medical and physical sciences.

No further discussion seems necessary because this is a point on which apparently most agree; indeed, almost all the positive comments on Lee and Nelder (1996) were on praising their promotion and formulation of models via unobservables.

3.2 Line Two: H-likelihood for Fixed Parameter

The authors' Section 3 is where I saw the definition of h-likelihood for the first time. Using the authors' initial notation, y denotes observed data, θ is the fixed parameter, and v I infer is what the authors regarded as a random "unobservable." The h-loglikelihood is simply defined as $h(\theta, v) = \log f_{\theta}(y, v)$ where $f_{\theta}(y, v)$ is the joint probability distribution/density of $\{y, v\}$.

In the rejoinder of Lee and Nelder (1996), the authors argued that the definition of h-likelihood is as logical as Fisher's likelihood. I agree. In fact, this point was well recognized in Berger and Wolpert's (1988) monograph on likelihood principle (LP) where they wrote (page 21.2), "...the LP should be formulated in such a way that θ consists of *all* unknown variables and parameters that are relevant to the statistical problem." (Emphasis is original.) They proceeded to devote an entire section to the successes and challenges in extending the LP to include what they call "unobservable variables," just as in the authors' formulation. In fact, in addition to the observable X , they wrote (pages 36–37) $\theta = (z; \omega) = (y, w; \xi, \eta)$, "where

$z = (y, w)$ is the value of an unobservable variable Z with y being of interest and w being a nuisance variable, and where $\omega = (\xi, \eta)$ is the parameter that determines the distribution of both X and Z , with ξ being of interest and η being a nuisance parameter." This quote shows that Berger and Wolpert's (1988) definition is the same as the authors', other than it takes a more explicit form by recognizing two different kinds of unobservables, y and w , just as we often distinguish between primary parameter ξ and nuisance parameter η .

The key question here, therefore, is *what to do with it* once it is defined. I shall discuss this point in Section 5. Here it suffices to note that the authors' initial proposal to maximize $h(\theta, v)$ jointly over $\{\theta, v\}$, which they label MHLE (maximum h-likelihood estimation) as in Section 2.2 of Lee and Nelder (1996), can clearly lead to grossly inconstant or even meaningless estimators if it is taken as a *general procedure*. This was pointed out by the majority of the discussants of Lee and Nelder (1996); as the authors stated later in the rejoinder of Lee and Nelder (2005), "The discussion was a disaster because everybody took the worst possible case of binary data and described difficulties with it. Nobody said it worked in other cases." The example of Bayarri et al. (1988), reviewed in authors' Section 4.2, demonstrated that the defect has little to do with binary data.

Indeed, earlier Little and Rubin (1983) provided four examples, three using standard univariate or bivariate (regression) normal models and one with a censored exponential model, to show that MHLE (though of course not in that term since Little and Rubin, 1983 predates Lee and Nelder, 1996) resulted in seriously flawed/inconsistent estimators, unless the amount of missing data is (asymptotically) negligible. The underlying issue is essentially the same as with the well-known Neyman–Scott problem (Neyman and Scott, 1948). The message here is loud and clear: maximizing over unobservable/missing data, *in general*, is not a valid method.

Evidently, the message has been appreciated by the authors, as they now make it explicit that for the "fixed parameters," their method is the same as Fisher's MLE, that is, maximizing the marginal log likelihood $\ell(\theta) = \log f_{\theta}(y)$. This certainly should help to avoid the type of mis-communications the authors described in the paper (e.g., about Rubin and Little's 2002 comments). But this also means that no further discussion is needed either because there is no new advance here.

However, for the sake of discussion, let me pick up on the authors' statement that "We view the marginal

likelihood as an adjusted profile likelihood eliminating nuisance unobservables v from the h-likelihood.” The issue is not much of the re-labeling itself, but rather that by making such a statement, the authors might be in danger of falling into the same trap that they have correctly warned others to avoid. The authors’ “adjusted profile h-likelihood (APHL),” as far as I am able to understand, simply uses a Laplace approximation to replace the integration called for by Bayesian marginalization (for nuisance parameter/unobservables). Whereas such an approximation indeed is very useful and appealing for practical purposes *when the approximation is reasonable*, it does not constitute a *principled* statistical method in its own right unless a sound *inferential principle* is articulated for the approximation itself. Without such a principle, its performance can only be judged by how close the approximation is to the Bayesian target it approximates. In this sense, comparisons such as those given in the authors’ Figure 2 say little about the merit of the h-likelihood methods, but only reconfirm the usefulness of the Laplace approximations, or demonstrate the impact of the prior (which of course is not a part of the h-likelihood formulation). In other words, mixing a *computation/approximation method* with a *statistical method* is as troublesome to me as mixing an *estimation method* with a *statistical model* is to the authors (and to me of course).

Enough painless/itchless quibbles; let us get to the heart of the authors’ proposal, that is, making inference about the unobservables via h-likelihood!

4. WHAT ARE THE PRINCIPLES BEHIND THE H-LIKELIHOOD METHODS?

4.1 Distinguishing Likelihood Principle, Likelihood Inference, and MLE

The authors invoked several times the likelihood principle (LP) to justify their h-likelihood methods. But all the LP says, broadly speaking, is that if two data sets lead to the same likelihood, then they contain the same information, assuming the underlying model for each data set is correctly specified. The LP eliminates any procedure that violates it, but it says nothing about how to conduct a *likelihood inference*. As Berger and Wolpert [(1988), Chapter 5] put it, “The LP strikes us as correct, and behaving in violation of it would be a source of considerable discomfort. Yet the LP does not tell one what to do (although insisting on methods based on the observed likelihood function certainly reduces the possibilities).”

Indeed, there is a long list of methods in the domain of “utilization of the likelihood function,” too long even for Berger and Wolpert’s (1988) monograph. I shall avoid repeating Berger and Wolpert’s argument that the full Bayesian inference is actually *the most principled* likelihood inference, since clearly the authors’ intention here is to achieve what Bayesian methods achieve but without adopting the Bayesian philosophy; or, to self quote again (Meng, 2008), “enjoying the Bayesian fruits without paying the B-club fee.” But it is worthwhile to re-emphasize that the notion of *likelihood inference* is a very elusive one—any method that does not violate LP can be legitimately included (see Berger and Wolpert, 1988).

In contrast, maximal likelihood estimation (MLE) is a well-defined method, telling us exactly what to do with the likelihood function. It is this specific method that the authors’ MHLE mimics. The aforementioned counterexamples demonstrate clearly that in general this imitation is only mathematical. The key question then is whether it is possible to find a set of useful and general conditions under which the imitation is more fundamental, that is, under which MHLE preserves the underlying properties of MLE that guarantee its validity and efficiency? The answer turns out to be an intriguing “yes and NO.” But before we get to that punch line, we will need the wisdom of an old friend, Mr. Bartlett.

4.2 Do Bartlett Identities Hold for H-likelihood?

Finding the *most likely* parameter value that could have produced the observed data is intuitively very appealing—what else could be better? But of course as statisticians we know such reasoning by itself is flawed, because it puts us squarely in the hands of the Devil of Overfitting! There is clearly much more to Fisher’s MLE than this flawed intuition.

