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A further note on the variance of a background-corrected OSL count

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Abstract

Galbraith (2002) gave formulae for calculating the relative standard error of a background-corrected optically stimulated luminescence (OSL) count. This note extends those formulae to the case where the number of channels used to estimate the background is not necessarily a multiple of (and may indeed be less than) the number used to estimate the signal. The theoretical formulae are unchanged, but the estimate of the background is expressed in a more general notation and I comment further on how the Poisson over-dispersion may be estimated. I will use the same notation as in Galbraith (2002) and will repeat enough of the text there for this note to be self-contained.

Derivation

The usual scenario is as follows. Optical stimulation of an aliquot of quartz produces a series of counts —a number of recorded photons for each of N equal length consecutive time intervals (channels). The optically stimulated luminescence (OSL) "signal" is measured from the total count in the first n channels minus an estimate of the contribution to this count from "background" sources, which here are taken to include all sources other than the signal to be estimated. The background emission rate is assumed to be constant over the whole period used, and is estimated from counts later in this period, where the contribution from the signal is assumed to be negligible.

Mathematically, the above may be expressed as follows. Let y_i denote the OSL count from channel i, for i = 1, 2, ..., N, and let $Y_0 = y_1 + y_2 + ... + y_n$ be the total count over the first n channels. Write

$$Y_0 = S_0 + B_0$$

where S_0 and B_0 are the contributions to Y_0 from the signal (or source of interest) and background respectively. Of course S_0 and B_0 are not observed directly. Assume that S_0 and B_0 are independent random quantities with expectations μ_S and μ_B , and variances σ_S^2 and σ_B^2 , respectively. Then the

observed count Y_0 will have expectation $\mu_S + \mu_B$ and variance $\sigma_S^2 + \sigma_B^2$. An estimate of the signal μ_S is thus obtained by subtracting an estimate of μ_B from Y_0 , i.e.,

$$\hat{\mu}_S = Y_0 - \hat{\mu}_B$$

We want to calculate the relative standard error of this estimate. An estimate of μ_B is usually obtained from the formula

$$\widehat{\mu}_B = \frac{n}{m} Y_1 = \frac{1}{k} Y_1$$

where Y_1 denotes the total count over m later channels chosen so that the mean count per channel can be assumed to equal that for B_0 , and k = m/n. It is desirable to choose m to be large enough to provide a sufficiently precise estimate of μ_B and it is convenient to choose m = nk for some integer k that is large enough to assess any over-dispersion (with respect to Poisson variation) in total background counts made over different sets of n channels. However, k need not be an integer and the data used to estimate any overdispersion need not be exactly the same as those used to estimate μ_B . Furthermore, k could be less than 1. That is, m could be chosen to be smaller than n, though the smaller m is, the less precise is the estimate of μ_B (other things being equal) and hence of μ_{S} . We here adapt the formulae of Galbraith (2002) to include this case explicitly.

Assume that all counts from individual channels that contribute to the background are independent random quantities from a distribution with mean μ_b and variance σ_b^2 . This includes the y_i s for the m channels that contribute to Y_1 as well as the unobserved counts that contribute to B_0 . Then $\mu_B = n\mu_b$ and $\sigma_B^2 = n\sigma_b^2$ and the expected value and variance of Y_1 are $m\mu_b = k\mu_B$, and $m\sigma_b^2 = k\sigma_B^2$, respectively. So $\hat{\mu}_B$ has expectation μ_B and variance

$$\operatorname{var}(\widehat{\mu}_B) = \left(\frac{1}{k}\right)^2 k \sigma_B^2 = \sigma_B^2 / k$$

Hence the variance of the estimated signal (corrected for background) is

$$\operatorname{var}(\widehat{\mu}_S) = \operatorname{var}(Y_0) + \operatorname{var}(\widehat{\mu}_B) = \sigma_S^2 + \sigma_B^2 + \sigma_B^2 / k \quad (1)$$

and the relative standard error is

$$\operatorname{rse}\left(\widehat{\mu}_{S}\right) = \frac{\sqrt{\sigma_{S}^{2} + \sigma_{B}^{2} + \sigma_{B}^{2}/k}}{\mu_{S}}$$
 (2)

These formulae agree exactly with equations (1) and (2) of Galbraith (2002). In order to calculate this relative standard error in practice, we need estimates of σ_S^2 and σ_B^2 in addition to the estimate of μ_S .

If S_0 , B_0 and Y_1 are all assumed to have Poisson distributions, then $\sigma_S^2 = \mu_S$ and $\sigma_B^2 = \mu_B$, and Equ. 1 becomes $var(\hat{\mu}_S) = \mu_S + \mu_B + \mu_B/k$, which may be estimated as $Y_0 + \hat{\mu}_B/k = Y_0 + Y_1/k^2$. Substituting these estimates into Equ. 2 gives the following estimated relative standard error:

$$\operatorname{rse}\left(\widehat{\mu}_{S}\right) \approx \frac{\sqrt{Y_{0} + Y_{1}/k^{2}}}{Y_{0} - Y_{1}/k} \tag{3}$$

This is the same as equation (3) of Galbraith (2002) with \overline{Y} replaced by Y_1/k .

