Ancient TL

www.ancienttl.org · ISSN: 2693-0935

Peng, J. and Dong, Z., 2014. *A simple Bayesian method for assessing the standard error of equivalent dose estimates.* Ancient TL 32(2): 17-23. https://doi.org/10.26034/la.atl.2014.480

A simple Bayesian method for assessing the standard error of equivalent dose estimates

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(Received 8 August 2014; in final form 17 November 2014)

Abstract

Estimating the equivalent dose (ED) value is critical to obtaining the burial dose for Optically Stimulated Luminescence (OSL) dating. In this study, a simple Bayesian method is used to assess the standard error of an ED value in a linear or an exponential model. An ED value is treated as a stochastic node that depends on a random variable whose posterior distribution can be constructed and sampled. The results show that the Bayesian approach may improve the precision of an ED estimate by avoiding the repeated curve-fitting procedure employed in the routine "parametric bootstrap" Monte Carlo method.

Key words: Bayesian method; Markov chain Monte Carlo; equivalent dose; standard error

Introduction

In the commonly adopted single aliquot regenerative-dose (SAR) protocol (Murray and Wintle, 2000; Murray and Wintle, 2003), the standardized natural OSL signal is projected onto the growth curve that is constructed using a series of sensitivity-corrected regenerative OSL signals to calculate the corresponding ED value. A maximum likelihood method was used by Yoshida et al. (2000) to fit the growth curve with an exponential-plus-linear model in which the true ED value was treated as an unknown parameter, and the standard error of the ED value was estimated through the profile likelihood function. However, this method may result in unreliable estimates (Yoshida et al., 2003) as the number of points is not many more than the dimension of the problem under consideration (Galbraith and Roberts, 2012). This problem led Yoshida et al. (2003) to use a "parametric bootstrap" method to simulate and fit a number of growth curves repeatedly to obtain a more reliable estimate of the standard error of an ED value. Duller (2007a) gave a detailed introduction about how to estimate an ED value and outlined two protocols (i.e. simple transformation and Monte Carlo simulation) to assess its standard error. Berger (2010) outlined methods that incorporate the contribution of errors from the characteristic parameters of a growth curve and their covariances to estimate standard errors of ED values. Classic numeric techniques such as non-linear parameter optimization and interpolation are routinely employed in these procedures (Peng et al., 2013). In this study, a simple Bayesian method was constructed to estimate ED values and their standard errors using measured datasets. The Gibbs sampler ***WinBUGS*** (Lunn et al., 2013) was employed to perform the Bayesian Markov chain Monte Carlo sampling, and the estimates were compared to those assessed using the ***Analyst*** software (Duller, 2007b).

Methods

We use x_i and y_i to denote the *i-th* regenerative dose and measured standardized (i.e. sensitivity corrected) OSL, respectively, for each of the *i=1 to n* observations. A saturating exponential growth curve may be described as:

$$\hat{y}_i = a(1 - e^{-bx_i}) + c \qquad \textbf{(Eqn. 1)}$$

where $\hat{y}_i$ denotes the *i-th* fitted standardized OSL and *a,b,c* are parameters to be optimized. Here *a* is the saturation level (maximum value) of the standardized OSL, *b* is the reciprocal of the saturation dose, and *c* is an offset accounting for potential "recuperation" effects. Let y_0 and x_0 denote the natural standardized OSL and the corresponding ED value respectively. An estimate of the ED value can be obtained by inversing Eqn. 1 analytically:

$$x_0 = -\frac{\ln[(a - y_0 + c)/a]}{b} \qquad \textbf{(Eqn. 2)}$$

Eqn. 2 is justified only if $a + c > y_0$, that is, the natural standardized OSL y_0 must not exceed the saturation level of the growth curve. It should be noted that even if the natural standardized OSL y_0 is close to (but does not exceed) the saturation level, the randomly selected quantity $Y_0 \sim N(y_0, \sigma_0)$ (see below) may exceed the maximum due to random errors controlled by its standard error σ_0. For this reason, it is best to ensure that the dose to be estimated does not exceed the double value of the saturation dose (Wintle and Murray, 2006).