Probabilistically, a backbone of Fisher’s ML method is the Bartlett identities, especially the first two. That is, for the (marginal) log-likelihood $\ell(\theta; y)$, under the usual regularity condition that the support of $f_\theta(y)$ does not depend on $\theta \in \Theta$, we have

$$(4.1) \quad E_\theta \left[\frac{\partial \ell(\theta; y)}{\partial \theta} \right] = 0 \quad \forall \theta \in \Theta,$$

$$(4.2) \quad E_\theta \left[\frac{\partial^2 \ell(\theta; y)}{\partial \theta^2} \right] + E_\theta \left[\left(\frac{\partial \ell(\theta; y)}{\partial \theta} \right) \left(\frac{\partial \ell(\theta; y)}{\partial \theta} \right)^\top \right] = 0 \quad \forall \theta \in \Theta$$

where E_θ denotes the expectation under $f_\theta(y)$. Here identity (4.1) guarantees that the normal/score equation

underlying the MLE method,

$$(4.3) \quad S(\theta; y) \equiv \frac{\partial \ell(\theta; y)}{\partial \theta} = 0,$$

is an *unbiased estimating equation*. Identity (4.2) is the basis for the asymptotic efficiency of MLE (under regularity conditions, of course) because it reduces the general “sandwich” variance formula to the inverse of Fisher information, the Cramér–Rao lower bound.

For these reasons, generalizations of (maximal) likelihood methods have largely tried to preserve these two identities, such as with the quasi-likelihood method (e.g., McCullagh and Nelder, 1989, Chapter 9); see Mykland (1994, 1999) for other examples. It is therefore difficult to imagine that the issue of preserving them has not been investigated in general in the context of h -likelihood, given it is essentially a minimal requirement; indeed, when Engle and Keen, the lead discussants of Lee and Nelder (1996), wrote, “. . . the usual first- and second moment properties exactly hold for h -scores, for example, for normal-normal and Poisson-Gamma models. . .” I believe they were referring to the two identities above. I therefore surmise that it is my haphazardly selective reading that makes the existing investigations unobservable to me. So I must offer my apologies to anyone, especially the authors, if I am reinventing the wheel below. But in any case I hope the material presented in the rest of this discussion will help to establish a firmer theoretical ground for investigating the virtues and limitations of MHLE and other h -likelihood methods.

Specifically, as we all know, identities (4.1) and (4.2) are consequences of

$$(4.4) \quad \int_{\Omega_y} e^{\ell(\theta; y)} \mu(dy) = \int_{\Omega_y} f_\theta(y) \mu(dy) = 1 \quad \forall \theta \in \Theta$$

by repeatedly differentiating under the integral sign with respect to θ , which is legitimate when the support Ω_y is free of θ (and assuming the usual continuous differentiability of $\ell(\theta; y)$ as a function of θ ; such conditions will be assumed below whenever needed). For log h -likelihood, $h(\theta, v; y) = \log f_\theta(y, v)$, clearly we still have

$$(4.5) \quad \int_{\Omega_{y,v}} e^{h(\theta, v; y)} \mu(dy, dv) = \int_{\Omega_{y,v}} f_\theta(y, v) \mu(dy, dv) = 1 \quad \forall \theta \in \Theta.$$

However, whereas we can still take (partial) derivatives with respect to θ on both sides of (4.5) to arrive at useful identities, obviously taking the derivative

of both sides with respect to v would produce $0 = 0$. This death of the old trick signifies a key difference between the h -likelihood and Fisher’s likelihood, even if we put aside cases where v is discrete and hence taking derivatives is not even an option. Here we remark that unlike Fisher’s likelihood where discrete parameters are rare (other than with model selection problems), discrete unobservable/missing data are common which poses an additional challenge to the MHLE method. But clearly the authors’ current proposal focuses on continuous v , so we will proceed in this setting.

5. ENCOURAGING NEWS: H-LIKELIHOOD IS BARTLIZABLE

5.1 Necessary and Sufficient Conditions for Bartlett Identities

Without the old trick, we have to directly investigate if and when (4.1) and (4.2) can be extended to h -likelihood. Specifically, when we let $\phi = \{\theta, v\}$, and write

$$(5.1) \quad h(\phi; y) = \log f_\theta(y|v) + \log f_\theta(v),$$

we see the “troublemaker” is the second term because for the first term, v plays the same role of a fixed parameter for the conditional distribution $f_\theta(y|v)$, and hence the old trick of differentiating under integration is applicable. In particular, as an application of (4.1) and (4.2) when conditioning on v and assuming the support of $f_\theta(y|v)$ does not depend on either θ or v , we have, for any $\theta \in \Theta$,

$$(5.2) \quad E_\theta \left[\frac{\partial \log f_\theta(y|v)}{\partial \phi} \Big| v \right] = 0,$$

$$(5.3) \quad E_\theta \left[\frac{\partial^2 \log f_\theta(y|v)}{\partial \phi^2} \Big| v \right] + E_\theta \left[\left(\frac{\partial \log f_\theta(y|v)}{\partial \phi} \right) \left(\frac{\partial \log f_\theta(y|v)}{\partial \phi} \right)^\top \Big| v \right] = 0.$$

Consequently, under the additional assumption that the support of $f_\theta(v)$ does not depend on θ , (5.1) and (5.2) imply that, for any $\theta \in \Theta$,

$$(5.4) \quad E_\theta \left[\frac{\partial h(\phi; y)}{\partial \phi} \right] = E_\theta \left[\frac{\partial \log f_\theta(v)}{\partial \phi} \right] = \begin{pmatrix} 0 \\ E_\theta \left[\frac{\partial \log f_\theta(v)}{\partial v} \right] \end{pmatrix} \equiv \begin{pmatrix} 0 \\ \int_{\Omega_v} \frac{\partial f_\theta(v)}{\partial v} \mu(dv) \end{pmatrix}.$$

Furthermore, noting that the cross terms in the quadratic expansion below are zero by first conditioning on v , we have from (5.1)–(5.3),

$$\begin{aligned}
 & E_{\theta} \left[\frac{\partial^2 h(\phi; y)}{\partial \phi^2} \right] + E_{\theta} \left[\left(\frac{\partial h(\phi; y)}{\partial \phi} \right) \left(\frac{\partial h(\phi; y)}{\partial \phi} \right)^{\top} \right] \\
 &= E_{\theta} \left[\frac{\partial^2 \log f_{\theta}(v)}{\partial \phi^2} \right] \\
 (5.5) \quad & + E_{\theta} \left[\left(\frac{\partial \log f_{\theta}(v)}{\partial \phi} \right) \left(\frac{\partial \log f_{\theta}(v)}{\partial \phi} \right)^{\top} \right] \\
 & \equiv \begin{pmatrix} A & B \\ B^{\top} & C \end{pmatrix}.
 \end{aligned}$$

