# Objective Inference for Climate Parameters: Bayesian, Transformation of Variables and Profile Likelihood Approaches

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## Abstract

Insight is provided into the use of objective Bayesian methods for estimating climate sensitivity by considering their relationship to transformations of variables in the context of a simple case considered in a previous study, and some misunderstandings about Bayesian inference are discussed. A simple model in which climate sensitivity (*S*) and effective ocean heat diffusivity ($K_v$) are the only parameters varied is used, with 20th century warming attributable to greenhouse gases (AW) and effective ocean heat capacity (HC) being the only data-based observables. Probability density functions (PDFs) for AW and HC are readily derived that represent valid, independent, objective Bayesian posterior PDFs, provided the error distribution assumptions involved in their construction are justified. Using them, a standard transformation of variables provides an objective joint posterior PDF for *S* and $K_v$; integrating out $K_v$ gives a marginal PDF for *S*. Close parametric approximations to the PDFs for AW and HC are obtained, enabling derivation of likelihood functions and related noninformative priors that give rise to the objective posterior PDFs that were computed initially. Bayes' theorem is applied to the derived AW and HC likelihood functions, demonstrating the effect of differing prior distributions on PDFs for *S*. Use of the noninformative Jeffreys' prior produces an identical PDF to that derived using the transformation of variables approach. It is shown that quite similar inference for *S* to that based on these two alternative objective Bayesian approaches is obtained using a profile likelihood method on the derived joint likelihood function for AW and HC.

# 1. Introduction

Estimates of climate sensitivity often use global energy balance or other simple climate models with a limited number of adjustable parameters, and compare modeled and observed values of multidecadal warming and other climate variables. Such estimates play an important role in assessment of climate sensitivity (Hegerl et al., 2007; Bindoff et al., 2013). Most of these studies use a Bayesian framework as a basis for assessing uncertainty and developing a probability density function (PDF) for climate sensitivity. This paper addresses the methodological challenge of selecting the appropriate Bayesian prior distributions for climate sensitivity and other parameters employed in simple climate model analyses.

Deriving valid probabilistic estimates for climate sensitivity and other uncertain parameters such as effective ocean diffusivity has proved challenging. These challenges primarily arise from the strongly nonlinear relationships between observable variables and these climate system parameters, combined with large observational uncertainties. Such factors make selection of appropriate Bayesian prior distributions for the parameters crucial but non-obvious. In suitable cases, the problem of prior selection may be addressed by considering Bayesian parameter inference as consisting of first generating probabilistic estimates for the 'true' values of the observable variables – those corresponding to what would have been observed in the absence of uncertainty – and then performing a transformation of variables from the observables to the parameters.

Frame et al. (2005; hereafter Fr05) was a seminal paper that addressed the role of prior assumptions regarding climate sensitivity, and is particularly well-suited for illustration of a transformation of variables approach. Fr05 used probabilistic observationally-derived estimates of 20th century warming attributable to greenhouse gas increases and of effective heat capacity to estimate a probability density function (PDF) for climate sensitivity (and implicitly also for effective ocean diffusivity) on different sampling strategies, representing different prior assumptions. Such an analysis can only be viewed in Bayesian terms, since in frequentist statistics there is no role for prior assumptions, nor is putting a probability distribution on a fixed but unknown parameter permitted.

Bayes' theorem (Bayes, 1763) states that the (posterior) PDF, $p_\theta(\boldsymbol{\theta} \mid \boldsymbol{y})$, for a parameter vector $\boldsymbol{\theta}$ on which observed data $\mathbf{y}$ depend, is proportional to the probability density of the data $p_y(\boldsymbol{y} \mid \boldsymbol{\theta})$ (termed the likelihood function when considered as a function of $\boldsymbol{\theta}$, with $\mathbf{y}$ fixed) multiplied by the density of a prior distribution (prior) for $\boldsymbol{\theta}$, $p_\theta(\boldsymbol{\theta})$, reflecting relevant existing knowledge:

$$p_\theta(\boldsymbol{\theta} \mid \boldsymbol{y}) \propto p_y(\boldsymbol{y} \mid \boldsymbol{\theta})\, p_\theta(\boldsymbol{\theta}) \qquad (1)$$

where the subscripts indicate which variable a density is for.

In subjective Bayesian analysis, the prior purely reflects existing knowledge about $\boldsymbol{\theta}$. In objective Bayesian analysis, where such knowledge is disregarded or nonexistent, the prior is designed to be noninformative so that the data dominates inference about $\boldsymbol{\theta}$. Noninformative priors depend on the characteristics of the data and experiment concerned and have no probability interpretation (Bernardo and Smith, 1994). The likelihood function required to apply Bayes' theorem is a probability density for data, $p_y(\boldsymbol{y}, \boldsymbol{\theta})|_{y=y_0}$, albeit expressed as a function of the parameter vector with the data fixed at $\boldsymbol{y}_0$, the actually observed $\boldsymbol{y}$. Typically, $\boldsymbol{y}$ will reflect some function of $\boldsymbol{\theta}$ and a random error

$\boldsymbol{\varepsilon}$: $\boldsymbol{y} = g(f(\boldsymbol{\theta}), \boldsymbol{\varepsilon})$, reducing to $\boldsymbol{y} = f(\boldsymbol{\theta}) + \boldsymbol{\varepsilon}$ where errors are additive and their distribution is independent of $\boldsymbol{\theta}$.

It is implicit in the foregoing formulation that $\boldsymbol{y}$ is not simply a deterministic function of $\boldsymbol{\theta}$, $\boldsymbol{y} = f(\boldsymbol{\theta})$. In such a case, $\boldsymbol{y}$ has a fixed value for any given $\boldsymbol{\theta}$ and thus no likelihood function exists. Therefore, Bayes' theorem is not required and instead one simply uses $f(\boldsymbol{\theta})$ to transform between data and parameter spaces. Where the dimensionality of $\boldsymbol{y}$ and $\boldsymbol{\theta}$ are the same, as they are in Fr05, and provided that in the region where $p_{\theta}(\boldsymbol{\theta}) > 0$, $f(\boldsymbol{\theta})$ is a smooth invertible one-to-one function with both $f(\boldsymbol{\theta})$ and $f^{-1}(\boldsymbol{y})$ continuously differentiable, the standard transformation-of-variables formulae for converting a PDF for $\boldsymbol{\theta}$ into a PDF for $\boldsymbol{y}$ and *vice versa* are:

$$p_y(\boldsymbol{y}) = p_{\theta}(f^{-1}(\boldsymbol{y}))\ J_{f^{-1}} \tag{2}$$

where $J_{f^{-1}}$ is the absolute value of the determinant of the Jacobian of $f^{-1}$ with respect to $\boldsymbol{y}$, and conversely:

$$p_{\theta}(\boldsymbol{\theta}) = p_y(f(\boldsymbol{\theta}))\ J_f \tag{3}$$

where $J_f$ is the absolute value of the determinant of the Jacobian of $f$ with respect to $\boldsymbol{\theta}$ (Mardia et al., 1979).

If the dimensionality of the observables exceeds that of the parameters, a dimensionally-reducing version of the transformation of variables PDF conversion formula may be used (Mardia et al, 1979; Lewis, 2013b), provided the observables can first be whitened (made independent and of equal variance, as in optimal fingerprint methods: Hegerl et al., 1996).

The primary aims of this paper are to provide insight into the use of objective Bayesian methods for estimating climate sensitivity by considering their relationship to transformations of variables in the context of the simple case considered in Fr05, discussing also estimation using profile likelihood methods, and to dispel some misunderstandings about Bayesian inference.

Although the Fr05 authors had no intention of using an objective Bayesian approach, they stated 'Unless they are warned otherwise, users will expect an answer to the question "what does this study tell me about X, given no knowledge of X before the study was performed?"', going on to assert that 'This requires sampling nonobservable parameters to simulate a uniform distribution in X, the forecast quantity of interest, before other constraints are applied,…'. By contrast, the objective approach presented here, which is intended not to incorporate any prior knowledge as to the values of the parameters involved, is equivalent to advocating a uniform prior, not in the forecast quantity, but in a transformation of observables that has errors with a Gaussian or other fixed distribution.

The data, model and model parameters used in this paper's analysis follow Fr05, although several inconsistencies and misinterpretations in Fr05 are pointed out. Fr05 mistakenly derived distributions for its observables that, as will be seen, equated to estimated posterior PDFs for them rather than likelihood functions. Accordingly, Fr05 is not fully consistent with Bayes theorem. Moreover, the Fr05 authors misinterpreted the ocean heat content change estimate they used, which pertains to a 44-year period, as covering only the somewhat shorter period used in Fr05. These errors, which have a relatively modest net effect, are addressed in a corrigendum (Frame et al., 2014).

The material is organized as follows. Section 2 summarizes the methods used and discusses their implications. Section 3 evidences replication of Fr05's original results. Section 4 deals with inference based on likelihood functions derived for the observables. Section 5 discusses climate sensitivity estimation and various misconceptions about it.

# 2. The observables, model and model parameters

## *a. Overview*

The analysis uses a global energy balance model (EBM) with a diffusive ocean (Andrews and Allen, 2008). The EBM uses given values of climate sensitivity, $S$, and effective ocean vertical diffusivity, $K_v$, and a greenhouse gas (GHG) forcing time series estimated by the Met Office HadCM3 model (Gordon et al. 2000), to simulate global surface temperature and ocean heat content changes over 1861 to 2000. The EBM is believed to be equivalent to, and to employ the same forcing series, as that used in Fr05, and is run at the same $S$ and $K_v$ values.