Software ***Analyst*** (Duller, 2007b) employs the Levenberg-Marquardt algorithm to estimate the parameters of a saturating exponential growth curve. Once the parameters are determined, an ED value can be calculated with Eqn. 2 or an interpolation procedure using the natural standardized OSL. The "parametric bootstrap" Monte Carlo method that assesses the standard error of the ED value involves fitting the growth curve and calculating the ED value repeatedly using random natural and regenerative standardized OSL signals simulated from normal distributions whose widths are determined by the relevant standard deviations (see Duller, 2007a for details). In the following part, we derive a simple alternative that avoids the repeated fitting process needed in the routine Monte Carlo procedure for obtaining the sampling distribution of an ED value of a saturating exponential growth curve using the Bayesian approach. The ED value whose distribution is determined is treated as a stochastic node that depends on parameters whose sampling distributions can be simulated via a Markov chain Monte Carlo method.

Firstly, note that it is possible to reduce the dimension of the problem under consideration to contain only parameter b via a linear algebraic method (Peng et al., 2013), just as that used in deconvolution of decay curves in previous studies (Bluszcz, 1996; Bluszcz and Adamiec, 2006). Let w_i be the weight of y_i . For a number of observations and a given b value, parameter a can be calculated as:

$$a = \frac{\sum_{i=1}^{n} w_i \sum_{i=1}^{n} w_i (1-e^{-bx_i}) y_i - \sum_{i=1}^{n} w_i (1-e^{-bx_i}) \sum_{i=1}^{n} w_i y_i}{\sum_{i=1}^{n} w_i \sum_{i=1}^{n} w_i (1-e^{-bx_i})^2 - [\sum_{i=1}^{n} w_i (1-e^{-bx_i})]^2}$$

(Eqn. 3)

Similarly, parameter c can be determined by:

$$c = \frac{\sum_{i=1}^{n} w_i y_i - a \sum_{i=1}^{n} w_i (1-e^{-bx_i})}{\sum_{i=1}^{n} w_i}$$

(Eqn. 4)

In a weighted nonlinear least-squares estimation we wish to minimize $\chi^2 = \sum w_i (y_i - \hat{y}_i)^2$, where the weight w_i are equal to $1 / \sigma_i^2$. The estimates obtained with a least-squares estimation will be identical to those given by a maximum likelihood estimation if we suppose that each of the *i-th* regenerative standardized OSL is independent of the others and follows a normal distribution with mean $\hat{y}_i$ and standard error σ_i, i.e., $y_i \sim N(\hat{y}_i, \sigma_i)$. Note that $\hat{y}_i$ is the model based (fitted) standardized OSL and σ_i is the standard error (based on photon counting statistics and measurement error) for the measured y_i. Combining Eqn. 1, 3 and 4, we can treat $\hat{y}_i$ as a function of the observations (x_i, y_i, w_i) and parameter b, which we denote as $\hat{y}_i = F(x_i, y_i, w_i, b)$. *prob(x,y,w|b)* is the probability for observing the standardized OSL signals y with fixed weights w at doses x if the reciprocal saturation dose has the value of b, it can be written as:

$$prob(x, y, w \mid b) = \prod_{i=1}^{n} \frac{\sqrt{w_i}}{\sqrt{2\pi}} e^{\frac{-w_i [y_i - F(x_i, y_i, w_i, b)]^2}{2}}$$

(Eqn. 5)

Similar to Eqn. 5, *prob*(b|x,y,w) is the probability that b has a given value if the observations are *x,y,w,* and it is called the posterior distribution of b. From Eqn. 1-5, it can be seen that if one is able to simulate a random variable b based on its posterior distribution, then variables *a, c, x_0* can be regarded as stochastic nodes that depend on the value of b. According to Bayes' theorem (Sivia, 1996), the posterior distribution of b under condition of the observed values is:

$$prob(b \mid x, y, w) \propto \text{pr}ob(x, y, w \mid b) prob(b)$$

(Eqn. 6)

prob(b) is the so-called prior of b, and if it follows a uniform distribution (i.e. *prob(b)* is a constant), then sampling a random variable b from its posterior distribution is equal to sampling a b value according to the joint-likelihood function determined by Eqn. 5. A good choice for the prior of b is the uniform distribution $U(0,1)$, which is equal to 1 for all values of b between 0 and 1, and 0 for all other values.

