Quaternary Geochronology 28 (2015) 62–70

Contents lists available at ScienceDirect

Quaternary Geochronology

journal homepage: www.elsevier.com/locate/quageo

Research paper

A Bayesian central equivalent dose model for optically stimulated luminescence dating

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ARTICLE INFO

Article history:
Received 10 March 2014
Received in revised form
27 March 2015
Accepted 1 April 2015
Available online 2 April 2015

Keywords:
Optically stimulated luminescence
Chronometric dating
Bayesian analysis

ABSTRACT

In this study, we propose and implement a Bayesian model to estimate a central equivalent dose from a set of luminescence measurements. This model is based on assumptions similar to the ones used in the standard statistical pipeline (typically implemented in the Analyst software followed by a subsequent central equivalent dose analysis) but tackles some of its main limitations. More specifically, it consists of a three-stage hierarchical model that has two main advantages over the standard approach: first, it avoids the introduction of auxiliary variables (typically mean and variance), at each step of the inference process, which are likely to fail to characterise the distributions of interest; second, it ensures a homogeneous and consistent inference with respect to the overall model and data. As a Bayesian model, our model requires the specification of prior distributions; we discuss such informative and non-informative distributions and check the relevance of our choices on synthetic data. Then, we use data derived from Single Aliquot and Regenerative (SAR) dose measurements performed on single grains from laboratory-bleached and dosed samples. The results show that our Bayesian approach offers a promising alternative to the standard one. Finally, we conclude by stressing that, relying on a Bayesian hierarchical model, our approach could be modified to incorporate additional information (*e.g.* stratigraphic constraints) that is difficult to formalise properly with the existing approaches.

1. Introduction

Radiometric dating methods generally rely on the observation of a time-varying physical quantity. However, in most cases these observations are noisy and sometimes ambiguous or even contradictory. The development of procedures to deal with such datasets and to produce suitable easy-to-interpret results is therefore essential. In such a context, Bayesian approaches are particularly suited and have already been applied for example to radiocarbon (Buck et al., 1991), electron spin resonance (Millard, 2006b), thermo-luminescence (Millard, 2006a) and uranium series (Millard, 2006a) data.

In this paper, we propose to deal with Optically Stimulated Luminescence (OSL, (Huntley et al., 1985)) data acquired with the Single Aliquot Regenerative (SAR) dose protocol (Murray and Wintle, 2000). Essentially, this protocol provides a set of luminescence signals together with their associated radiation doses for a given grain or set of grains called an **aliquot**. Obtaining an age from these data involves linking these paired datasets through a **dose–response function** in order to estimate the individual **equivalent dose** (for each aliquot, this is the laboratory dose equivalent to that accumulated since the last luminescence signal resetting event - typically exposure to daylight, *i.e.* the laboratory dose inducing the same OSL signal as that induced by the natural dose). For a given sample whose luminescence signal was well reset before burial, it is common to analyse a large set of aliquots from which a single equivalent dose is ultimately estimated together with a confidence interval. This characteristic equivalent dose is defined through a statistical model; different models can be used, from the simplest one, a plain average of individual equivalent doses, to more sophisticated ones such as the common equivalent dose model or the central equivalent dose model (see (Galbraith et al., 1999; Galbraith and Roberts, 2012) for a review of the most commonly used equivalent dose models). The age of sediment deposition can then

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http://dx.doi.org/10.1016/j.quageo.2015.04.001
1871-1014/

be obtained by dividing the characteristic equivalent dose by the average environmental dose rate received by the grains.

In practice, the statistical analysis of such data is not an easy task. Indeed, many sources of dispersion in the data (*e.g.* luminescence measurement errors, reproducibility of the instrument) interact with each other and some of them are shared by different variables of the problem. A standard procedure to deal with this interdependency consists in sequentially propagating the uncertainties using classical rules of combination or through Monte-Carlo methods (Duller, 2007) and, in a final step, in estimating a maximum likelihood characteristic equivalent dose together with a confidence interval that is then converted into an age using the environmental dose rate. In this article, this approach is referred to as the standard approach (a technical and critical review is provided in Section 2).

In our opinion, the complexity of the previously described data model naturally calls for a hierarchical decomposition through a Bayesian formalism as an alternative to the standard approach. Indeed, such a hierarchical decomposition leads to a complete model relating all the variables to one another, to produce a homogeneous and consistent inference. By contrast, because the standard approach decomposes the global inference into a set of consecutive assessments, it is likely to lead to a significant loss of information at each step of the process, and can result in an inference of limited coherency with respect to the original data.

Some Bayesian models for OSL dating (Sivia et al., 2004; Zink, 2013) have already been proposed. However, these models did not include the assessment of the individual equivalent doses but focused on determining a characteristic equivalent dose or age from already assessed individual or central equivalent doses. In our opinion, individual equivalent dose assessment is one of the most critical aspects of the statistical processing as it relates most of the experimental variables (individual equivalent doses, measured luminescence signals and dose–response curves) to one another through non-linear terms, leading to complex probability distributions. Moreover, all tasks have to be merged into a single model encapsulating all the statistical relationships in order to lead to a fully informative inference. Following this approach, Huntriss (Huntriss, 2007) proposed a Bayesian model including the overall process but through modelling choices impractical for applications to the dating of Quaternary sediments (a discussion is provided in Section 2.3).