The observables used are 20th century warming attributable to greenhouse gases (attributable warming), $T_A$, and effective heat capacity – the ratio of changes in ocean heat content and global surface temperature – $C_H$. Thus, $\boldsymbol{y}$ and $\boldsymbol{\theta}$ are both bivariate, with observables $\boldsymbol{y} = (T_A, C_H)$ and parameters $\boldsymbol{\theta} = (S, K_v)$. Although $K_v$ usually denotes effective ocean vertical diffusivity, for notational convenience here $K_v$ represents the square root of effective ocean vertical diffusivity, which controls $C_H$ in an approximately linear manner (Sokolov et al., 2003) and in effect is treated as being the parameter.

Model accuracy is assumed, with there being a 'true' setting $(S^t, K_v^t)$ of model parameters that simulates 'true' (error-free) values $(T_A^t, C_H^t)$. As the EBM is deterministic, the dispersion of the estimated PDFs for $S$ entirely reflects uncertainties in the observationally-based estimates of $T_A$ and $C_H$.

EBM simulations are run using all parameter value combinations lying on a grid that is uniformly spaced in terms of $S$ and $K_v$. The ranges used are sufficiently wide for there to be negligible probability of the true values of $S$ or $K_v$ lying outside them. The annual model-simulation time series are used to compute $T_A^m$ and $C_H^m$, $T_A^m$ as the 20th century linear trend in global temperature and $C_H^m$ as the ratio of changes in ocean heat content and global temperature over 1957-94.

Since the EBM is a deterministic rather than a statistical model, and given the relationships of the $T_A^m$ and $C_H^m$ values to the parameters, there is a smooth invertible both-ways differentiable one-to-one functional relationship between joint model parameter settings, $(S^m, K_v^m)$, and joint values of $(T_A^m, C_H^m)$: each $(S^m, K_v^m)$ combination corresponds to a unique value of $(T_A^m, C_H^m)$ and vice versa. Given the assumption of model-accuracy the same relationship exists between the true joint values $(T_A^t, C_H^t)$ of ($T_A$, $C_H$), and the true joint values $(S^t, K_v^t)$ of $(S, K_v)$. It follows from (3) that the estimated joint posterior PDF for $(S^t, K_v^t)$ is determined by that for $(T_A^t, C_H^t)$:

$$p_{S^t, K_v^t}(S, K_v) = p_{T_A^t, C_H^t}(f(S, K_v))\, J_f \tag{4}$$

where $f$ is the functional relationship between $(S^m, K_v^m)$ and $(T_A^m, C_H^m)$ and $J_f$ is the absolute Jacobian determinant, given by:

$$J_f = \text{absolute value of} \left| \begin{pmatrix} \dfrac{\partial T_A^m}{\partial S^m} & \dfrac{\partial T_A^m}{\partial K_v^m} \\ \dfrac{\partial C_H^m}{\partial S^m} & \dfrac{\partial C_H^m}{\partial K_v^m} \end{pmatrix} \right|_{S^m = S, K_v^m = K_v} \tag{5}$$

The derivatives can be estimated by numerical differentiation using the EBM output at grid points. It follows that were an estimated joint posterior PDF for $(T_{\mathrm{A}}^{\mathrm{t}}, C_{\mathrm{H}}^{\mathrm{t}})$ available, it would provide through (4) and (5) and the model-accuracy assumption a unique corresponding joint posterior PDF for $(S^{\mathrm{t}}, K_{\mathrm{v}}^{\mathrm{t}})$.

*b. Derivation of climate sensitivity PDFs from the observables*

The attraction of using $C_{\mathrm{H}}$ rather than ocean heat content is that $C_{\mathrm{H}}$ should be independent of the change in global surface temperature and hence of $T_{\mathrm{A}}$. On the basis of independence between its observables $C_{\mathrm{H}}$ and $T_{\mathrm{A}}$, which holds for similar variables in the HadCM3 control run, their joint density can be obtained by multiplying their individual densities. In order to undertake Bayesian inference for the parameters, that joint density (*l_hood*) would need to be the likelihood at any selected ($T_{\mathrm{A}}$, $C_{\mathrm{H}}$) combination (and hence at the corresponding $(S, K_v)$ combination) of having obtained the actual observations, $(T_{\mathrm{A}}^{\mathrm{o}}, C_{\mathrm{H}}^{\mathrm{o}})$, reflecting the observed level of model-data discrepancy. That is to say, *l_hood* must represent the joint density for $(T_{\mathrm{A}}^{\mathrm{o}}, C_{\mathrm{H}}^{\mathrm{o}})$ on the conjecture that $(S^{\mathrm{m}}, K_{\mathrm{v}}^{\mathrm{m}})$ equal their 'true' values, $(S^{\mathrm{t}}, K_{\mathrm{v}}^{\mathrm{t}})$ and hence that $(T_{\mathrm{A}}^{\mathrm{m}}, C_{\mathrm{H}}^{\mathrm{m}})$ equal $(T_{\mathrm{A}}^{\mathrm{t}}, C_{\mathrm{H}}^{\mathrm{t}})$, the 'true' values of $T_{\mathrm{A}}$ and $C_{\mathrm{H}}$.

The EBM simulation runs and interpolation from ($T_{\mathrm{A}}$, $C_{\mathrm{H}}$) space onto the $(S, K_v)$ grid can be used to derive the value of *l_hood* at all $(S, K_v)$ grid combinations. By integrating the resulting *l_hood* values over all $K_{\mathrm{v}}$ values, a posterior distribution for $S$ based on assuming a uniform initial distribution in sensitivity can be derived, provided *l_hood* is a likelihood. Alternatively, the impact of different prior distributions can be simulated by weighting in different ways when interpolating between the $(S, K_v)$ and

($T_A$, $C_H$) grids. Provided *l_hood* is a likelihood this procedure is equivalent to using differing prior distributions in Bayes' theorem and thereby obtaining different marginal posterior PDFs for *S*.

However, for Bayes theorem to be applied, *l_hood* must be a likelihood as defined above, and not a posterior PDF. In the latter case, Bayes' theorem is not applicable and instead the standard Jacobian determinant rule applicable to transformations of variables enables computation of a posterior PDF for $(S^t, K_v^t)$, and hence for *S* upon integrating out $K_v$.

*c. Methods used to derive the observables from the data and their resulting status*

$C_H^o$ is inferred from the observed change in global ocean heat content $(\Delta\text{OHC})$ of 144.7 ZJ (Levitus et al., 2005) divided by the corresponding change in decadal-mean surface temperature ($\Delta T_G$) of 0.338 K over the 1957-94 period stated in Fr05, allowing for the uncertainty in both quantities (respectively 45 ZJ and 0.066 K standard errors, assumed independent and Gaussian). As discussed in Section 1, the ΔOHC estimate actually related to a longer period, resulting in an overestimate of $C_H^o$, and hence of *S* and $K_v$, but it is used in order to provide comparability with Fr05. Section 5 gives an estimate of *S* with ΔOHC and $\Delta T_G$ determined (as respectively 128.3 ZJ and 0.360 K) over matching 1957–96 periods. Since the ΔOHC estimate used does not represent total heat uptake, a small allowance for omitted elements should perhaps be added; consideration of that issue is beyond the scope of this paper.

Where, as for ΔOHC and $\Delta T_G$, the observed value $z^o$ of a variable with true value $z^t$ is subject to an additive error $\varepsilon$ having a fixed distribution, a location parameter model applies:

$$z^o = z^t + \varepsilon \text{ where } \varepsilon \sim e(\mu_\varepsilon, \sigma_\varepsilon) \tag{6}$$

Here, only the difference $(z^o - z^t)$ between the true and observed value affects the probability of the observation. That being so, the likelihood function is a mirror-image of the error distribution centered on the observed value. Where the error distribution is Gaussian, as here, the likelihood function – the density for the observed value at the value actually observed, as a function of the true value – is identical to the error distribution, centered on the observed value:

$$p_{z^o}(z^o, z^t)\Big|_{z^o} = \frac{1}{\sigma_\varepsilon \sqrt{2\pi}} \exp[-(z^t - z^o)^2 / 2\sigma_\varepsilon^2] \tag{7}$$

(This applies for any symmetric zero-mean error distribution.) It is well known (e.g., Datta and Sweeting, 2005) that in such cases a uniform prior in the variable is completely noninformative for Bayesian inference, and gives rise to an objective posterior density for the true variable, identical to the likelihood function, that provides exact probability matching with frequentist confidence intervals:

$$p_{z^t}(z^t \mid z^o) = \frac{1}{\sigma_\varepsilon \sqrt{2\pi}} \exp[-(z^t - z^o)^2 / 2\sigma_\varepsilon^2] \tag{8}$$

From the Bayesian perspective, the $N(144.7,\ 45)$ ZJ and $N(0.338,\ 0.066)$ K distributions involved accordingly not only represent independent likelihood functions for the observed values of ΔOHC and $\Delta T_G$ but also independent objective posterior PDFs, derived using uniform priors, for the true values of those variables.