In the above expression,

$$\begin{aligned}
 A &= E_{\theta} \left[\frac{\partial^2 \log f_{\theta}(v)}{\partial \theta^2} \right] \\
 (5.6) \quad & + E_{\theta} \left[\left(\frac{\partial \log f_{\theta}(v)}{\partial \theta} \right) \left(\frac{\partial \log f_{\theta}(v)}{\partial \theta} \right)^{\top} \right] = 0
 \end{aligned}$$

by applying (4.2) to $\log f_{\theta}(v)$. For the term B , one can easily verify that

$$\begin{aligned}
 B &= E_{\theta} \left[\frac{\partial^2 \log f_{\theta}(v)}{\partial \theta \partial v} \right] \\
 (5.7) \quad & + E_{\theta} \left[\left(\frac{\partial \log f_{\theta}(v)}{\partial \theta} \right) \left(\frac{\partial \log f_{\theta}(v)}{\partial v} \right)^{\top} \right] \\
 &= \frac{\partial}{\partial \theta} \left\{ E_{\theta} \left[\left(\frac{\partial \log f_{\theta}(v)}{\partial v} \right)^{\top} \right] \right\} \quad \forall \theta \in \Theta,
 \end{aligned}$$

and hence it will also be zero if $E_{\theta} \left[\frac{\partial \log f_{\theta}(v)}{\partial v} \right] = 0$ for all $\theta \in \Theta$. Finally, simple algebra shows

$$\begin{aligned}
 C &= E_{\theta} \left[\frac{\partial^2 \log f_{\theta}(v)}{\partial v^2} \right] \\
 (5.8) \quad & + \left(\frac{\partial \log f_{\theta}(v)}{\partial v} \right) \left(\frac{\partial \log f_{\theta}(v)}{\partial v} \right)^{\top} \\
 & \equiv \int_{\Omega_v} \frac{\partial^2 f_{\theta}(v)}{\partial v^2} \mu(dv).
 \end{aligned}$$

Combining (5.4)–(5.8) yields the following straightforward but key result.

THEOREM 1. *Let $h(\phi; y) = \log f_{\theta}(y, v)$ be a log h-likelihood where $\phi = \{\theta, v\}$, $\theta \in \Theta$ is the model parameter, v is a continuous unobservable with density $f_{\theta}(v)$ with respect to a measure μ , and let $\mathcal{S}_{\theta}(v) = \frac{\partial \log f_{\theta}(v)}{\partial v}$. Furthermore, assume the support of $f_{\theta}(y|v)$ does not depend on either θ or v (almost surely with respect to μ), the support of $f_{\theta}(v)$, denoted by Ω_v , is free*

of θ , and all continuity and differentiability conditions hold whenever needed. Then the first Bartlett identity holds for the h-likelihood, that is

$$(5.9) \quad E_{\theta} \left[\frac{\partial h(\phi; y)}{\partial \phi} \right] = 0 \quad \forall \theta \in \Theta$$

if and only if

$$(5.10) \quad E_{\theta}[\mathcal{S}_{\theta}(v)] \equiv \int_{\Omega_v} \frac{\partial f_{\theta}(v)}{\partial v} \mu(dv) = 0 \quad \forall \theta \in \Theta.$$

Assuming (5.10), then the second Bartlett identity holds for the h-likelihood; that is,

$$\begin{aligned}
 & E_{\theta} \left[\frac{\partial^2 h(\phi; y)}{\partial \phi^2} \right] \\
 (5.11) \quad & + E_{\theta} \left[\left(\frac{\partial h(\phi; y)}{\partial \phi} \right) \left(\frac{\partial h(\phi; y)}{\partial \phi} \right)^{\top} \right] \\
 &= 0 \quad \forall \theta \in \Theta
 \end{aligned}$$

if and only if

$$\begin{aligned}
 & E_{\theta} \left[\frac{\partial \mathcal{S}_{\theta}(v)}{\partial v} + \mathcal{S}_{\theta}(v) \mathcal{S}_{\theta}^{\top}(v) \right] \\
 (5.12) \quad & \equiv \int_{\Omega_v} \frac{\partial^2 f_{\theta}(v)}{\partial v^2} \mu(dv) = 0 \quad \forall \theta \in \Theta.
 \end{aligned}$$

5.2 Yes: It is Easy for H-likelihood to Produce “Un-sandwiched” Estimating Equation

Theorem 1 is somewhat remarkable because the necessary and sufficient conditions (5.10) and (5.12) are determined purely by the marginal distribution of the unobservable v , and hence they are easy to check. For example, in Bayarri’s example quoted by the authors, the marginal density of the unobservable u is exponential with mean $\lambda = \theta^{-1}$. Consequently, $\mathcal{S}_{\theta}(u) = -\theta$, and hence condition (5.10) is violated for all $\theta > 0$, as is condition (5.12). This means that whenever u is used for the h-likelihood, the resulting h-score will never form an unbiased estimating equation, regardless of the model for $f_{\theta}(y|u)$! Indeed, we have seen from the authors’ Section 4.2 that the corresponding MHLE leads to meaningless estimates.

In contrast, when we use $v = \log u$, $f_{\theta}(v) = \theta e^{v-\theta e^v}$, and hence $\mathcal{S}_{\theta}(v) = 1 - \theta e^v = 1 - u/\lambda$ and $\mathcal{S}'_{\theta}(v) + \mathcal{S}_{\theta}^2(v) = -\theta e^v + (1 - \theta u)^2 = -u/\lambda + (u - \lambda)^2/\lambda^2$. Both conditions (5.10) and (5.12) then follow trivially because $E_{\theta}(u) = \lambda$ and $V_{\theta}(u) = \lambda^2$. Consequently, the authors’ h-score is not only an unbiased estimating equation but also an “optimal” one in the sense that we do not need the usual “sandwich” formula, but only the

Hessian matrix, for “valid” variance estimation. Unfortunately, I have to put both “optimal” and “valid” in quotes because of the *bad news* I will deliver in the next section. But as far as for preserving Bartlett identities goes, *which by itself does not guarantee valid statistical inferences*, I can share the authors’ optimism for the future of MHLE, especially because of the following somewhat even more surprising result, which says that conditions (5.10) and (5.12) hold quite easily for many unobservables or their simple transformations.

THEOREM 2. *Under the same setting as in Theorem 1, suppose the support of $f_\theta(v)$, $\Omega_v \subset \mathbb{R}^d$, takes a rectangle form, $\Omega_v = \prod_{j=1}^d [a_j, b_j]$, where a_j or b_j is permitted to take the value of $+\infty$ or $-\infty$. Let $\partial\Omega_v$ be the boundary set of Ω_v (i.e., the set of all points whose coordinates contain at least one a_j or b_j), and assume the dominating measure μ is the Lebesgue measure on \mathbb{R}^d . We then have:*

(I) *If $f_\theta(v) = 0$ for all $v \in \partial\Omega_v$, then condition (5.10) holds, and hence the first Bartlett identity (5.9) holds.*

(II) *If in addition $\frac{\partial f_\theta(v)}{\partial v} = 0$ also holds for all $v \in \partial\Omega_v$, then condition (5.12) holds, and hence the second Bartlett identity (5.11) holds.*

PROOF. For (I), because of (5.10), if v is univariate, that is, if $d = 1$, then

$$\begin{aligned} \int_{\Omega_v} \frac{\partial f_\theta(v)}{\partial v} dv &= \int_{a_1}^{b_1} df_\theta(v) \\ (5.13) \qquad \qquad \qquad &= f_\theta(b_1) - f_\theta(a_1) \\ &= 0, \end{aligned}$$

under our assumption that $f_\theta(v)$ vanishes on the boundary. For $d > 1$, we apply the same argument to each of the d integrations that form the leftmost vector in (5.13), that is, $\int_{\Omega_v} \frac{\partial f_\theta(v)}{\partial v_k} dv, k = 1, \dots, d$, by integrating with respect to v_k first to conclude that it is zero for all θ .