This simulation can be easily performed with a general Markov chain Monte Carlo sampler, in our case the software ***WinBUGS*** (Lunn et al., 2013). ***WinBUGS*** requires as input (1) the measured values (x,y,w), (2) the model (i.e. Eqn. 1), (3) the prior distribution for the parameter to be simulated, in our case $U(0,1)$ for parameter b, (4) Eqn. 3-4 to reduce the dimension of the model, and (5) Eqn. 2 to allow calculation of the node x_0. The software creates automatically a random b value according to Eqn. 5. Parameters a, c depend on the value of b (see Eqn. 3-4). They are the by-product of the simulation and are regarded as nodes. By using randomly generated natural standardized OSL values $Y_0 \sim N(y_0,\sigma_0)$ and the nodes a and c, the sampling distribution of ED values (i.e. x_0) can be monitored according to Eqn. 2. That means the distributions of these quantities can be obtained iteratively, i.e. each time a value of b is generated and the values of a and c are calculated, and the value of the ED can be monitored. After a large number of simulations, we can infer statistical quantities such as the mean, the median, the standard deviation, and the 95% confidence interval of these parameters. There are certain benefits to reduce the dimension of the problem to contain only one independent variable. Firstly, this makes the posterior distribution of b be mainly dominated by the likelihood function and the prior is almost irrelevant, as a number of data points are used to simulate only one parameter. Another advantage of reducing the dimension lies in that it facilitates the sampling process. The Gibbs sampler may fail to converge and the generated samples may have poor mixing properties if there are many quantities that need to be sampled, as parameters in this model are highly correlated with each other.

The same methodology would apply to a linear growth curve by setting the slope as the independent variable and treating the intercept and ED value as nodes that depend on the value of the slope. Also, the procedure may be modified to apply to a quadratic growth curve. However, this method is inapplicable to an exponential plus linear model, as this model cannot be inversed analytically as $x = f^{-1}(y)$ and software ***WinBUGS*** does not have a standard function to do interpolation of this kind.

Results of Comparisons and Discussions

Measured datasets from 35 aliquots of samples GL1-1 and 36 aliquots of sample GL1-2 (Peng and Han, 2013) were analyzed. Decay curves of these two samples have variable OSL intensities (Peng et al., 2014). The net OSL intensity was calculated using integration of the first 0.64s after subtracting background from the last 50 channels in a decay curve. The standard error of the sensitivity-corrected OSL was based on counting statistics and a measurement error of 2%. Datasets from sample GL1-1 and GL1-2 were fitted with a saturating exponential and a linear growth curve, respectively. We compared the estimates derived from the Bayesian method outlined above using software ***WinBUGS*** (version 1.4.3) with the results of the "parametric bootstrap" Monte Carlo method described by Duller (2007a) using software ***Analyst*** (version 4.12). Software ***WinBUGS*** was called in batch model via the package ***R2WinBUGS*** (version 2.1-19) (Sturtz et al., 2005) for the ***R*** statistical software so that datasets can be easily loaded and analyzed. The outputs are summary statistics (the mean, the standard deviation, the 95% confidence interval, etc.) for the relevant parameters of the growth curve and the desired ED value. Scripts for running the models are presented in the supplementary. In software ***Analyst***, the number of Monte Carlo iterations was set equal to 1,000. In software ***WinBUGS***, each dataset was simulated through 50,000 iterations and the posterior inference was based on 8,000 iterations. As is common procedure with these types of simulations the initial 10,000 iterations were discarded ("burn-in") and every 5-th iteration was retained ("thinning"). The kernel density plots of the parameters derived from the exponential model simulation for an aliquot of sample GL1-1 are shown in Figure 1. Related trace plots of the variations of parameters and ED value with the number of iterations are shown in Figure 2. The unimodal and symmetric distribution pattern (Figure 1) and good mixing property (Figure 2) demonstrated in the simulated b value (also shown in the ED value) indicate that the simulation appears to converge. To test the program we also attempted to fit an exponential model to a number of linear growth curves. Our analysis suggests that for a growth curve that is linear or approximately linear, the sampling distribution of the saturating OSL (i.e. parameter a) may seem to be very inhomogeneous and highly variable if an exponential model is applied. But even in this case, the posterior of b and the resultant ED values can still converge to a unimodal distribution.