I derive an estimated PDF for the true effective heat capacity, $C_H^t$, from the PDFs for ΔOHC and $\Delta T_G$ by calculating the quotients of many pairs of random samples taken from them and computing their histogram. This is essentially an identical method to that used in Gregory et al (2002) directly to compute a PDF for $S$ from the error distributions for the relevant observables. The sampling-based method provides a correctly calculated, objective Bayesian, estimated posterior density for $C_{\mathrm{H}}^{\mathrm{t}}$, that is $p_{C_{\mathrm{H}}^{t}}(C_{\mathrm{H}}^{t} \mid C_{\mathrm{H}}^{o})$. This density for $C_{\mathrm{H}}^{\mathrm{t}}$ cannot be regarded as a likelihood function for $C_{\mathrm{H}}^{\mathrm{o}}$ – the density for the "observed" value of $C_{\mathrm{H}}$ at varying values of $C_{\mathrm{H}}^{\mathrm{t}}$, $p_{C_{\mathrm{H}}^{o}}(C_{\mathrm{H}}^{o} \mid C_{\mathrm{H}}^{t})\big|_{C_{\mathrm{H}}^{o}}$. Unlike for PDFs, one cannot derive a likelihood function for the ratio of the true values of two independent variables by sampling from their likelihood functions, calculating quotients and computing their histogram. However, as shown in Section 4, it is possible to estimate a likelihood function for $C_{\mathrm{H}}^{\mathrm{o}}$ by other means.  Since a location parameter model does not apply to $C_{\mathrm{H}}$, its likelihood function differs from the posterior density for $C_{\mathrm{H}}^{\mathrm{t}}$.

The other observable, $T_{\mathrm{A}}^{\mathrm{o}}$, represents attributable warming. $T_{\mathrm{A}}^{\mathrm{o}}$ is a modified version of $T_{\mathrm{A\_SK}}$, attributable warming estimated from simulations by the HadCM3 AOGCM, observationally-constrained using a pattern-based attribution analysis (Stott and Kettleborough, 2002), which gives a distribution of scaling factors for the forced response (Stott et al., 2004). Data available for $T_{\mathrm{A\_SK}}$ constitute a cumulative distribution function (CDF), which is derived from the estimated error distribution for a regression coefficient and hence is objective. I differentiate the CDF to obtain an objective estimated posterior PDF for $T_{\mathrm{A\_SK}}^{\mathrm{t}}$, the true value of $T_{\mathrm{A\_SK}}$. The derivative of the CDF is not a likelihood function, since it does not represent a density for observed data. I then sample the $T_{\mathrm{A\_SK}}^{\mathrm{t}}$ values and add a ±10% divisive allowance for forcing uncertainty, matching what was done in Fr05.  Doing so replaces the initial (posterior) probability density for

$T^{\mathrm{t}}_{\mathrm{A\_SK}}$ with a density for $T^{\mathrm{t}}_{\mathrm{A}}$, the ratio of $T^{\mathrm{t}}_{\mathrm{A\_SK}}$ to another variable having a uniform [0.9, 1.1) PDF; it does not transform the posterior PDF into a likelihood.

It follows that *l_hood* actually represents a joint posterior density for $(T^{\mathrm{t}}_{\mathrm{A}}, C^{\mathrm{t}}_{\mathrm{H}})$, the true values of the observables $C_{\mathrm{H}}$ and $T_{\mathrm{A}}$, not a likelihood (the joint density for the observations, $(T^{\mathrm{o}}_{\mathrm{A}}, C^{\mathrm{o}}_{\mathrm{H}})$, at differing candidate true values).

*d. Implications of using a joint posterior PDF instead of a likelihood*

Since the density *l_hood* for the observables is a joint posterior PDF for $(T^{\mathrm{t}}_{\mathrm{A}}, C^{\mathrm{t}}_{\mathrm{H}})$, not a likelihood, no subsequent application of Bayes' theorem is required in order to obtain an estimated joint posterior PDF for $(S^{\mathrm{t}}, K^{\mathrm{t}}_{\mathrm{v}})$. Rather, the joint posterior PDF for $(S^{\mathrm{t}}, K^{\mathrm{t}}_{\mathrm{v}})$ is given by the transformation-of-variables method, applying (4) and (5) to *l_hood*, and (for the EBM model used) is unique. The PDF $p_{T^{\mathrm{t}}_{\mathrm{A}}, C^{\mathrm{t}}_{\mathrm{H}}}(f(S, K_{\mathrm{v}}))$ in (4) is given here by $l\_hood(T_A(S, K_{\mathrm{v}}), C_{\mathrm{H}}(S, K_{\mathrm{v}}))$. The known values of $(T^{\mathrm{m}}_{\mathrm{A}}, C^{\mathrm{m}}_{\mathrm{H}})$ at each setting of $(S^{\mathrm{m}}, K^{\mathrm{m}}_{\mathrm{v}})$ provide the conversion between $(T_{\mathrm{A}}, C_{\mathrm{H}})$ space and $(S, K_{\mathrm{v}})$ space and enable computation of the Jacobian determinant $J_f$. The marginal PDF for $S^{\mathrm{t}}$ is then obtained by integrating out $K_{\mathrm{v}}$.

In geometrical terms, $J_f$ represents the volume of a region $dT^{\mathrm{m}}_{\mathrm{A}} dC^{\mathrm{m}}_{\mathrm{H}}$ in $(T_{\mathrm{A}}, C_{\mathrm{H}})$ space relative to that of the region $dS^{\mathrm{m}} dK^{\mathrm{m}}_{\mathrm{v}}$ in $(S, K_v)$ space to which it corresponds. High value of $J_f$ indicate that the observable variables change rapidly with the parameter values at those points in parameter space; low values indicates the opposite.

The shape of the Jacobian determinant surface is shown in Figure 1. It is highest in the low $S$, low $K_v$ corner and declines with both $S$ and $K_v$, declining faster when the other variable is high.

The PDF for $(S^t, K_v^t)$ and hence the marginal PDF for $S^t$ obtained as set out above are valid Bayesian posterior densities notwithstanding that *l_hood* is a posterior density not a likelihood, since its character as such is unaltered by a transformation of variables. Therefore, the uncertainty ranges for $S^t$ are Bayesian credible intervals with estimated probabilities that $S^t$ lies above or below them matching the specified probabilities. By contrast, a confidence interval (CI) is constructed so that the estimated proportions of occasions that $S^t$ would lie above or below it match the specified probabilities on repeated sampling of data from the same distributions. Noninformative priors for objective Bayesian inference often produce credible intervals that approximately match confidence intervals, and may be judged by their ability to do so; in some common cases matching is exact. Confidence intervals for a single parameter may be obtained using profile likelihoods, and although in general likewise not exact they provide both an alternative objective parameter inference method and a simple check on the frequentist validity of credible intervals derived from Bayesian analysis.

# 3. Inference for *S* using a transformation of variables

In this section, I use a transformation of variables approach to infer $S$ and demonstrate replication of two Fr05 PDFs for $S$ – those stated to correspond to uniform initial distributions respectively in TCR/attributable warming (jointly with effective heat capacity) and in climate sensitivity (jointly with $K_v$). Given the linear response to transient forcing, TCR and attributable warming are approximately linearly related, hence the PDFs for *S* in Figure 1(c) of Fr05 based on uniform initial distributions in each of them are indistinguishable. Although Fr05 was not an objective Bayesian study, it unintentionally used incorrect methods for the calculation of the likelihood functions, namely the methods set out in Section 2 for the derivation of objective Bayesian posterior PDFs for the observables. As a result, the correctness of my emulation of Fr05's model-simulations and other calculations can be tested by comparing its (uncorrected) PDFs for *S* based on uniform initial distributions respectively in TCR/attributable warming and in climate sensitivity with those I compute using a transformation of variables approach to convert the PDFs for the observables respectively using, and omitting, the applicable standard Jacobian determinant factor. The uncorrected Fr05 PDFs – which do not accurately reflect the stated intentions of its authors – are shown only to demonstrate that the computations in this study match those in Fr05.

*a. Replication of PDFs for S*

Figure 2 shows marginal posterior PDFs for *S* after (as in Fr05) integrating out $K_v$. The black line, computed by transforming the posterior PDF for $(T_A^t, C_H^t)$ to one for $(S^t, K_v^t)$ using the Jacobian determinant, is almost identical to the green line, reproduced from Figure 1(c) of Fr05, evidencing accurate replication of Fr05's calculations. The green line is stated there to be based on a simulated uniform initial distribution in TCR; it samples uniformly also in $C_H$, and presumably overlays the non-visible line based on uniform sampling in $(T_A, C_H)$. Uniform sampling in $(T_A, C_H)$ weights *l_hood*, the PDF for $(S^t, K_v^t)$, by reference to volumes in $(T_A, C_H)$ space relative to corresponding volumes in $(S, K_v)$ space. It thus equates to multiplication by the Jacobian determinant required upon the change of variables from $(T_{\mathrm{A}}, C_{\mathrm{H}})$ to $(S, K_{\mathrm{v}})$.