If the background counts do not have a Poisson distribution, but are over-dispersed, we may write, as in Galbraith (2002),

$$\sigma_B^2 = \mu_B + \sigma^2$$

for some positive value of σ^2 to be estimated. There are several possible ways to estimate σ^2 . One is to use

$$\hat{\sigma}^2 = s_V^2 - \overline{Y} \tag{4}$$

provided that this is positive, where \overline{Y} and s_Y denote the sample mean and standard deviation of total counts for sets of n channels that contribute to Y_1 . (There are [k] such total counts, where [k] denotes the largest integer less than or equal to k.) This is the same as Equ. 4 of Galbraith (2002), but, as pointed out there, we would like an estimate based on a reasonable number of degrees of freedom, and it makes sense to obtain a pooled estimate from several different series. Such a pooled estimate of over-dispersion could be used for each series, while at the same time using separate estimates of background level.

Another method is to use

$$\hat{\sigma}^2 = n\left(s_y^2 - \bar{y}\right) \tag{5}$$

provided that this is positive, where \bar{y} and s_y denote the sample mean and standard deviation of the mcounts for single channels that contribute to Y_1 . This has the advantage of having more degrees of freedom, but the possible drawback of being based on variation between single channels rather than between sums over n channels. In theory, if the individual y_i s are independent with constant variance σ_b^2 , then sums of them over non-overlapping sets of *n* channels will be independent with variance $n\sigma_b^2$. However, in practice it is possible that the estimates based on Equ. 4 and Equ. 5 may not agree, and it is really Equ. 4 that is more relevant here. In any case, if m is small, a more reliable estimate of σ^2 may again be obtained by averaging the estimates for several series.

It is not so straightforward to obtain a corresponding estimate of σ_S^2 because the expected counts change rapidly at the start of the stimulation period. But there is perhaps a case for assuming that S_0 does have a Poisson distribution, while B_0 does not. The former comes from pure OSL emissions while the latter comes, at least partly, from other sources such as scattered light and instrument noise, which may not exhibit Poisson variation. Then we still have $\sigma_S^2 = \mu_S$ and the resulting estimated relative standard error is

$$\operatorname{rse}(\hat{\mu}_{S}) \approx \frac{\sqrt{Y_{0} + Y_{1}/k^{2} + \hat{\sigma}^{2}(1 + 1/k)}}{Y_{0} - Y_{1}/k}$$
 (6)

This is the same as equation (6) of Galbraith (2002) with \overline{Y} replaced by Y_1/k .

Further comments

Li (2007) discussed the estimation of the error variance of background-corrected OSL counts, where he distinguished between two sources of background — namely, the "slow" component of the signal and "instrumental background". On the basis of laboratory experiments, he argued that it was just the counts from the latter source that were over-dispersed with respect to Poisson variation, and furthermore that such over-dispersion would be approximately the same for all analyses that used the same instrumental conditions. He therefore advocated the use of his Equation 6, which is equivalent to equation (6) of Galbraith (2002) and Equ. 6 above, with $\hat{\sigma}^2$ obtained from appropriate laboratory experiments

and used for all analyses made under the same instrumental conditions. For his experiments, the estimate of over-dispersion based on variation between single channels was very similar to that based on variation between totals for sets of n channels.

Experiments to identify and measure specific sources of variation are to be encouraged, though it is also good practice to check that empirical estimates, such as those based on Equ. 4 or 5 or averages of them from several series, agree with those obtained from such experiments.

Finally, in practice an estimated background-corrected signal is usually divided by a similar background-corrected estimate obtained from a response to a test dose, in order to allow for a possible "sensitivity change" in the response to optical stimulation. The resulting quantity is usually denoted by L_x/T_x and its relative standard error may be calculated as the sum in quadrature of the separate relative standard errors of L_x and T_x . That is,

$$\operatorname{rse}\left(\frac{L_x}{T_x}\right) \approx \sqrt{\left[\operatorname{rse}(L_x)\right]^2 + \left[\operatorname{rse}(T_x)\right]^2}$$

where $rse(L_x)$ and $rse(T_x)$ are each given by $rse(\hat{\mu}_S)$ in Equ 6 applied to the appropriate series of counts.

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Reviewer

G.A.T. Duller

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Obituary

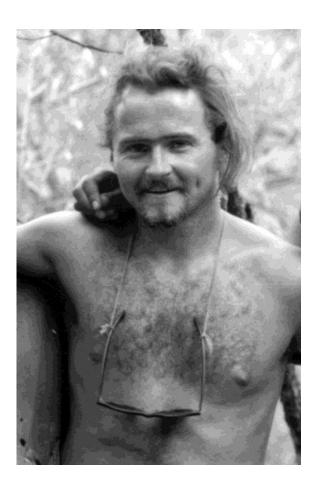
Stephen Stokes (1964-2014)

Stephen Stokes, luminescence chronologist and Quaternary scientist, passed away on Monday 24 March 2014 after a long illness at the age of 50: Stephen had been diagnosed with amyotrophic lateral sclerosis, also known as motor neurone disease.