For (II), we first note that for any $\{k, s\}$,

$$\begin{aligned} I_{k,s} &\equiv \int_{\Omega_v} \frac{\partial^2 f_\theta(v)}{\partial v_k \partial v_s} dv \\ (5.14) \qquad \qquad \qquad &= \int_{\Omega_v} \frac{\partial}{\partial v_k} \left(\frac{\partial f_\theta(v)}{\partial v_s} \right) dv. \end{aligned}$$

Hence, using the same argument as above but with $f_\theta(v)$ replaced by $\frac{\partial f_\theta(v)}{\partial v_s}$, we can conclude $I_{k,s} = 0$ for all $k, s = 1, \dots, d$. Consequently, condition (5.12) holds. \square

What this result says is that as long as the marginal density of the unobservable v vanishes on the boundary of its support, the first Bartlett identity holds for h-likelihood. In addition, if its derivative also vanishes on the boundary, then the second Bartlett identity holds. This provides an even easier way to verify Bayarri’s example. For the original unobservable u , $f_\theta(u) = \theta e^{-\theta u}$, with boundary points $u = 0$ and $u = \infty$. But since $f_\theta(0) = \theta$, the vanishing condition is violated as long as $\theta > 0$. In contrast, for $v = \log u$, $f_\theta(v) = \theta e^{v-\theta e^v}$, with boundary points $v = -\infty$ and $v = +\infty$. It is easy to see that $f_\theta(-\infty) = f_\theta(+\infty) = 0$ for all θ . Furthermore, since

$$\frac{\partial f_\theta(v)}{\partial v} = \theta(e^{v-\theta e^v} - \theta e^{2v-\theta e^v}),$$

the derivative also vanishes at both $v = -\infty$ and $v = \infty$. Therefore, both Bartlett identities hold for h-likelihood when $v = \log u$ is used as the unobservable. For simplicity, we will label the process of finding a transformation that makes Bartlett identities hold *Bartlization* (“Bartlettization” is too much of a tongue twister!).

An astute reader may have noticed that I did not say that failing the vanishing condition is the reason for the failing of the Bartlett identities for the original scale u . The vanishing condition is sufficient, but not necessary. This can easily be seen in (5.13), which only requires $f_\theta(a_1) = f_\theta(b_1)$. Indeed, the Bartlett identity fails for the original scale u precisely because $f_\theta(u = +\infty) = 0$ but $f_\theta(u = 0) = \theta$, and hence $E_\theta[\mathcal{S}_\theta(u)] = 0 - \theta = -\theta$, as verified directly previously. A necessary and sufficient condition via integration on $\partial\Omega_v$ is not hard to obtain, but it requires a bit more mathematical treatment than is needed for most practical applications, for which Theorem 2 is adequate. Here we just mention that we can generalize Theorem 2 by allowing Ω_v to be an arbitrary *simply connected* manifold in \mathbb{R}^d (i.e., a manifold with “no hole”), and then invoke the generalized Stokes’ theorem (see Marsden and Tromba, 2003) to equate the integration of dw on Ω_v to that of w on the boundary $\partial\Omega_v$ where w is a so-called $d - 1$ differential form which can be taken in terms of $f_\theta(v)$ or its derivative as needed.

The authors stated in the rejoinder of Lee and Nelder (2005) that “We do not say that the current h-likelihood method will always perform the best, but we believe that it can always be modified to give an improvement, as has been done with Fisher’s likelihood method.” I believe the alluded-to improvements lie in using higher order Bartlett identities, such as the third identity for “Bartlett correction” for the likelihood ratio

tests (e.g., McCullagh, 1987). Clearly Theorem 1 and Theorem 2 have their higher order generalizations, but it is already 9:14 pm of the *second* Sunday. My teenagers' visit to Dr. Langdon is already postponed for another week, so I had better leave such generalizations to a future paper. More importantly, as much as I am enjoying discovering the "Bartlizability" of h-likelihood, I do not see a way to correct the more fundamental problem described in the next section, which potentially makes "Bartlett-corrected h-likelihood" an exercise that is literally just a homework exercise.

6. BAD NEWS AND A PUZZLE: FISHY OR FIDUCIAL?

6.1 NO: It is Hard for log H-likelihood to be Summarizable Quadratically

Having the Bartlett identities is only a part of the story. What it guarantees is that *if the log h-likelihood can be approximated quadratically*, then the mode and the Hessian matrix derived from it will provide an approximately correct estimator and its associated (inverse) variance. To examine this issue more clearly, let us mimic the formal asymptotic argument behind the estimating equation approach which relies on the expression

$$(6.1) \quad \hat{\phi} - \phi = I_h^{-1}(\theta)S(\phi; y) + R,$$

where $\hat{\phi}$ is the MHLE, $S(\phi; y) = \frac{\partial h(\phi; y)}{\partial \phi}$ is the h-score, and $I_h(\theta)$ is the h-likelihood extension of the expected Fisher information, the expected Hessian,

$$(6.2) \quad I_h(\theta) \equiv E_{\theta} \left[-\frac{\partial^2 h(\phi; y)}{\partial \phi^2} \right].$$

We emphasize here that unlike the original Fisher information, $I_h(\theta)$ is not generally guaranteed to be positive definite (so $I_h^{-1}(\theta)$ may not even exist) *unless condition (5.12) holds*; see Section 7 for an example.

Expression (6.1) by itself is tautological, because there is always an R to make it hold; in particular it can be derived from a remainder term in the Taylor expansion of $S(\hat{\phi}; y) - S(\phi; y)$. However, *when R is (asymptotically) negligible*, (6.1) allows us to conclude that the distribution of $\hat{\phi} - \phi$ can be approximated by that of $T(\theta; y) \equiv I_h^{-1}(\theta)S(\phi; y)$ which has mean zero when the first Bartlett identity holds and variance $I_h^{-1}(\theta)$ when the second Bartlett identity holds.

When h is a regular Fisher's likelihood, under regularity conditions, the R term is asymptotically negligible compared with the first term on the right-hand

side of (6.1). A key reason for this is the *accumulation of information* as we collect more data; eventually we will have zero uncertainty about the parameter, at least in theory. Unfortunately, for h-likelihood, this cannot be true *in general* even in theory because no matter how much data we accumulate, it cannot possibly eliminate the uncertainty, say, in predicting a *future outcome*, such as in the authors' Example 4. This lack of accumulation of information for unobservables is essentially the key problem pointed out by multiple discussants (e.g., both lead discussants) of Lee and Nelder (1996), with both theoretical and empirical examples.

Without the accumulation of information to justify the central limit theorem or the law of large numbers, we actually will run into two problems with the standard asymptotic arguments for (6.1), even if the first two Bartlett identities hold. The most obvious and critical one is that since R is not negligible, we cannot approximate the distribution of $\hat{\phi} - \phi$ by that of $T(\theta; y) = I_h^{-1}(\theta)S(\phi; y)$; indeed, without R being negligible, the MHLEs are not guaranteed to be consistent, as in all examples of Little and Rubin (1983). It is of critical importance to stress that the Bartlizability property of h-likelihood itself has little bearing on the issue of being quadratically summarizable, that is, the R term being negligible. Indeed, in all normal examples of Little and Rubin (1983), the h-likelihood is naturally Bartlized because clearly the normal density and any of its derivatives vanish on the boundary of its support, yet the MHLE produces inconsistent estimators because of the nonnegligibility of the R term. The more subtle one is that regardless of whether R is negligible or not, we may not be able to justify the usual normal approximation $T(\theta; y) \sim N(0, I_h^{-1}(\theta))$, even if $T(\theta; y)$ has mean zero and variance matrix $I_h^{-1}(\theta)$. (Of course, when R is not negligible, the properties of T are not really relevant.) Section 7 will illustrate all these points via a simple but very informative example.