The Figure 2 grey line shows a PDF for *S* computed by restating, in terms of $(S, K_v)$, the posterior PDF for $(T_{\mathrm{A}}^{\mathrm{t}}, C_{\mathrm{H}}^{\mathrm{t}})$ and renormalizing. It differs from the black line due to omitting the multiplication by the Jacobian determinant required upon the change of variables from $(T_{\mathrm{A}}, C_{\mathrm{H}})$ to $(S, K_{\mathrm{v}})$, and hence does not correctly reflect the posterior PDF for $(T_{\mathrm{A}}^{\mathrm{t}}, C_{\mathrm{H}}^{\mathrm{t}})$. The red line in Fr05 Figure 1(c), stated there to be based on assuming a uniform initial distribution in sensitivity and reproduced as the coral line in Figure 2, was effectively likewise derived just by restating *l_hood* in terms of $(S^{\mathrm{t}}, K_{\mathrm{v}}^{\mathrm{t}})$ and is shown as a dashed coral line in Figure 2. The close matching of the grey and coral lines provides further evidence of correct replication of Fr05.

Percentile points of the posterior PDFs give Bayesian credible intervals for *S*, shown by the box plots in Figure 2 for 10–90% and 5–95% ranges.

### *b. Discussion of the climate sensitivity PDF obtained by the transformation of variables approach*

In a first stage, I derived, using a sampling-based objective Bayesian approach, a joint posterior PDF for $(T_{\mathrm{A}}^{\mathrm{t}}, C_{\mathrm{H}}^{\mathrm{t}})$. In a second stage I carried out a transformation of variables from $(T_{\mathrm{A}}, C_{\mathrm{H}})$ to $(S, K_{\mathrm{v}})$, using the appropriate Jacobian determinant, thereby obtaining a posterior PDF for $(S^{\mathrm{t}}, K_{\mathrm{v}}^{\mathrm{t}})$. The marginal PDF for *S* – the black line in Figure 2 – follows upon applying the standard Bayesian method of integrating out $K_{\mathrm{v}}$.

If one accepts that the posterior PDF derived for $(T_A^t, C_H^t)$ correctly reflects the uncertainty distributions of the observations, then since the PDFs for $(T_A^t, C_H^t)$ and $(S^t, K_v^t)$, are related by the standard transformation-of-variables Jacobian conversion factor, the posterior PDF for $(S^t, K_v^t)$ derived in the above way correctly reflects the observational uncertainties.

The sampling-derived estimated posterior PDF for $C_H^t$ appears objectively correct provided that the underlying estimates and Gaussian error assumptions for ΔOHC and $\Delta T_G$ are valid: it corresponds with repeated sampling results. Moreover, it is implicitly assumed in Fr05 that, after the additional allowance is made for forcing uncertainty, the objective observationally-constrained estimated PDF for attributable warming derived from simulations by the HadCM3 AOGCM, $T_{A\_SK}^t$, provides a valid estimated PDF for $T_A^t$. From a scientific viewpoint, it seems difficult (unless other external information is to be incorporated) to argue for the use of any prior in a direct Bayesian derivation of a PDF for $(S^t, K_v^t)$ – one not involving a transformation-of-variables approach – other than that which produces a posterior that is consistent, upon transformation to $(T_A, C_H)$ space, with the posteriors derived here for $C_H^t$ and $T_A^t$. That is because those posteriors correctly reflect the assumed data error characteristics.

# 4. Inference based on likelihood functions

I have shown that objective posterior PDFs for $T_A$ and $C_H$ can readily be derived from the data used in Fr05, a joint PDF for $(T_A^t, C_H^t)$ formed and an objective PDF for $(S^t, K_v^t)$ derived from it by effecting a transformation-of-variables, with a marginal posterior PDF for $S^{t}$ being obtained by integrating out $K_v$. By comparison, the usual Bayesian approach would be to derive PDFs for $(S^{t}, K_v^{t})$, and hence for $S^{t}$, directly from likelihood functions for $T_A$ and $C_H$ without any transformation-of-variables.

In objective Bayesian terms, it is possible to regard the posterior PDFs for $T_A^{t}$ and $C_H^{t}$ as each equating to a likelihood function corresponding to some distribution for $T_A^{o}$ or $C_H^{o}$ and a particular observation, multiplied by a prior that is noninformative for inference from the distribution concerned (Hartigan, 1965). Estimation of such likelihood functions may be practicable if a suitable family of parameterized distributions is selected and a noninformative prior for it derived. The distribution parameters can then be selected so that the product of the likelihood function and noninformative prior closely matches the relevant posterior PDF. For $C_H$ a more direct, non-Bayesian method, of deriving an approximate likelihood function can also be used, but for $T_A$ the data used in Fr05 do not provide the necessary information.

*a. Deriving a joint likelihood function for S and $K_v$ and related noninformative priors*

Normally, where – as here – estimated objective posterior PDFs for the observables are already available, or can be easily and exactly calculated, there would be no reason to derive corresponding likelihood functions and to carry out Bayesian inference using them. Rather, one would just carry out a transformation of variables to parameter space. The reason for doing so here is partly to provide insight into the nature of Bayesian inference, partly to show that sampling uniformly in the observables at the likelihood function level may not provide satisfactory results, and partly in order to present comparative, purely likelihood-based, inference results.

When employing the parameterized-distributions approach to deriving likelihood functions set out above, the matching process can be simplified by restricting the considered likelihood functions to simple transformations of standard location distributions. That is because a uniform prior is known to be noninformative for a location parameter. In such cases the required noninformative prior is simply the derivative of the transform involved, and is the Jeffreys' prior (the square root of the Fisher information matrix) (Jeffreys, 1946). The Jeffreys' prior can be thought of as a uniform sampling of Gaussian-distributed data, subsequently transformed.

With suitable choices of parameters, assigning non-central *t*-distributions to the logs of upwards-shifted versions of $T_{\mathrm{A}}$ and $C_{\mathrm{H}}$ provides likelihood functions for them that give rise, using the Jeffreys' prior, to posterior densities that are extremely close fits to the posterior PDFs for $T_{\mathrm{A}}^{\mathrm{t}}$ and $C_{\mathrm{H}}^{\mathrm{t}}$. Thus, for $C_{\mathrm{H}}$ the likelihood is chosen as

$$p_{C_H^o}(C_H^o, C_H^t)\Big|_{C_H^o} = f(t,\nu) \quad \text{where} \quad t = (\log(C_H^t + a) - b)/c \tag{9}$$

$f(t,\nu)$ being the density for a Student's *t* distribution with *v* degrees of freedom. Here, (a,b,c,*v*) are selected to minimize the sum of squared differences between the actual PDF for $C_{\mathrm{H}}^{\mathrm{t}}$ and the fitted PDF derived by multiplying the parameterized likelihood function by the corresponding noninformative Jeffreys' prior, $\pi_{C_H}^J$. That prior can be seen, upon differentiating, to be the reciprocal of the argument of the log, here the sum of the parameter value and a positive constant (the shift).

$$\pi_{C_H}^J \propto \frac{\partial t}{\partial C_H^t} \quad = \frac{1}{C_H^t + a} \tag{10}$$

As a check on the objective validity of the calculated noninformative priors, PDFs were computed from the estimated likelihood functions (in which this reciprocal factor does not appear) both using Bayes' theorem with the Jeffreys' priors and directly, by sampling randomly from the appropriate *t*-distribution and then exponentiating and shifting the samples. Figure 3 shows that both ways of deriving posterior PDFs for $T_A$ and $C_H$ give such close approximations to the PDF to be matched that the three PDFs are visually indistinguishable. The relevant likelihood functions are also shown (cyan lines). The PDFs are each shifted leftwards relative to, and at the right are slightly better constrained than, the corresponding likelihood functions. That is consistent with each prior being monotonically declining with its parameter value. The variation in each prior reflects the fact that, as the parameter value varies, the likelihood function measures density at the fixed value of the observation, while the posterior measures density at the varying value of the parameter.

In the case of $C_H$ only, the underlying data error distributions are available, providing likelihood functions for ΔOHC and $\Delta T_{G,}$ and – since these are assumed independent – upon their multiplication for (ΔOHC, $\Delta T_G$). A frequentist profile likelihood can then be obtained for $C_H$ by taking, at each $C_H$ value, the maximum across all ΔOHC and $\Delta T_G$ combinations whose quotient equals that $C_H$ value (as is done in the Frame et al, 2014, corrigendum). Profile likelihood is a pragmatic approach that typically provides a reasonable, although not exact, likelihood (Pawitan, 2001). The profile likelihood for $C_H$ closely matches the likelihood obtained from fitting a shifted log-*t* distribution: the likelihoods have indistinguishable modes and shapes apart from the profile likelihood being fractionally wider. For consistency, the likelihoods derived from the shifted log-*t* distribution fits are used for both $C_H$ and $T_A$ in carrying out the Bayesian inference discussed next.

*b. Bayesian inference for S based on likelihood functions for $T_A$ and $C_H$*

Having derived likelihood functions for $T_A$ and $C_H$, Bayes' theorem can now be validly applied to derive marginal posterior PDFs for $S$ based on various joint prior distributions. In particular, it is of interest to consider the following: a uniform joint prior distribution in $S$ and $K_v$; a joint prior equivalent to a uniform initial distribution in $T_A$ and $C_H$; and a computed noninformative prior. Doing so requires conversion of the joint likelihood function and of the noninformative prior – formed by multiplication, given the assumption of conditional independence of $T_A$ and $C_H$ – from $(T_A, C_H)$ to $(S, K_v)$ space. Since likelihood functions do not change upon reparameterisation, their values are simply restated in terms of $(S, K_v)$ coordinates, by interpolating between EBM simulation runs. The joint prior for $(T_A, C_H)$ must additionally be multiplied by the applicable Jacobian determinant: noninformative Jeffreys' priors convert from one parameterization to another using the standard method of converting PDFs on a transformation of variables.