In the present paper, we follow a similar approach but based on choices dedicated to the dating of Quaternary sediments. The resulting Bayesian model can be used to infer a central equivalent dose from the observed luminescence signals of a set of aliquots. Then, we use measurements performed on single grains from laboratory-dosed samples to validate this model; we observe that it provides better accuracy and robustness than those provided by the standard approach (summary in Figs. 3 and 5).

The outline of this paper is as follows: In Section 2, we present the standard approach to estimate a central equivalent dose together with a confidence interval from luminescence measurements acquired through the SAR protocol. This approach is typically implemented in the Analyst software (Duller, 2001) followed by a central equivalent dose analysis, or in the R package for luminescence analysis (Kreutzer et al., 2012). In this section, we underline the potential weaknesses of this approach and try to isolate the hypotheses it relies on. In Sections 3 and 4, we present our Bayesian model based on hypotheses similar to the ones used in the standard approach. In Section 5, we validate a Markov Chain Monte-Carlo sampler for our posterior density and we compare, using experimental data, the standard and the Bayesian approach. Finally, in Section 6, we stress the differences between our approach and the standard one and give some perspectives to improve the ability of the Bayesian model to deal with wider hypotheses.

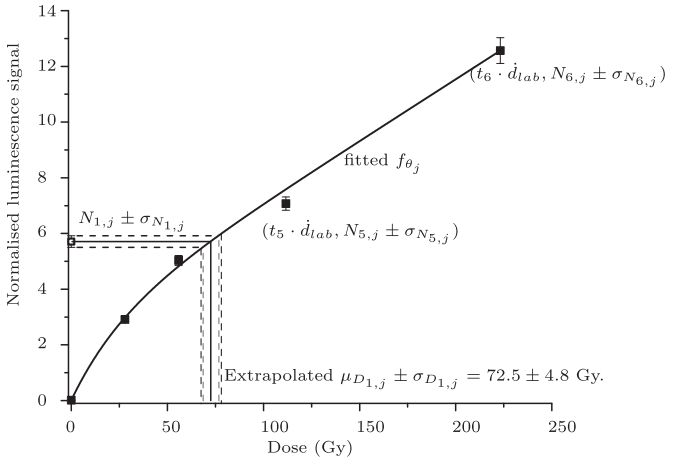

Fig. 1. Illustration of the individual equivalent dose assessment (Step 1) obtained with the Analyst software (modified to include our notations): For a given aliquot j, the dose–response function f_{θ_j} with $f_{\theta_j=(a_j,b_j,c_j,d_j)} : \mathcal{D}_{k,j} \mapsto a_j \left(1 - \exp\left(\frac{-(\mathcal{D}_{k,j}-d_j)}{b_j}\right)\right) + c_j \mathcal{D}_{k,j}$ is fitted in the least-squares sense into the pairs $(t_{k,j} \cdot \dot{d}_{lab}, N_{k,j})_{k \geq 2}$ so that $N_{1,j}$ can be used to estimate the mean $\mu_{\mathcal{D}_{1,j}}$ and standard deviation $\sigma_{\mathcal{D}_{1,j}}$ of the individual equivalent dose $\mathcal{D}_{1,j}$. The vertical grey dashed lines represent the standard deviation $\sigma_{\mathcal{D}_{1,j}}$ estimate accounting only for the measurement standard deviations $(\sigma_{N_{k,j}})_{k \in [1:K]}$ while the vertical black dashed lines represent the estimate by also taking account of the goodness of the fit.

2. Existing approaches

In this section, we first introduce the SAR acquisition protocol used to measure the normalised luminescence signals (Section 2.1). Then, we detail and discuss the standard statistical approach to produce a single central equivalent dose together with a confidence interval from a set of luminescence measurements (Section 2.2). Finally, we discuss an already existing Bayesian approach (Section 2.3).

2.1. The SAR acquisition process

A key concept in luminescence dating is that of **equivalent dose** (denoted $\mathcal{D}_{1,j}$). For a given grain or set of grains, usually called an aliquot (denoted j), it is the laboratory dose needed to generate a luminescence signal equivalent to the measured **normalised natural luminescence** (denoted $N_{1,j}$).

To evaluate the equivalent dose characteristic of an aliquot j using the SAR protocol, one generates a sequence of **normalised regenerated luminescence** signals (denoted $N_{k,j}$, $k \geq 2$) for different known laboratory doses - called **regenerative doses**, $\mathcal{D}_{k,j} = t_{k,j} \cdot \dot{d}_{lab}$, $k \geq 2$ ($t_{k,j}$ being the irradiation time and $\dot{d}_{lab}$ the dose-rate of the laboratory source). Then these paired data $(\mathcal{D}_{k,j}, N_{k,j})_{k \geq 2}$ can be used in a calibration step to determine the equivalent dose $\mathcal{D}_{1,j}$ from the natural normalised luminescence $N_{1,j}$. How this determination is typically dealt is detailed in the next subsection.

In practice, the normalised luminescence signals $(N_{k,j})_{k \in [1:K], j \in [1:J]}$ are defined as the ratio of a luminescence signal $L_{k,j}$ corresponding to the regenerated or natural delivered dose $\mathcal{D}_{k,j}$ and of a luminescence signal $T_{k,j}$ corresponding to a constant test dose. This normalisation by the response to a fixed test dose is needed to monitor sensitivity changes throughout the measurement sequence (Murray and Wintle, 2000). Given the two signals $L_{k,j}$ and $T_{k,j}$, an empirical estimate of the mean experimental noise $B_{k,j}$ and the instrument reproducibility error F_e (Thomsen et al., 2005; Jacobs et al., 2006), one can compute the measured