Figure 3 (A-B) shows a linear growth curve for an aliquot of sample GL1-2 and an exponential growth curve for an aliquot of sample GL1-1 that are fitted using the Bayesian approach. A comparison of ED values and their standard errors estimated using the "parametric bootstrap" Monte Carlo method and the simple Bayesian method is presented in Figure 3 (C-F). A paired two-tailed t-test with a 1% significance level is used to test the significance of difference between the results of the two methods. For datasets from sample GL1-1 that are fitted with an exponential model, the t-values calculated using the difference of ED values and the difference of errors of ED values are 0.16 and 5.06, respectively,

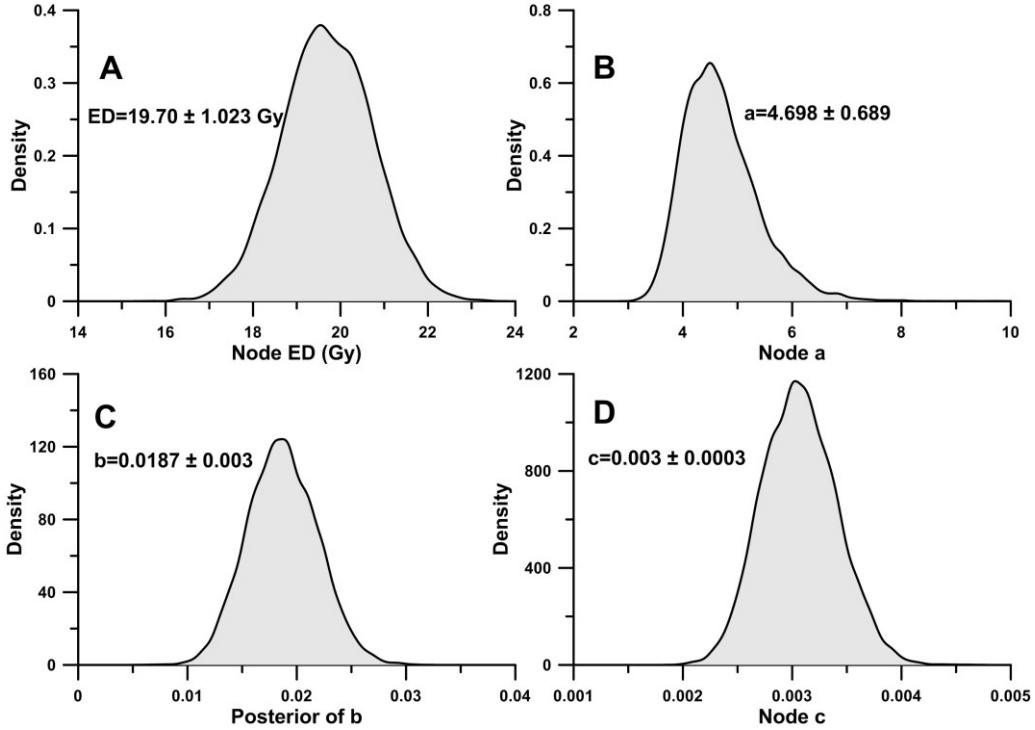

Figure 1: *Kernel density plots for the ED value and characteristic parameters of a saturating exponential growth curve using an aliquot from sample GL1-1. Each plot is drawn using 8,000 samples. The plots show unimodal distributions. Note: The density values plotted on the y-axis should not be confused with probability distributions and can have values larger than 1.*

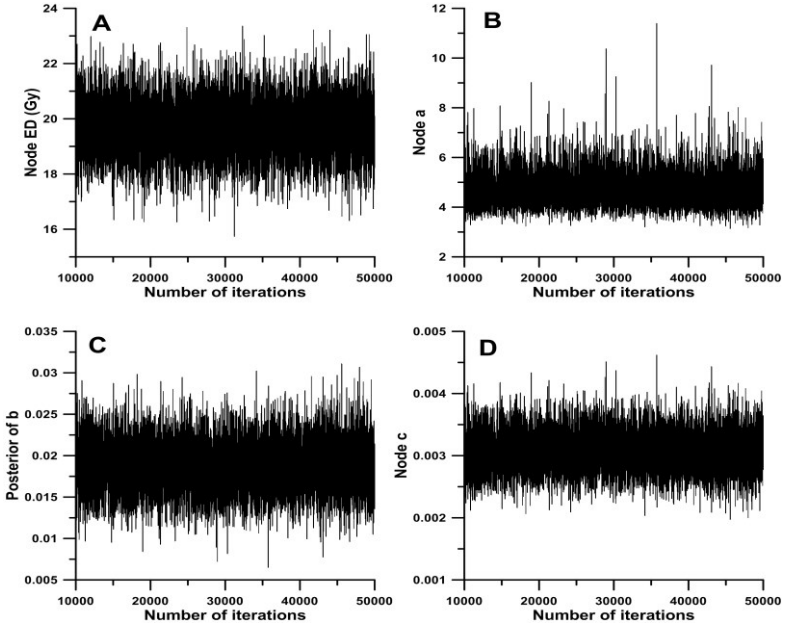

Figure 2: *Variations of simulated ED values and characteristic parameters with the number of iterations in an exponential model for an aliquot from sample GL1-1. Each plot is drawn using 8,000 samples. Throughout the simulation variables are evenly spread over their feasible spaces, reflecting good mixing properties.*