The resulting shape of the noninformative Jeffreys' prior in $(S, K_v)$ space is shown in Figure 4. It is very highly peaked in the low $S$, low $K_V$ corner, and has an extremely small value (slightly higher at very low $K_V$ values) when $S$ is high. The idea that a prior having such a shape *a priori* assumes an upper bound on climate sensitivity, or discriminates against high sensitivity values, is mistaken. A valid noninformative prior asserts nothing about the value of the parameters concerned. Rather, it primarily represents how informative the data are expected to be about the parameters in different regions of parameter space. That depends both on how responsive the data are to variations in parameter values in different parts of parameter space and on how precise the data are in the corresponding parts of data space. Here, the responsiveness of the combined data variables $(T_{\mathrm{A}}, C_{\mathrm{H}})$ to the parameters $(S, K_{\mathrm{v}})$ is reflected in the Jacobian determinant shown in Figure 1, while the declining precision of the data variables as $(S, K_{\mathrm{v}})$ – and hence $(T_{\mathrm{A}}, C_{\mathrm{H}})$ – increase is reflected in the joint noninformative prior for inference in $(T_{\mathrm{A}}, C_{\mathrm{H}})$ space being the product of reciprocals of the shifted data variables.

It may be asked why parameter values falling in a range in which observed quantities are fairly insensitive to parameter changes should be considered improbable relative to the data likelihood value – be down weighted by the noninformative prior having a low value – simply for that reason. The answer is that unless posterior probability is scaled down relative to likelihood in such a parameter-range, more probability will be assigned to parameter values within it than corresponds to the probability of the quantities that have been observed having resulted from such parameter values, given their assumed error distributions. Viewing probabilities in terms of CDFs rather than densities makes this clear. For example, if what is observed varies linearly with the climate feedback parameter $\lambda$, the reciprocal of $S$, and thus is insensitive to $S$ at high $S$ levels, then provided that $\lambda$ can be estimated sufficiently accurately to put a positive lower bound $\lambda_L$ on it at an acceptable confidence level, $S$ can be constrained above at $1/\lambda_L$ with the same confidence. However, one should be aware that the magnitude of an objective-Bayesian posterior PDF reflects how responsive the observed quantities are to parameter changes in various parameter-ranges as well as to how likely it was the observed values would be obtained given each possible parameter value combination. In strongly affected cases care should therefore be taken in interpreting objective-Bayesian posterior PDFs, but the uncertainty ranges derived from them are nevertheless valid.

Marginal posterior PDFs for $S$ derived on the selected bases from the joint likelihood function for $T_A$ and $C_H$ are shown in Figure 5. The black line uses the Jacobian determinant to convert the joint posterior PDF for $T_A$ and $C_H$ into a joint posterior PDF for $S$ and $K_v$, as in Figure 2. The red line shows the result of applying Bayes' theorem to the joint likelihood function for $T_A$ and $C_H$ using the Figure 4 noninformative prior, which gives an objective Bayesian posterior PDF. The green line is the published Fr05 PDF stated to be based on a uniform initial distribution in TCR. These three posterior PDFs are almost identical. Indeed, the black and red line PDFs would be identical in the absence of discretization errors. The identity of these two PDFs confirms that the highly peaked Figure 4 noninformative prior does not convey an initial assumption that $S$ is very low, but rather has the shape required to achieve objective inference about $S$.

The coral line in Figure 5 assumes a uniform initial distribution in TCR/attributable warming and effective heat capacity, using the same weighting method as for the green line, but weighting $S$ values by the joint likelihood function for $T_A$ and $C_H$ rather than by their joint posterior density. That is, carrying out Bayesian inference using a uniform joint prior for $T_A$ and $C_H$, or sampling uniformly in the observables. The form of the prior used corresponds to that in Figure 1 rather than Figure 4. The resulting PDF is significantly worse constrained above than are the black, red and green PDFs. The reason is that, although assuming a uniform joint prior in $T_A$ and $C_H$ effectively incorporates the Jacobian determinant factor necessary for correctly converting a joint density in $(T_A, C_H)$ space to one in $(S, K_v)$ space, it does not also provide a noninformative joint prior for $T_A$ and $C_H$ in their own space.

If errors in estimating $T_A$ and $C_H$ were Gaussian, $t$-distributed or otherwise independent of the values of those variables, so that $T_A$ and $C_H$ themselves were location parameters, uniform priors in $(T_A, C_H)$ space would be noninformative for those variables and their resulting objective posterior PDFs would have the same shapes as their likelihood functions. In such a case, sampling uniformly in the observables would provide an objective Bayesian posterior PDF for $(S, K_v)$. However, since the fitted *t*-distribution applies to log transforms of $T_A$ and $C_H$, suitably shifted, a uniform prior is not noninformative, the likelihood functions for $T_A$ and $C_H$ are not identical to their objective posterior PDFs and sampling uniformly in the observables does not provide an objective posterior PDF for $(S, K_v)$. In effect, the log transforms reflect multiplicative elements in the estimation errors for $T_A$ and $C_H$.

The dashed grey line in Figure 5 is the same as the grey line in Figure 2, and is shown for the purposes of comparison. The blue line shows the posterior PDF resulting from applying Bayes' theorem to the joint likelihood function for $T_A$ and $C_H$ using a uniform joint prior in $S$ and $K_v$. It is substantially worse constrained even than the dashed grey PDF, since the latter effectively employs noninformative priors for inferring posterior PDFs for $T_A$ and $C_H$ from their likelihoods whereas the blue line does not.

Although under a subjective Bayesian approach all the prior distributions considered here are in principle acceptable, it would be incorrect to argue – based on deriving a climate sensitivity PDF using a prior that samples uniformly in $S$ and $K_v$ – that we cannot from the data available rule out high sensitivity, high heat uptake cases that are consistent with, but nonlinearly related to, 20th century observations. All high sensitivity, high heat uptake cases would have given rise to an increase in ocean heat content that is inconsistent with observations at a high confidence level, and so can logically be ruled out (with the implication that use of a uniform in $S$ and $K_v$ prior is inappropriate).

*c. Profile likelihood inference for S*

Figure 5 also shows, in cyan, confidence intervals (CIs) for *S* derived by employing the frequentist signed-root-likelihood-ratio (SRLR) profile likelihood method on the joint likelihood for $T_A$ and $C_H$, restated in $(S, K_v)$ coordinates. Only a box plot is shown, since profile likelihoods are not comparable with PDFs. The SRLR method, which depends on an asymptotic normal approximation to the probability distribution involved, provides CIs for individual parameters from their joint likelihood function. The method is exact in cases involving a normal distribution or a transformed normal distribution. Unlike objective Bayesian approaches, it does not require computation of a noninformative prior. The SRLR method was employed in Allen et al. (2009). That study used exactly the same approach as set out here, of carrying out many EBM simulations and comparing their results with estimates of $T_A$ and $C_H$. However, it used parameterized lognormal distributions for those variables rather than estimating actual distributions, correctly calculating therefrom the likelihood functions required for its profile likelihood inference.

Credible intervals from the objective Bayesian PDF for *S* derived from the posterior PDFs for $T_A$ and $C_H$, using the standard method for converting PDFs on a transformation of variables – shown by the black box plot in Figure 5 – may properly be used to judge profile likelihood SRLR-derived CIs, since the posterior PDFs for $T_A$ and $C_H$ are objectively and exactly derived from the original data used as the basis for inference. Although the SRLR method gives CIs that correspond fairly closely to credible intervals implied by the posterior PDFs for $(T_A, C_H)$, the correspondence is not exact. The peak of the profile likelihood closely matches the median of the objective Bayesian posterior PDF. However, the distances from there to the 5% and, particularly, 95%

bounds are somewhat smaller when using the SRLR method. Part of the difference may be due to the fitted shifted log-*t* distributions not being exact. But most of it likely relates to the shapes of the posterior PDFs for $T_A$ and $C_H$ being best matched by transforming *t*-distributions with modest degrees of freedom (10 for $T_A$, 17 for $C_H$), which is consistent with neither of those PDFs closely corresponding to a transform of a normal distribution.

An illuminating comparison between profile likelihood and Bayesian inference based on various priors, including Jeffreys' prior, in a case corresponding to that in Allen et al. (2009) is given in Rowlands (2011), which also contains other analyses of relevance. It found nearer identity between profile likelihood derived CIs and Bayesian credible intervals derived using Jeffreys' prior than here. Since the SRLR profile likelihood method is based on a normal approximation, it performs very well where the likelihood functions are normal or (as in Rowlands, 2011) transformed normal distributions. Where data–parameter relationships are strongly nonlinear and/or data uncertainties have unsuitable forms, a simple SRLR method may not always provide acceptably accurate CIs. In such cases one of the various modified versions of the SRLR method may be employed in order to improve accuracy (see, e.g., Cox and Reid, 1987). Modified profile likelihood based inference has close links to objective Bayesian inference, and often gives results closely corresponding to those from objective Bayesian marginal posterior PDFs (Bernardo and Smith, 1994, Section 5.5 and Appendix B.4).