6.2 And a Puzzle: The Meaning of the H-distribution

Even if R is exactly zero and all Bartlett identities hold, the h-likelihood method, as a method for predicting the unobservables v , still faces a fundamental challenge. That is, what is the meaning of the resulting distribution $f(v|y)$, which I shall term the *h-distribution* for obvious reasons? If one is willing to assume a constant prior on θ , then of course this has a Bayesian interpretation as a posterior predictive distribution or an

approximation to it. But the authors specifically emphasized that they did not want to specify a prior on θ , for their goal is to provide an alternative method to the Bayesian approach.

Some Bayesians may be agitated by having a method that is mathematically or numerically equivalent, in general, to a Bayes method (perhaps under a particular prior), but is labeled as something else. I am much less troubled, provided that (1) the connection is clearly spelled out, and (2) there is a well-articulated non-Bayesian principle justifying the method. The authors clearly have done (1), but for (2) all I can find is authors' desire to conduct a *probabilistic inference* for v without having to specify a prior for θ . At the conceptual level, I have the very same desire because of my frustration, which I am sure some share, with the apparent impossibility of constructing a truly "noninformative" prior (for continuous parameters, at least). I also very much appreciate the authors' emphasis that the "plug-in" empirical Bayes is not a satisfying method, precisely because "plug-in" is an ad hoc method. So indeed I was quite excited when I thought that the authors had found a way to meaningfully specify a *probabilistic* $f(v|y)$, without considering θ as a random variable.

At a practical level, the authors did provide a number of "well-specified" h-distributions, either via (the implied) normal approximation with mean and variance obtained from the MHLE/Hessian matrix for v or the APHL approximation by profiling out θ . But without spelling out the probabilistic meaning of such resulting distributions, it is essentially impossible to answer the criticism that the label of h-likelihood is a red herring because they are just approximations to Bayesian solutions instead of the products of a genuine competing method as claimed. More importantly, without knowing what "gold standard" they aim to approximate, we have no meaningful ways to evaluate how good the approximations are, or even to specify a probabilistic evaluation mechanism; in what real or thought experiment can it be realized?

Indeed, the lack of a distinct and justifiable meaning of the h-distribution apparently has put the authors in an awkward position in terms of demonstrating the merit of their methods. From the papers I read, it appears that the authors have two kinds of comparisons. The first is to compare an h-distribution to a Bayesian one, and to "validate" the h-distribution by showing how close it is to the Bayesian counterpart. But this only strengthens the aforementioned "red herring" criticism, and provides evidence for—not against—the

kind of statements made by my twin brother quoted previously. Clearly this is contrary to the authors' intention, and I believe is part of the reasons for the continuing discrepancy between the authors' enthusiasm for and others' reluctance toward the h-likelihood methods.

The second type is something that I have not seen before, at least not in academic publications. The authors seem to take their methods as the standard, and compared everything else to it, as suggested by the statement, "In the salamander data, among other methods considered, the MCEM of Vaida and Meng (2005) gives the closest estimates to the h-likelihood estimators." Such comparisons would be meaningful if the superiority of the h-likelihood results had already been demonstrated either by theoretical proof (e.g., optimality of some sort) or by a distinctive principle that is not subsumed or invalidated by accepted ones. But even in such cases, the value of this type of comparison is to demonstrate the performance of *other methods*, not the merit of the h-likelihood method itself.

6.3 Fiducial Argument via Predictive Pivotal Quantity?

As I tried in vain to form a thought experiment that would meaningfully define the h-distribution $f(v|y)$ without slipping into the Bayesian mode, I looked hard into the authors' writings for clues about what they had in mind. The first clue came from Section 3.1 of Lee and Nelder (1996), where they showed that, in the context of the models they were investigating, a log h-likelihood expression in their (3.2) can be expanded into their expression (3.3) which is a quadratic term $-(\tilde{v} - v)'D^*(\tilde{v} - v)/2$ plus a term that depends on y only (their \tilde{v} is the same as the \hat{v} notation here). They then wrote, "Ignoring the constant term, which depends only on y and not on v , expressions (3.2) and (3.3) imply that

$$v|y \sim N(\tilde{v}, D^{*-1})$$

would be a good approximation for the distribution of $v|y$." With apologies to the authors in case I misunderstand their notation or there was a misprinting, this reasoning smells either fishy or fiducial, depending on the meaning of "the distribution of $v|y$."

First, if by "the distribution of $v|y$ " is meant the sampling distribution of v given both y and θ , then the reasoning underlying the above statement would contain the elementary flaw of confusing a *marginal* distribution of $X_1 - X_2$ with the *conditional* distribution of $X_1 - X_2$ given X_1 . This is because, even if the normal

approximation is justified, the quadratic term above is for the *marginal* distribution of $\tilde{v} - v$, as v and \tilde{v} , which is a function of y only, vary *jointly* according to $f(y; v|\theta)$. [I switch the notation from $f_\theta(y; v)$ to $f(y; v|\theta)$ to emphasize the conditioning on θ , even though the latter notation may imply that θ is a *variable* being conditioned upon, something the authors' approach aims to avoid.] This marginal distribution clearly is not the same, in general, as the *conditional* distribution $f(\tilde{v} - v|\tilde{v}, \theta)$ or $f(\tilde{v} - v|y, \theta)$ (note in general that these two distributions are also different unless y and v are independent given θ). This can be most clearly seen from (6.1) where all the distributional calculations are with respect to the joint distribution $f(y; v|\theta)$, *not* the conditional distribution $f(v|y; \theta)$.

Of course, this is unlikely to be what the authors intended, since their goal is to capture $v|y$ without conditioning on θ . But the notation $f(v|y)$ has no definition or meaning under the authors' joint modeling specification $f(y, v|\theta)$ because θ is treated as fixed. This brings me to the second "smell," that is, the authors were invoking a fiducial-like argument, by implicitly *defining* their *conditional h-distribution* $v|y$ as the *sampling marginal distribution* of $\hat{v} - v$ under the joint distribution $f(y, v|\theta)$, and getting rid of its dependence on θ when $\hat{v} - v$ is (asymptotically) a *predictive pivotal quantity*, meaning that its distribution is free of any unknowns. We can also think of this way of eliminating the nuisance parameter θ for the purpose of prediction as seeking *predictive ancillarity*, that is, a function of both y and v whose distribution is free of θ . See the example in Section 7 for an illustration.