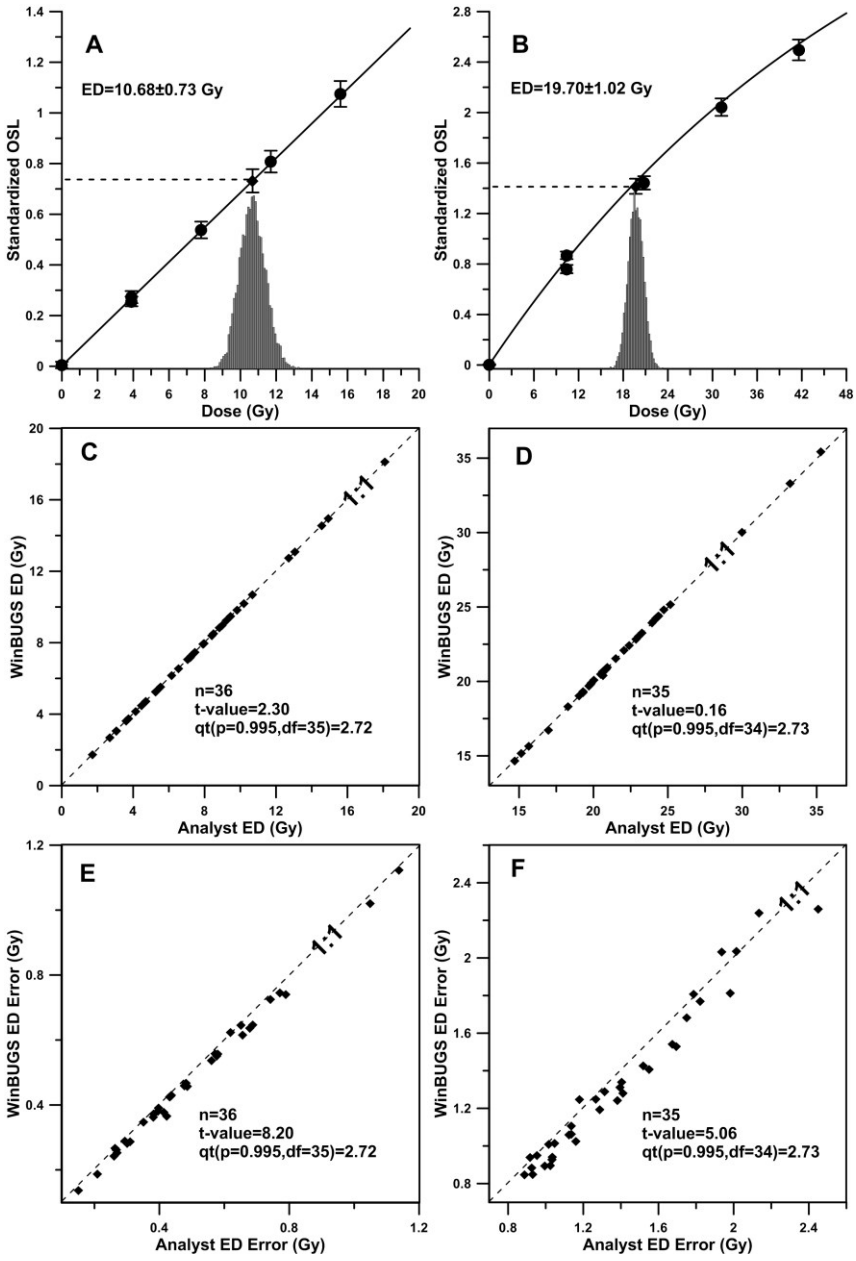

Figure 3: *A linear growth curve for an aliquot of sample GL1-2 (A) and an exponential growth curve for an aliquot of sample GL1-1 (B) that are fitted using the Bayesian method. C and D: Comparisons of ED values obtained using the Monte Carlo method and the Bayesian method for samples GL1-2 and GL1-1, respectively. E and F: Comparisons of standard errors of ED values assessed using the Monte Carlo method and the Bayesian method for samples GL1-2 and GL1-1, respectively.*