# 5. Discussion

The various methods for estimating climate sensitivity from the data used in Fr05 and the resulting estimates are summarised in Table 1. Using objective methods and with the ΔOHC error corrected, a median estimate of 2.2 K and 5–95% bounds of 1.2–4.5 K (uncorrected: 2.4 K and 1.2–5.2 K) are obtained using the transformation-of-variables method, based on the initial, objective Bayesian, posterior PDFs for $T_A$ and $C_H$. Although this estimate is objective given the data, the data it reflects are somewhat dated and may have shortcomings. For instance, Gillett et al. (2012) found that using (as in this case) temperature data spanning just the twentieth century, the first two decades of which were anomalously cool, produced a high estimate for attributable warming, which would bias estimation of *S* upwards. However, the main object of this paper is to illustrate the relative effects of various methods of inference for climate sensitivity, which are unaffected by such bias.

Since the best estimated PDF for a parameter value does not depend on the use to which that estimate is put (Bernardo and Smith, 1994, Section 3.4 and Bernardo, 2009), one should use the same prior assumptions for estimating climate sensitivity irrespective of for what purpose the resulting PDF is used. Differing loss functions associated with differing purposes may lead to the same probabilistic estimate then being used in different ways.

Most climate sensitivity studies have embodied a subjective Bayesian perspective, in which probability represents a personal degree of belief as to uncertainty and prior distributions represent subjective assumptions of the investigators. However, for scientific reporting, it is usual to assume no prior information as to the value of unknown parameters being estimated in an experiment. To achieve that using Bayesian methods, a "noninformative" prior distribution must be mathematically derived from the assumed statistical model. That corresponds to an objective Bayesian approach, results from which, like frequentist results, depend only on the assumed model and the data obtained (Bernardo, 2009). A proposal for adapting the objective Bayesian approach to allow for incorporation of probabilistic prior information, represented as if derived from data, is set out in Lewis (2013a).

In cases where a prior that is noninformative for inference about the observables is easily identified, and the observables are independent (or can be transformed to be independent, as by whitening in optimal fingerprint methods), an objectively-correct joint posterior PDF for the observables may be derived and hence, via a transformation of variables, a joint posterior PDF for the parameters computed. In many cases it may be easier to adopt an objective Bayesian approach by performing Bayesian inference in observation-space and then effecting a transformation of variables, than by deriving a noninformative joint prior for the parameters. The climate model simulations that are generally performed can be used to convert the joint posterior PDF from observation space to parameter space through a transformation of variables. The objectivity of the inference procedure may be more obvious with such a two stage procedure than when the parameters are inferred directly from the observables' likelihoods using Bayes' theorem with a highly non-uniform noninformative prior. And in some cases, as here, the available data more readily provides objective posterior PDFs for the observables than accurate likelihood functions for them, so the use of a transformation of variables approach is particularly advantageous.

The transformation of variables approach can be employed even where the model used is not deterministic, provided a location parameter relationship applies between actual and true observables, since the effects of model noise on simulated observables and measurement error plus internal climate variability on actual observables are then equivalent. Where, as in the case considered here, the dimensionality of the observables and the parameters is the same, the PDF conversion factor is the absolute Jacobian determinant. The transformation of variables approach should produce an equivalent result to computing a noninformative joint prior for the parameters (Lewis, 2013b).

If there are more observables than parameters, a dimensionally-reducing transformation of variables PDF conversion formula may be used, after whitening the observables. To facilitate doing so, it may be possible to transform individual observable variables having non-Gaussian (e.g., lognormal) uncertainty so that their distributions are at least approximately Gaussian, although transformations estimated from data are themselves uncertain.

Whether objective Bayesian inference is undertaken using a transformation of variables approach or not, it should be appreciated that the prior or PDF conversion factor is a function of all parameters (here $S$ and $K_v$) jointly: it does not vary with the parameter of interest alone.

Objective Bayesian methods are not a universal, perfect solution to the issue of quantifying uncertainty or the only objective approach to estimating climate sensitivity. Nor, when there are multiple parameters, is Jeffreys' prior always the best noninformative prior to use for marginal parameter inference (see, e.g., Bernardo and Smith, 1994, Sections 5.4 and 5.6). There is always merit in reporting likelihood functions and prior distributions as well as posterior PDFs, which enables the effect of the prior to be seen, and in appropriate cases exploring the effects of different prior distributions may be helpful. Exploring data error assumptions, which affect the shape of noninformative priors used for objective Bayesian inference as well as the likelihood functions, is also advisable.

Profile likelihood methods of varying complexity offer a viable objective alternative to Bayesian methods where likelihood information about sensitivity jointly with other climate system parameters is obtained. The basic SRLR profile likelihood method has the advantage of being simpler to apply than objective Bayesian approaches, but may be less accurate. It is worth undertaking even if Bayesian methods are used, as it provides a cross-check on uncertainty bounds given by Bayesian credible intervals. That profile likelihood only provides CIs is not a real drawback, since – if one accepts the Bayesian paradigm although not its methods – a PDF may be obtained by computing one-sided CIs at all values of *S* and differentiating. However, for many purposes the combination of a best estimate (50th percentile or likelihood peak) and uncertainty ranges may provide as much useful information as a PDF does, and is less susceptible to misinterpretation.

Whatever method of inference is used, there are many other subjective choices to be made, such as the observables, datasets, error distribution assumptions and model which will all affect the results. But the objective Bayesian approach does offer a solution to the issue of the relevant prior to use when estimating climate sensitivity.

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FIG. 3: Posterior PDFs and likelihood functions for attributable 20th century warming $T_A$ and effective heat capacity $C_H$. The overlying black, red and green lines show PDFs respectively calculated as set out in Section 2, derived by sampling from the shifted log-t distributions and derived by multiplying the estimated likelihood function by the related Jeffreys' prior, applying Bayes' theorem. The cyan lines show the estimated likelihood functions. The Fr05 version of $C_H$, which does not correctly match the OHC and $T_G$ data, has been used in order to give a like-for-like comparison with Fr05.

FIG. 4: Noninformative (Jeffreys') joint prior for $S$ and $K_v$ for inference from $T_A$ and $C_H$ likelihoods. The much sharper peak in the low climate sensitivity, low effective ocean diffusivity corner and lower values elsewhere than in Figure 1 reflects the fact that the observational data is most precise in the region that corresponds to that corner of parameter space and becomes increasingly less precise away from it, in addition to the responsiveness of the observations to changes in the parameters reducing as they move away from the low climate sensitivity, low effective ocean diffusivity corner. When performing Bayesian inference about the parameters from $T_A$ and $C_H$ likelihoods, rather than using the objective estimated PDFs for their true values and undertaking a transformation of variables to parameter space, a noninformative prior will reflect that declining precision in addition to the Jacobian determinant applicable to the transformation of variables.

FIG. 5. Estimated marginal PDFs for climate sensitivity derived on various bases. The match between the overlying black and red lines shows that the conversion of the joint posterior PDF for the observables into a PDF for the parameters $S$ and $K_v$ by a transformation of variables using the Jacobian determinant, giving the black line, and objective Bayesian inference from the combined likelihood functions for $T_A$ and $C_H$ using

the Figure 4 noninformative prior, giving the red line, are equivalent. The coral line shows that assuming a uniform initial distribution in the observables does not give the same result. The blue line shows how poorly the PDF is constrained when an informative, subjective, uniform prior in the parameters is used. Two other PDFs are given for comparison. The green line is the same as the dashed green line in Figure 2. The (dashed) grey line is the same as the grey line in Figure 2. The box plots indicate boundaries, to the nearest grid value, for the percentiles 5–95 (vertical bar at ends), 10-90 (box-ends), and 50 (vertical bar in box), and allow for off-graph probability lying between *S* = 10 K and *S* = 20 K. The cyan box plot shows confidence intervals derived by a profile likelihood method (the vertical bar in the box showing the likelihood profile peak).

**Table 1.** Summary of different methods of estimating climate sensitivity from the data Fr05 used (with the ΔOHC error uncorrected unless otherwise stated) and their results

| Method of estimating climate sensitivity ($S$) and color of corresponding PDF line and box plot in Figure 5 where relevant | Median (K) | 5–95% range (K) |
|---|---|---|
| *Bayesian estimation based on sampling uniformly in terms of* ($S$,$K_v$)*: blue*<br>Sample joint ($T_A$,$C_H$) likelihood uniformly in terms of corresponding ($S$,$K_v$) values (equating to Bayesian inference using uniform priors in $S$ and $K_v$). | 3.5 | 1.6–15.1 |
| *What Fr05 actually did when sampling uniformly in terms of* ($S$,$K_v$)*: grey*<br>Derive (posterior) PDFs for $T_A$ and $C_H$, express their joint PDF in terms of the corresponding ($S$,$K_v$) values, sample it uniformly in terms of ($S$,$K_v$). | 2.9 | 1.4–12.6* |
| *Transformation of variables from joint posterior PDF for $T_A$ and $C_H$: black*<br>Transform joint posterior PDF for ($T_A$,$C_H$) into one for ($S$,$K_v$), using the Jacobian. [Fr05 effectively did this when sampling uniformly in ($T_A$,$C_H$)] | 2.4 | 1.2–5.2 |
| *Bayesian estimation based on sampling uniformly in terms of ($T_A$,$C_H$): coral*<br>Derive likelihoods for $T_A$ and $C_H$, sample their joint likelihood uniformly and transform to ($S$,$K_v$) space using the Jacobian | 2.6 | 1.4–6.5 |
| *Objective estimation of S from likelihoods for $T_A$ and $C_H$*<br>*a) Bayesian: red*. Express joint likelihood for ($T_A$,$C_H$) in terms of corresponding ($S$,$K_v$) values, multiply it by derived noninformative prior and sample uniformly in terms of ($S$,$K_v$) to obtain their joint posterior PDF.<br>*b) Frequentist: cyan*. Express joint likelihood for ($T_A$,$C_H$) in terms of the corresponding ($S$,$K_v$) values, compute a profile likelihood for $S$ and obtain confidence intervals from the signed log-likelihood ratio. | 2.4<br><br>2.4 | 1.2–5.2<br><br>1.3–4.8 |
| *What an objective Bayesian estimate for S using the correctly matched ΔOHC and Δ$T_G$ data would have been* | 2.2 | 1.2–4.5 |
| *The Frame et al (2014) corrigendum's estimate for S when using uniform priors in S and $K_v$ and correctly matched ΔOHC and Δ$T_G$ data* | n/a | 1.2–14.5 |

For consistency, all computations using the uncorrected ΔOHC data are based on the fitted parameterized distributions. Integration out of $K_v$ from the joint ($S$,$K_v$) posterior to obtain a marginal posterior for $S$ is taken as read.