6.4 A Duality or Prestidigitation?

The second piece of evidence from the authors' writing seems to confirm this interpretation. In the comparisons of their methods with the Empirical Bayesian method, they compared the Bayesian posterior predictive variance of $v|y$ with the estimator obtained from the Hessian matrix. To make this comparison more explicit, let us denote $\tau(\theta; y) = V(v|\theta; y)$ and $e(\theta; y) = \hat{v}(y) - E(v|\theta; y)$. Then by the law of iterated expectations (or the so-called EVE formula) and noting that \hat{v} is determined by y , we have

$$(6.3) \quad \begin{aligned} V(v|y) &= V(\hat{v} - v|y) \\ &= E[\tau(\theta; y)|y] + V[e(\theta; y)|y], \end{aligned}$$

$$(6.4) \quad V(\hat{v} - v|\theta) = E[\tau(\theta; y)|\theta] + V[e(\theta; y)|\theta].$$

The authors' argument seems to implicitly rely on a "duality," that is, the two mean terms on the right-hand

sides of (6.3) and (6.4) are (asymptotically or approximately) the same; so are the two variance terms. That is, we can switch the required mean and variance calculations under $f(y|\theta)$ in (6.3) to that under $f(\theta|y)$ in (6.4). Fisher's fiducial argument, as far as I can understand, aimed to establish the validity of this switching on its own without viewing it as an approximation to the Bayesian method (with a constant prior). There is nothing wrong with invoking the fiducial argument (well, actually there is but it depends on who one asks); indeed there has been a recent surge of interest in it, especially in connection with the "generalized confidence" approach [e.g., Hannig, Iyer and Patterson (2006) and Hannig (2009)]. Perhaps the authors' approach is the next step, that is, using the fiducial approach for prediction, not just for estimation. But without being told explicitly about this switching, a reader's reaction would be anybody's guess. A suspicion of prestidigitation? A *deja vu* feeling of reading *Deception Point* instead of *De Vinci Code*? Or even worse, an accusation of the prosecutor's fallacy?

Finally, even if we buy the fiducial argument, it does not follow that the left-hand side of (6.4) can be well approximated by (an appropriate element of) the inverse of the Hessian matrix because of the non-negligibility of the R term, as discussed before. The authors, of course, well recognized this, and hence invoked the APHL method to approximate (define?) the h -distribution $f(v|y)$ instead of relying on the normal approximation. While this approach indeed "works well," in the authors' example and in the example I am about to present, I have to put "works well" in quotes when the success is judged by comparing how close the h -distribution is to the posterior predictive distribution under the constant prior. But I'd be happy to remove the quotation marks if the evaluation is based on the aforementioned pivotal predictive framework, because that is a distinctive principle, regardless of whether one subscribes to it or not.

7. SHOW AND TELL: ESTIMATION AND PREDICTION WITH EXPONENTIAL DISTRIBUTION

To illustrate various general points made in Sections 4–6, let us consider a simple case where the data are an i.i.d. sample $y = \{y_1, \dots, y_n\}$ from an exponential distribution with mean λ with the unobservable being $u = y_{n+1}$, a future observation. This example is different from Bayarri's two-level exponential model because here we only have one level, as in the authors' Example 4. It is hard to have faith in a method for multi-level hierarchical models if it cannot handle single-level models.

7.1 Why does the Original Scale Fail?

As we discussed in Section 5.2, when the exponential variable $u = y_{n+1}$ is used as the unobservable, the Bartlett identities fail. In the current setting, this can be seen directly by noting that (where \bar{y}_n denotes the sample mean of $\{y_1, \dots, y_n\}$)

$$(7.1) \quad h(\lambda, u; y) = -(n+1) \log \lambda - \frac{n\bar{y}_n + u}{\lambda},$$

which clearly does not have an internal mode because it is linear in $u \geq 0$. Indeed, the h-score equation,

$$(7.2) \quad S(\phi; y) \equiv \begin{pmatrix} \frac{\partial h}{\partial \lambda} \\ \frac{\partial h}{\partial u} \end{pmatrix} = \begin{pmatrix} -\frac{n+1}{\lambda} + \frac{n\bar{y}_n + u}{\lambda^2} \\ -\frac{1}{\lambda} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix},$$

leads to the meaningless estimator $\hat{\lambda} = +\infty$. Incidentally, this is also an example that $I_h(\theta)$, as defined in (6.2), is not nonnegative definite because the second Bartlett identity fails. Specifically, by further differentiating the expressions in (7.2), it is easy to verify that

$$I_h(\theta) = E \left[- \begin{pmatrix} \frac{n+1}{\lambda^2} - 2\frac{n\bar{y}_n + u}{\lambda^3} & \frac{1}{\lambda^2} \\ \frac{1}{\lambda^2} & 0 \end{pmatrix} \right] = \begin{pmatrix} \frac{n+1}{\lambda^2} & -\frac{1}{\lambda^2} \\ -\frac{1}{\lambda^2} & 0 \end{pmatrix}$$

which clearly fails to be nonnegative definite.

7.2 A Simple Transformation is All it Takes

However, when the h-likelihood uses $v = \log(u)$ as unobservable, it satisfies both conditions of Theorem 2 as verified in Section 5.2, so the corresponding h-likelihood is Bartlized. To see this directly, because

$$(7.3) \quad h(\lambda, v; y) = -(n+1) \log \lambda - \frac{n\bar{y}_n + e^v}{\lambda} + v,$$

the h-score equation becomes

$$(7.4) \quad \begin{aligned} \frac{\partial h}{\partial \lambda} &= -\frac{n+1}{\lambda} + \frac{n\bar{y}_n + e^v}{\lambda^2} = 0, \\ \frac{\partial h}{\partial v} &= -\frac{e^v}{\lambda} + 1 = 0. \end{aligned}$$

This delivers the correct MLE for λ , $\hat{\lambda} = \bar{y}_n$, and a very sensible point prediction for the future observation, $\hat{u} = e^{\hat{v}} = \hat{\lambda} = \bar{y}_n$.

Furthermore, the expected Hessian matrix is

$$(7.5) \quad I_h(\lambda) = E_\lambda \left[- \begin{pmatrix} \frac{n+1}{\lambda^2} - 2\frac{n\bar{y}_n + e^v}{\lambda^3} & \frac{e^v}{\lambda^2} \\ \frac{e^v}{\lambda^2} & -\frac{e^v}{\lambda} \end{pmatrix} \right] = \begin{pmatrix} \frac{n+1}{\lambda^2} & -\frac{1}{\lambda} \\ -\frac{1}{\lambda} & 1 \end{pmatrix}.$$

It is easy to see that when evaluated at MLE (=MHLE), $\hat{\lambda}$, $I_h(\hat{\lambda})$ is identical to the *observed Hessian matrix* $I_h^{\text{obs}} = -\frac{\partial^2 h(\phi; y)}{\partial \phi^2} \Big|_{\phi=\hat{\phi}}$

$$(7.6) \quad I_h^{\text{obs}} \equiv - \begin{pmatrix} \frac{n+1}{\hat{\lambda}^2} - 2\frac{n\bar{y}_n + e^{\hat{v}}}{\hat{\lambda}^3} & \frac{e^{\hat{v}}}{\hat{\lambda}^2} \\ \frac{e^{\hat{v}}}{\hat{\lambda}^2} & -\frac{e^{\hat{v}}}{\hat{\lambda}} \end{pmatrix} = \begin{pmatrix} \frac{n+1}{\hat{\lambda}^2} & -\frac{1}{\hat{\lambda}} \\ -\frac{1}{\hat{\lambda}} & 1 \end{pmatrix},$$

where the equality holds because $\hat{\lambda} = \bar{y}_n = e^{\hat{v}}$. The fact that these two Hessian matrices coincide also gives us another indication that the MHLE/Hessian matrix can behave just like MLE/Fisher information for regular exponential families.