and the critical t-value is 2.73. This demonstrates that there is no significant difference between the two sets of ED values, but there are obvious differences between the standard errors at a significance level of 1%. Similar results are found in estimates from sample GL1-2 that have a theory t-value of 2.72. ED values estimated using the two different methods are comparable, though the ED value estimated by software ***Analyst*** is based on solely the natural standardized OSL while the ED value obtained from the Bayesian method is the mean value of all resulting samples in node ED. This consistency may result from the fact that software ***Analyst*** assigns unequal weights to the observations using inverse

variances so the shape of the resultant growth curve is akin to that fitted by a maximum likelihood estimation using Eqn. 5. However, it turned out that for the analyzed aliquots almost all standard errors of ED values assessed by the Bayesian method using software ***WinBUGS*** are smaller than that estimated by the "parametric bootstrap" Monte Carlo method using software ***Analyst***, though in general the differences are small. The uncertainties arising from photon counting statistics (Galbraith, 2002; Li, 2007; Adamiec et al., 2012; Galbraith, 2014), the instrument reproducibility (Truscott et al., 2000; Thomsen et al., 2005), and the growth-curve fitting error (Jacobs et al., 2006; Duller, 2007a) are the three major source of uncertainties involved in estimating an ED value. The differences of errors between the two methods cannot be caused by the first two sources of error that influence the uncertainty of the standardized OSL if the same dataset is analyzed. For a Monte Carlo method in which growth curves are simulated and fitted repeatedly, bias is introduced in each iteration. But the Bayesian method in which the ED value is treated as a node that depends on a single variable that can be sampled from its posterior distribution avoids the curve-fitting process and may result in a reduction in the standard error of an ED estimate hence an improvement in precision.

A predominate advantage of the simple Bayesian protocol is that a user need not pay much attention to the initialization of parameters, unlike that encountered when applying a classic nonlinear method (Peng et al., 2013). Another benefit of the Bayesian method is the flexibility with which posterior inferences can be summarized (Gelman et al., 2013). The Bayesian approach outlined above can be modified to be more flexible to obtain more variable ED distributions. McCoy et al. (2000) observed that individual grains of quartz exhibit log-norm distributions in their OSL intensities. Thus a log-norm distribution may be assumed for the standardized OSL (Yoshida et al., 2003) when simulating an ED value. Whether normal or log-normal distributions are assumed will make little difference if the uncertainty of a sensitivity-corrected OSL is relatively small (Galbraith and Roberts, 2012). It is also possible to specify the standardized OSL to have constant relative uncertainty (i.e.$\sigma_i = ky_i$), then the estimate will be equal to that given by a weighted nonlinear least-squares method with weights $1/y_i^2$ if we ignore the common constant (Thompson, 2007). Moreover, if few outliers are presented in a number of data points, the standardized OSL may be assumed to follow a heavily-tailed distribution (say, the *t*-distribution) so that outliers can be accommodated. Additionally, in all the preceding analysis, we have implicitly assumed that the regenerative dose values are known exactly. But in fact, this assumption may be far from the truth as the precision of a given dose is instrument-dependent. If the associated error-bars for the x-coordinate are not known, then we may perform the simulation by assuming that they have constant relative uncertainty, say, 1% or 2%, and the resultant ED values will be more variable in this way. However, it should be noted that the sensitivity of the model to the imposed assumptions needs to be carefully checked, and that any conflict between the assumptions and the data may crash the simulation or result in absurd posteriors within a Bayesian framework. It is essentially the user's responsibility to ensure that the resulting posterior distribution is correct when special priors or assumptions are assumed.

Conclusion

A simple Bayesian approach is used to estimate ED values and assess their standard errors for a linear and a saturating exponential growth curve. The resulting ED values are comparable to those obtained by a weighted nonlinear least-square fit. This method avoids the repeated curve-fitting procedures required by the "parametric bootstrap" Monte Carlo protocol in error assessments, and may result in an improvement in the precision of an ED value.

Acknowledgments

We would like to thank Dr Regina DeWitt for improving the language of this manuscript. Comments by Dr Regina Dewitt have substantially improved the manuscript. This work was funded by the Ministry of Science and Technology of the People's Republic of China (2013CB956000).

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Reviewer

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