* As is evident from Figure 2, this range differs somewhat from the range given in Fr05; the 95% bound is extremely sensitive to the total probability included in the calculation.

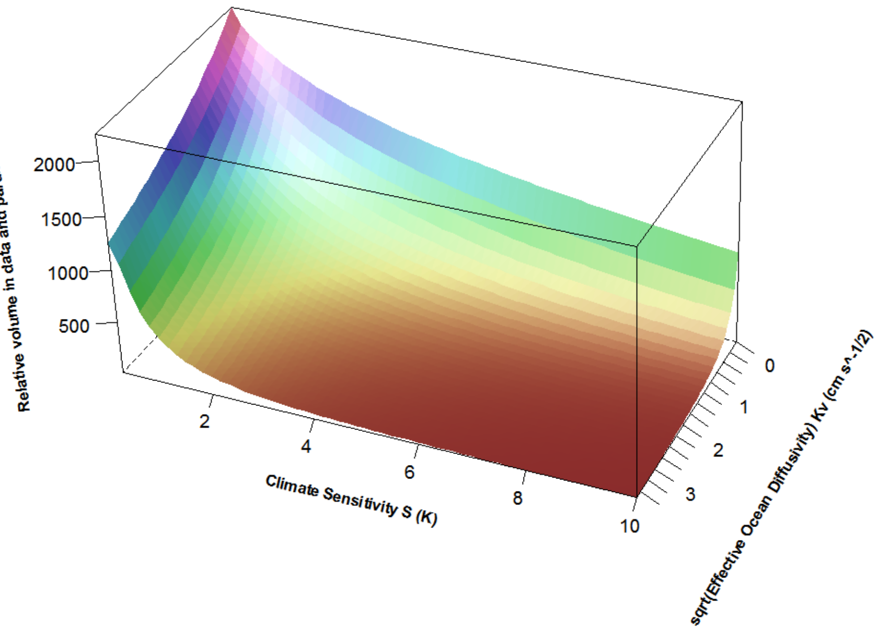


FIG. 1. Absolute Jacobian determinant of the transformation from $(S^{\mathrm{m}}, K_{\mathrm{v}}^{\mathrm{m}})$ to $(T_{\mathrm{A}}^{\mathrm{m}}, C_{\mathrm{H}}^{\mathrm{m}})$ space. Its value, the scale of which is arbitrary, represents the volume of the region in $(T_{\mathrm{A}}^{\mathrm{m}}, C_{\mathrm{H}}^{\mathrm{m}})$ space relative to that of the region in $(S^{\mathrm{m}}, K_{\mathrm{v}}^{\mathrm{m}})$ space to which it corresponds. The large values in the low climate sensitivity, low effective ocean diffusivity corner reflects high joint responsiveness there of attributable 20th century warming $T_{\mathrm{A}}$ and effective heat capacity $C_{\mathrm{H}}$ to changes in the parameters $S$ and $K_{\mathrm{v}}$. The converse is the case towards the opposite corner of parameter space.

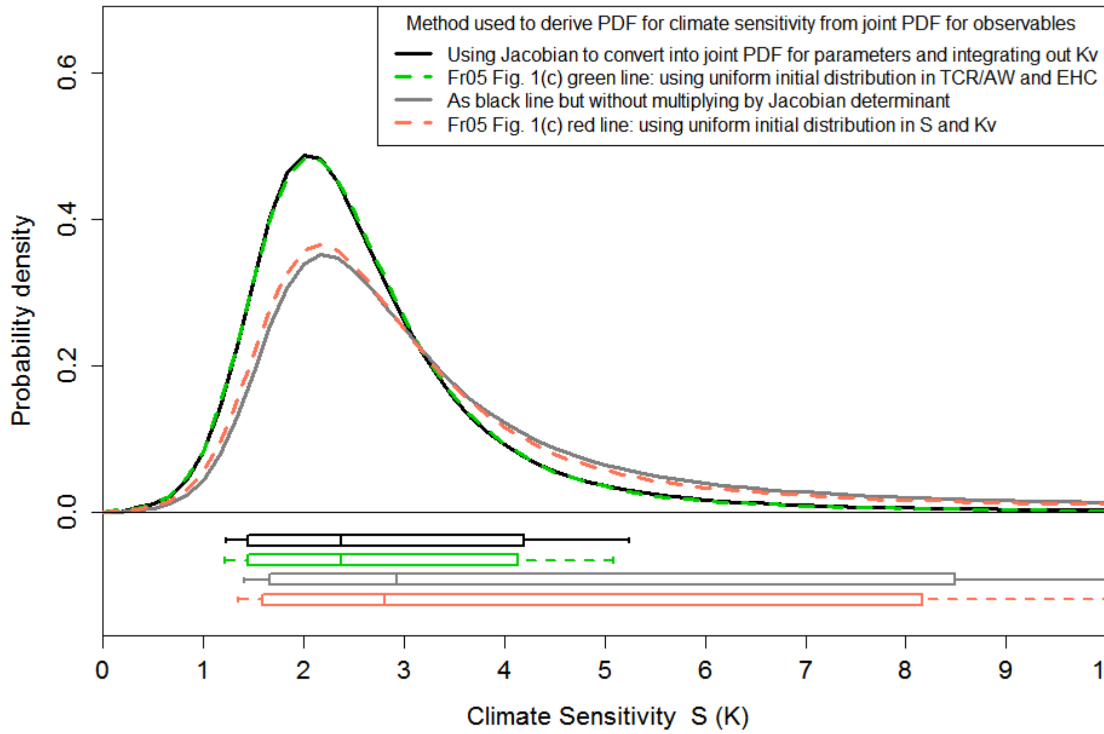


FIG. 2. Estimated marginal PDFs for climate sensitivity, after integrating out $K_{\mathrm{v}}$. The black line is derived by transforming the posterior PDF for the observables, $(T_{\mathrm{A}}^{\mathrm{t}}, C_{\mathrm{H}}^{\mathrm{t}})$, to one for $(S^{\mathrm{t}}, K_{\mathrm{v}}^{\mathrm{t}})$, using the Jacobian determinant. The near identical (dashed) green line is reproduced from Figure 1(c) of Fr05, where it is stated to assume a uniform initial distribution in TCR (and implicitly in $C_{\mathrm{H}}$). The grey line is computed by restating, in terms of $(S, K_v)$, the posterior PDF for $(T_{\mathrm{A}}^{\mathrm{t}}, C_{\mathrm{H}}^{\mathrm{t}})$, without multiplication by the Jacobian determinant, and renormalizing. The (dashed) coral line reproduces the red line in Fr05 Figure 1(c), stated there to be based on assuming a uniform initial distribution in sensitivity, shifted to the right by 0.083 K to correct an apparent plotting error in the Fr05 code. The two uncorrected Fr05 Figure 1(c) PDFs do not accurately reflect the stated intentions of its authors; they are shown to demonstrate that this study's computations

match those in Fr05. The box plots indicate boundaries, to the nearest grid value, for the percentiles 5–95 (vertical bar at ends), 10-90 (box-ends), and 50 (vertical bar in box), and allow for off-graph probability lying between $S$ = 10 K and $S$ = 20 K.