7.3 So How Good is the Approximation?

Now let us examine the inverse of $I_h(\lambda)$,

$$(7.7) \quad I_h^{-1}(\lambda) = \begin{pmatrix} \frac{\lambda^2}{n} & \frac{\lambda}{n} \\ \frac{\lambda}{n} & 1 + \frac{1}{n} \end{pmatrix} \equiv \begin{pmatrix} \tau_\lambda^2 & \tau_{\lambda,v} \\ \tau_{\lambda,v} & \tau_v^2 \end{pmatrix}.$$

If the R term in (6.1) is negligible, then the above matrix should provide the (asymptotic) value of $V_\lambda(\hat{\phi} - \phi)$ where $\phi = \{\lambda, v\}$ and the variance operator V_λ is with respect to the *joint sampling distribution* $f_\lambda(y, v)$. Clearly, $\tau_\lambda^2 = \lambda^2/n$ is exactly right because it is $V_\lambda(\hat{\lambda})$. To examine the other entries, we first recall that for *large* n , Taylor's expansion (i.e., the δ -method) justifies the approximation

$$(7.8) \quad \log(\bar{y}_n) - \log(\lambda) \approx \frac{\bar{y}_n - \lambda}{\lambda} \equiv z_n.$$

Adopting this approximation, and noting that $v = \log(y_{n+1})$ is independent of \bar{y}_n given λ , we have

$$(7.9) \quad \begin{aligned} \text{Cov}_\lambda(\hat{\lambda}, \hat{v} - v) &= \text{Cov}_\lambda(\bar{y}_n, \log(\bar{y}_n)) \\ &\approx \text{Cov}_\lambda(\bar{y}_n, z_n) = \frac{\lambda}{n} \end{aligned}$$

which is the same as $\tau_{\lambda,v}$.

Similarly, by (7.8), $V_\lambda(\log(\bar{y}_n)) \approx V(z_n) = 1/n$, and hence we have

$$(7.10) \quad \begin{aligned} V_\lambda(\hat{v} - v) &= V_\lambda(\log(\bar{y}_n)) + V_\lambda(\log(y_{n+1})) \\ &\approx \frac{1}{n} + V_\lambda(\log(y_{n+1})). \end{aligned}$$

This would be the same as τ_v^2 if $V_\lambda(\log(y_{n+1})) = 1$. But unfortunately this is where the MHLE/Hessian matrix approximation breaks down. One can directly verify or use the property of Gumbel distribution (recall log of an exponential variable is a Gumbel variable) to arrive at

$$(7.11) \quad V_\lambda(\log(y_{n+1})) = \frac{\pi^2}{6} = 1.6449\dots$$

which is considerably larger than 1. [Incidentally, the integrating moment generating function approach (Meng, 2005) can be used to calculate $V_\lambda(\log(\bar{y}_n))$ exactly for general n , if needed.]

7.4 So What Works and What Does Not?

To see more clearly what went wrong, let us write out the R term in (6.1) explicitly for the current model. Using (7.4) and (7.7), simple algebra reveals that (6.1) becomes

$$(7.12) \quad \begin{aligned} \begin{pmatrix} \hat{\lambda} - \lambda \\ \hat{v} - v \end{pmatrix} &\equiv \begin{pmatrix} \bar{y}_n - \lambda \\ \log(\bar{y}_n) - \log(y_{n+1}) \end{pmatrix} \\ &= \begin{pmatrix} \bar{y}_n - \lambda \\ \bar{y}_n - y_{n+1} \end{pmatrix} \frac{1}{\lambda} + \begin{pmatrix} 0 \\ R_{v,n} \end{pmatrix}, \end{aligned}$$

where $R_{v,n}$ obviously makes up the difference between $\hat{v} - v$ and $(\bar{y}_n - y_{n+1})/\lambda$, but it would be more useful to express it in the equivalent form

$$(7.13) \quad \begin{aligned} R_{v,n} &= \left[\log\left(\frac{\bar{y}_n}{\lambda}\right) - \frac{\bar{y}_n - \lambda}{\lambda} \right] \\ &\quad - \left[\log\left(\frac{y_{n+1}}{\lambda}\right) - \frac{y_{n+1} - \lambda}{\lambda} \right]. \end{aligned}$$

From these expressions, we see that the MHLE/Hessian matrix approach works perfectly for the estimation of λ —it is the same as MLE and with the correct variance estimator because its R term is exactly zero. However, for the prediction of v , two things went wrong, and both are due to the failure of accumulation of information. First, $R_{v,n}$ is not negligible compared with the leading term $Z_{v,n} = (\bar{y}_n - y_{n+1})/\lambda$. Indeed, as $n \rightarrow \infty$, $R_{v,n} \rightarrow R_\infty = \xi - 1 - \log(\xi)$ and $Z_{v,n} \rightarrow Z_\infty = 1 - \xi$ where ξ is an exponential variable with mean one. In

fact, while $E(Z_\infty) = 0$, $E(R_\infty)$ is far from zero, taking the value of Euler's constant, $\gamma = 0.5772\dots$. This failure obviously is due to the nonapplicability of the Taylor expansion (7.8) when $n = 1$; if this were applicable, then $V(\log(y_{n+1})) = V(v)$ would be approximated by $V(z_n) = 1$, leading to $\tau_v^2 = 1 + \frac{1}{n}$ for $V(\hat{v} - v)$ in (7.7).

Second, although Z_∞ has mean zero and variance one, its density function $f(z) = e^{z-1}$, with support $(-\infty, 1]$, is far from that of the normal. Indeed, $f(1)/\phi(1) > 5$, where $\phi(z)$ is the p.d.f. of $N(0, 1)$. But of course the distribution of Z_∞ or $Z_{v,n}$ is not even relevant because we cannot use either of them to approximate the sampling distribution of $\hat{v} - v$ due to the nonnegligibility of $R_{v,n}$.

7.5 3-in-1: Pivotal Predictive Distribution, Posterior Predictive Distribution, and H-distribution

The exact distribution of $\hat{v} - v$, of course, can be worked out easily in this case. But it is important to emphasize that by moving from the original $u = y_{n+1}$ scale to the $v = \log(y_{n+1})$ scale, we have obtained a *predictive pivotal quantity*. That is, whereas the sampling distribution of $u - \hat{u} = y_{n+1} - \bar{y}_n$ depends on the unknown λ , the distribution of $v - \hat{v} = \log(y_{n+1}/\bar{y}_n)$ is free of λ because it is canceled in the ratio as the scale parameter. Consequently, the v scale provides us a way to construct exact prediction intervals without having to worry about λ which is a *nuisance parameter for the purposes of prediction*. This is simply the predictive version of the usual inference of parameter of interest based on a pivotal quantity. Although such a construction is by nature a frequentist one, it should help to understand the importance of the choice of scale of the unobservables for the authors' approach. Evidently, this consideration of pivotal quantity greatly restricts the family of scales for unobservables, beyond the minimal requirement of preserving the (first two) Bartlett identities, as discussed in Section 5.