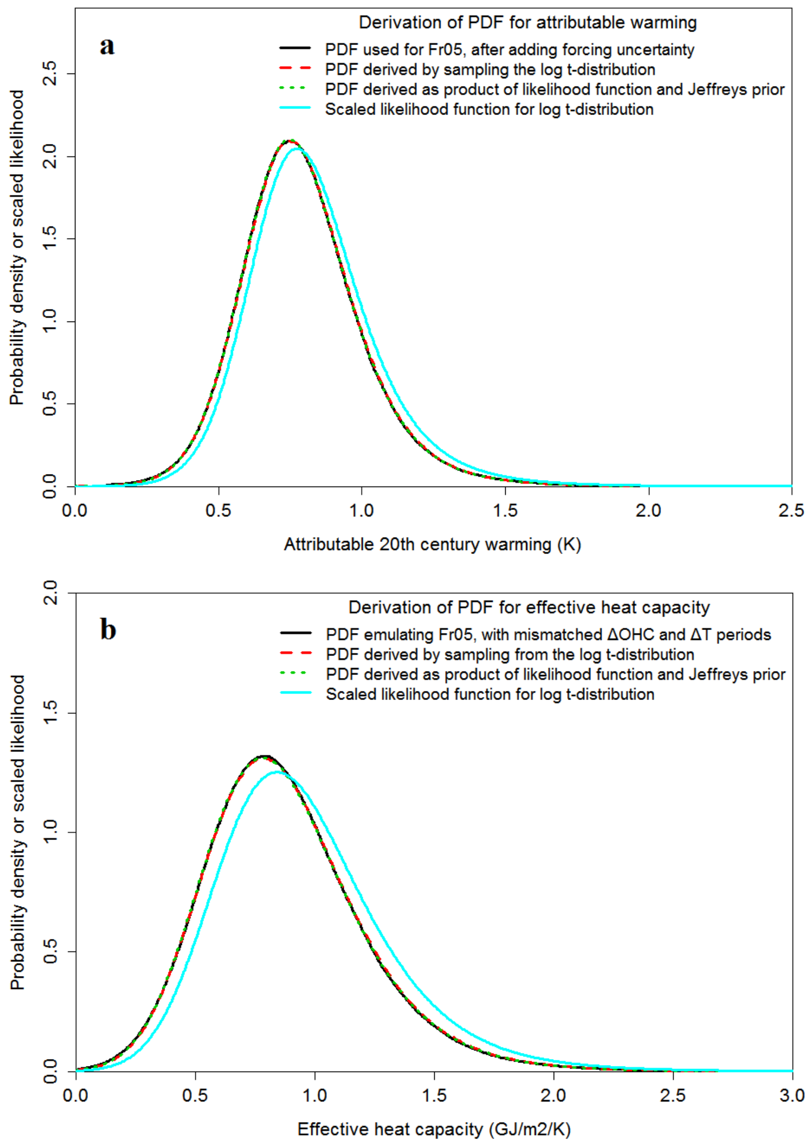


FIG. 3: Posterior PDFs and likelihood functions for attributable 20th century warming $T_A$ and effective heat capacity $C_H$. The overlying black, red and green lines show PDFs respectively calculated as set out in Section 2, derived by sampling from the shifted log-t

distributions and derived by multiplying the estimated likelihood function by the related Jeffreys' prior, applying Bayes' theorem. The cyan lines show the estimated likelihood functions. The Fr05 version of $C_H$, which does not correctly match the OHC and $T_G$ data, has been used in order to give a like-for-like comparison with Fr05.

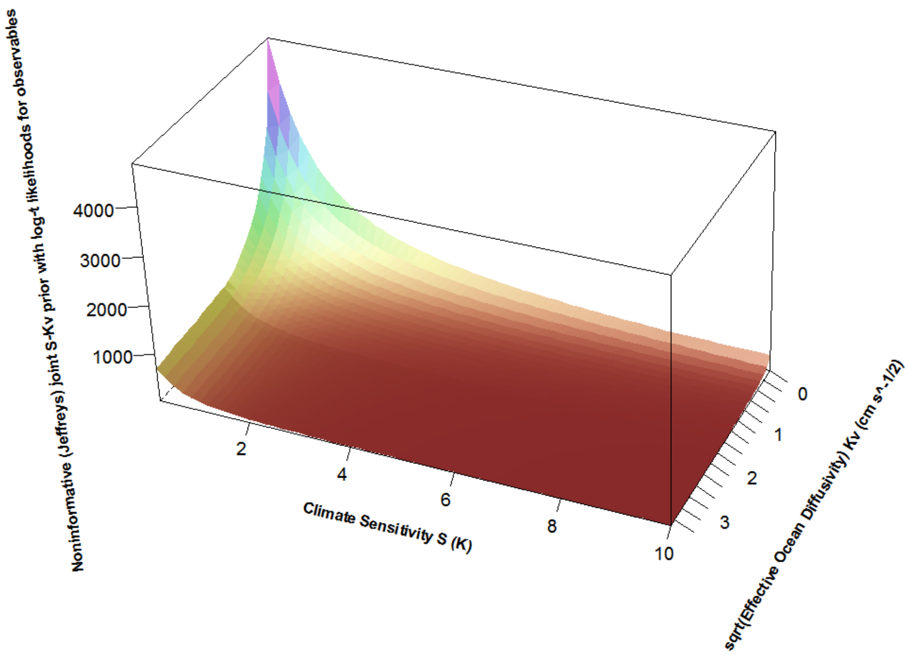


FIG. 4: Noninformative (Jeffreys') joint prior for $S$ and $K_v$ for inference from $T_A$ and $C_H$ likelihoods. The much sharper peak in the low climate sensitivity, low effective ocean diffusivity corner and lower values elsewhere than in Figure 1 reflects the fact that the observational data is most precise in the region that corresponds to that corner of parameter space and becomes increasingly less precise away from it, in addition to the responsiveness of the observations to changes in the parameters reducing as they move away from the low climate sensitivity, low effective ocean diffusivity corner. When performing Bayesian inference about the parameters from $T_A$ and $C_H$ likelihoods, rather than using the objective estimated PDFs for their true values and undertaking a

transformation of variables to parameter space, a noninformative prior will reflect that declining precision in addition to the Jacobian determinant applicable to the transformation of variables.

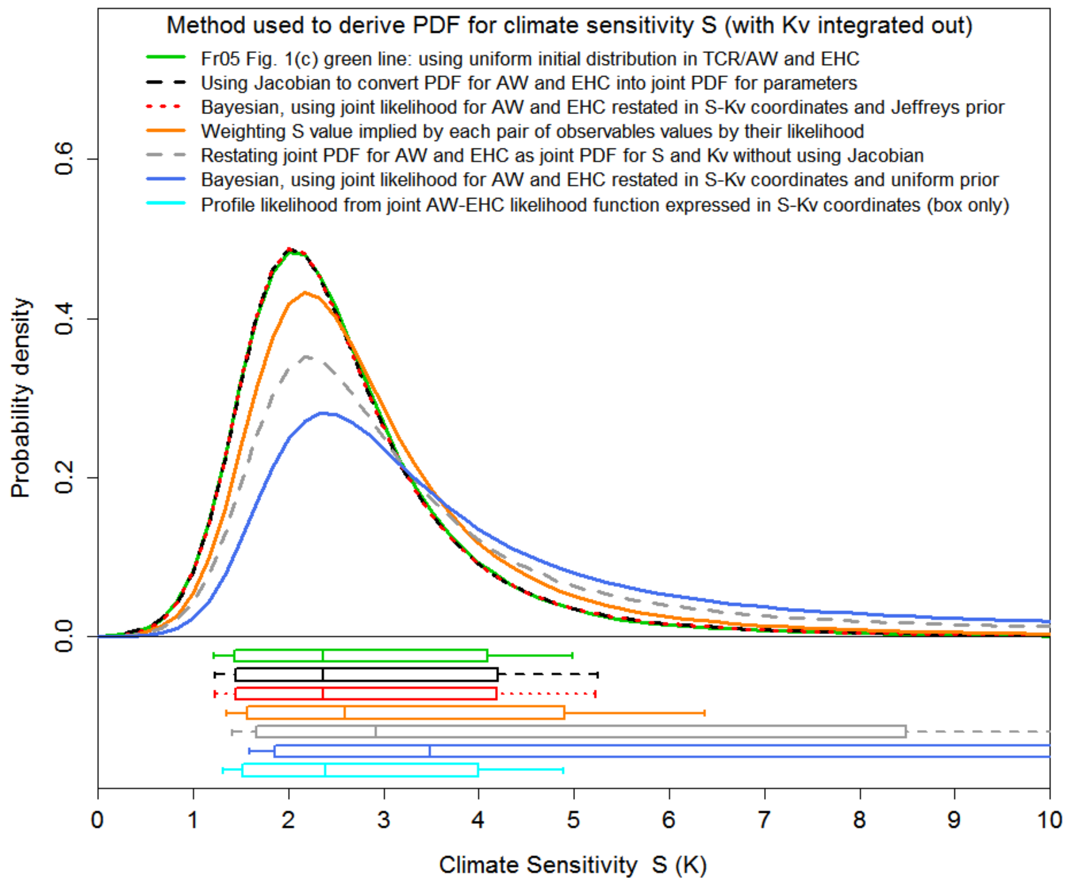


FIG. 5. Estimated marginal PDFs for climate sensitivity derived on various bases. The match between the overlying black and red lines shows that the conversion of the joint posterior PDF for the observables into a PDF for the parameters *S* and $K_v$ by a transformation of variables using the Jacobian determinant, giving the black line, and objective Bayesian inference from the combined likelihood functions for $T_A$ and $C_H$ using the Figure 4 noninformative prior, giving the red line, are equivalent. The coral line

shows that assuming a uniform initial distribution in the observables does not give the same result. The blue line shows how poorly the PDF is constrained when an informative, subjective, uniform prior in the parameters is used. Two other PDFs are given for comparison. The green line is the same as the dashed green line in Figure 2. The (dashed) grey line is the same as the grey line in Figure 2. The box plots indicate boundaries, to the nearest grid value, for the percentiles 5–95 (vertical bar at ends), 10-90 (box-ends), and 50 (vertical bar in box), and allow for off-graph probability lying between $S$ = 10 K and $S$ = 20 K. The cyan box plot shows confidence intervals derived by a profile likelihood method (the vertical bar in the box showing the likelihood profile peak).