Indeed, it is informative to compare the three distributions here: (I) the sampling distribution $f_\lambda(\hat{v} - v)$, (II) the posterior predictive distribution $f^B(v|y)$ under constant prior and (III) the h-distribution $f^H(v|y)$ derived from the authors' APHL method. For (I), because $U_n = \sum_{i=1}^n y_i \sim \text{Gamma}(n, \lambda)$ is independent of $u = y_{n+1} \sim \text{Gamma}(1, \lambda)$, we know the ratio $B_n = U_n/(U_n + u)$ is distributed as $\text{Beta}(n, 1)$. Consequently, $r = y_{n+1}/\bar{y}_n = n(B_n^{-1} - 1)$ follows a Pareto distribution of order $n + 1$, that is,

$$(7.14) \quad f(r) = \left(1 + \frac{r}{n}\right)^{-(n+1)}, \quad r \geq 0$$

which converges to e^{-r} as $n \rightarrow \infty$, as it should. [The distribution $f(r)$ obviously determines the distribution of $v - \hat{v} = \log(r)$.]

In comparison, for (II), because $f(y_1, \dots, y_n | \lambda) \propto \lambda^{-n} e^{-U_n/\lambda}$, a posteriori we can write $\lambda = U_n \gamma^{-1}$, where $\gamma \sim \text{Gamma}(n - 1, 1)$. Consequently, because $u = \lambda \xi$ where $\xi \sim \text{Gamma}(1, 1)$ and is independent of γ , a posteriori we have $u = U_n (\xi/\gamma)$. This implies $r \equiv nu/U_n = n\xi/\gamma = n(\tilde{B}_{n-1} - 1)$ where $\tilde{B}_{n-1} \sim \text{Beta}(n - 1, 1)$; here we assume $n > 1$ as the posterior is improper when $n = 1$ under the constant prior on λ . It follows that

$$(7.15) \quad f^B(r|y) = \frac{n-1}{n} \left(1 + \frac{r}{n}\right)^{-n}, \quad r \geq 0.$$

For (III), we note from the first equation of (7.4) that for any given v , the h-likelihood is maximized at

$$(7.16) \quad \lambda(v) = \frac{n\bar{y}_n + e^v}{n+1}.$$

From (7.3), the log profile h-likelihood then becomes, ignoring irrelevant constants,

$$(7.17) \quad h_\lambda(v; y) = -(n+1) \log \lambda(v) + v.$$

Using the authors' notation and (7.5), $D(h, \lambda) = -\frac{\partial^2 h(\lambda, v; y)}{\partial \lambda^2} = (n+1)/\lambda^2$ when $\lambda = \lambda(v)$, and hence the authors' (log) adjusted profile h-likelihood becomes, again ignoring irrelevant constants,

$$(7.18) \quad \begin{aligned} \tilde{h}_\lambda(v; y) &= -(n+1) \log \lambda(v) + v \\ &\quad - \frac{1}{2} \log(D(h, \lambda(v))) \\ &= -n \log \lambda(v) + v. \end{aligned}$$

The h-distribution for v then, as I understand from the authors' approach, is to set

$$(7.19) \quad \begin{aligned} f^H(v|y) &\propto e^{\tilde{h}_\lambda(v; y)} \\ &= e^v \lambda^{-n}(v) \propto e^v (U_n + e^v)^{-n}. \end{aligned}$$

Converting this to the distribution of $r = nu/U_n = ne^v/U_n$ and re-normalizing it to be a proper distribution, we have, again assuming $n > 1$,

$$(7.20) \quad f^H(r|y) = \frac{n-1}{n} \left(1 + \frac{r}{n}\right)^{-n}, \quad r \geq 0$$

which is identical to the posterior predictive distribution (7.15). This is expected because of the accuracy of the Laplace approximation (and by re-normalizing we eliminate the remaining approximation inaccuracy).

7.6 The Need of Choosing the Right Scale for the Fixed Parameter

A perceptive reader may realize that the small difference between (7.14) and (7.15) or (7.20), although of little practical consequence, nevertheless points to a deeper issue. Indeed, if we use the constant prior on $\log(\lambda)$, the most common “noninformative” prior for scale parameter, then $f^B(r|y)$ will be the same as $f(r)$ of (7.14). This suggests an intimate connection between posterior prediction and the pivotal approach on the joint space of $\{y, v\}$.

For h-likelihood, we have seen that choosing the right scale for the unobservable is crucial. However, the scale of the parameter also plays a role, especially for the adjusted profile h-likelihood because the value of $D(h, \alpha)$ depends on the scale of α . For example, in the current example, if we also choose the log scale for λ , that is, use $h(\eta, v; y)$ to carry out all the h-likelihood calculations where $\eta = \log(\lambda)$, then $D(h, \eta) = n + 1$. Consequently, the adjustment becomes immaterial, making the log APHL the same as (7.17), the original profiled log h-likelihood. This is easily seen to lead to

$$(7.21) \quad f^H(r|y) = \left(1 + \frac{r}{n}\right)^{-(n+1)}, \quad r \geq 0,$$

which is now identical to the pivotal predictive distribution $f(r)$ in (7.14), a truly 3-in-1!

This equivalence not only demonstrates the intimate connection among the three methods, but also suggest the possibility of providing a probabilistic meaning to h-distributions, at least in some cases. For example, under (7.14), a $1 - \alpha$ highest density predictive (HDP) interval is of the form

$$(7.22) \quad \text{HDP} = [0, c(\alpha, n)\bar{y}_n],$$

where $c(\alpha, n) = n(\alpha^{-1/n} - 1) \rightarrow -\log(\alpha)$.

This interval has both Bayesian interpretation and frequentist interpretation, the latter of which I believe is closer to what the authors have been seeking. The frequentist interpretation is simply that among repeated samples of $\{y_1, \dots, y_n, y_{n+1}\}$, the HDP in (7.22) covers y_{n+1} with frequency/probability $1 - \alpha$. Such interpretation perhaps is more appealing to some than its posterior predictive interpretation which in this case is actually not directly realizable with random λ because it is derived under the improper prior $\pi(\lambda) \propto \lambda^{-1}$. It is somewhat intriguing that this un-realizable posterior predictive distribution via random λ is easily realizable

via the pivotal predictive distribution. A general investigation of this connection may offer new insights into both the similarities and differences between Bayesian and sampling inferences.

8. EPILOGUE

Dan Brown concluded *Angels and Demons* with Dr. Langdon's religious experience with Vittoria, a yoga master. Although my pleasure is at an entirely different level, I must confess that my study of the h-likelihood framework is largely carried by both the authors' faith in their methods and my faith in the authors—they must have seen signs that most discussants did not. My Bayesian half urged me every weekend to seek Dr. Langdon's ambigram of "H," yet my other half kept seducing me with promises of hidden treasures. Indeed, a posteriori I am willing to move all probability from (V) to (IV), as well as to increase the probability of (II) over 50%, provided that we are always mindful of another "H" for h-likelihood—its Achilles' Heel—the potential (and often) non-negligibility of the R term. The Bartlizability and pivotal predictive interpretation of the h-likelihood methods could seduce someone to speculate that the "H" is *The Lost Symbol*, the eagerly awaited new thriller of Dan Brown. As a matter of fact, since I have already been seduced for the past five weekends, far exceeding the originally planned 3-day excursion, I may as well enjoy my earned fantasy, a spoonful of my colleague Dr. Langdon's new experience, divine or not. . . .

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