Stephen was born in Liverpool, England, on March 17th 1964. When he was 6, his family moved to New Zealand where he surfed through school and college, undertaking his BSc and Masters under the guidance of Professor David Lowe at Waikato. His first paper, Stokes and Lowe 'Discriminant function analysis of late Quaternary tephras from five volcanoes in New Zealand using glass shard major element chemistry' was published in Quaternary Research in 1988. Stephen returned to his birth land on securing a scholarship to study at Oxford where, under the tutelage of Martin Aitken, luminescence dating pioneer, and Andrew Goudie. desert geomorphologist, he gained his D.Phil. in 1994, having worked on the application of OSL to secure new chronologies of aeolian sedimentation in the southwest USA. Crucially, he showed the evolution of US sand seas to be more complex, and spread over more accumulation phases, than had previously been widely acknowledged. His thesis also pioneered technical advances in optical dating. His love of travel, fieldwork and technical challenges meant that he often got drawn into other projects while a doctoral student. This, and his wit, is captured in his thesis acknowledgement:

"Mandela is free, Nixon is dead, Thatcher is out of office, the Soviet Union has split, England are not in the World Cup, all my friends are marrying, Cliff Richard has (finally) stopped making records, and I have two grey hairs- it must be time to finish up!"

With his abundant talent and supreme ability to inspire students, it was no surprise that he continued in the School of Geography at Oxford, first as a Departmental Demonstrator then as a University Lecturer and Fellow of St Catherine's College. He was a true scholar and academician, equally at home with the most inexperienced undergraduates and senior academics alike, never afraid to challenge established theory and the establishment, to explore ideas, and to constantly push boundaries, especially in terms of the application of luminescence dating. Stephen was the first to apply OSL to marine



sediments, and the first to take its application into various desert realms, including parts of the Sahara and Sahel, Kalahari, and Arabia. He loved to talk science- his doctoral viva was over six hours long, not because there was a problem, but because he wanted to talk. He had extremely fruitful working relationships with established academics including Gary Haynes, Ashok Singhvi and Warren Wood, but most notably with students. His outstanding lectures inspired undergraduates such as Simon Armitage, Sallie Burrough, Sarah Feakins and Abi Stone, who went on to doctorates with other supervisors and then to their own academic careers. He directly or jointly supervised the doctorates of several now-established academics, such as Morteza Fattahi, Lee Arnold, Zhongping Lai, Julie Rich and Tom Stevens, while taking on others such as Richard Bailey and Chantal Tribolo in postdoctoral positions. All owe something, and often a lot, to the catalyst that was Stephen Stokes.

In the midst of his career, Stephen Stokes envisioned a somewhat different perspective in what could be his contribution to society. He was awarded an MBA in his mid-forties and joined the private sector. He brought a refreshing new angle to the issues of environmental assessment in a world

shifting from dire exploitation to sustainable development. In 2007, he joined AMR Research (Gartner) in Boston as a business analyst. As an Oxford academic and down-to-earth thinker, he helped redefine sustainability in the whole supply chain.

Stephen authored almost 80 papers in his short academic career. Many are landmark papers in luminescence dating and its application to dune and lake sediments, to major archaeological questions, and even to dating fault movements. His last paper (to date), Singhvi, Stokes et al. 'Changes in natural OSL sensitivity during single aliquot regeneration procedure and their implications for equivalent dose determination', was published in *Geochronometria* in 2011.

In 2003, Stephen's life changed irreversibly when a woman from Montreal happened to visit Oxford. Stephen and Marie-Josée Duquette embarked on an always-surprising adventure together that included the birth of a daughter, Laurence, now 9 years old. This small family brought Stephen immeasurable joy. He is also survived by family in New Zealand and London. Stephen's life was lived to the full, it burned bright and short, and his death leaves a gap that it will not be possible to fill.

David Thomas, University of Oxford Michel Lamothe, Université du Québec à Montréal

(The text of this obituary was originally published in *Quaternary Geochronology* and is reprinted here with kind permission of the editors of that journal and Elsevier)

Submission of articles to Ancient TL

Reviewing System

In order to ensure acceptable standards and minimize delay in publication, a modification of the conventional refereeing system has been devised for Ancient TL:

Articles can be sent directly by authors to a member of the Reviewers Panel chosen on the basis of the subject matter, but who is not in any of the authors' laboratories. At the discretion of the Editor, reviewers who are not listed in the Panel may be used.

The reviewing system aims to encourage direct dialogue between author and reviewer. The Editor should be kept advised of the progress of articles under review by sending him copies of all correspondence. He is available for advice where reviewing difficulties have arisen. Authors whose mother tongue is not English are required to have their manuscript revised for English *before* submitting it.

We ask reviewers to specify (where required) the minimum of revision that is consistent with achieving a clear explanation of the subject of the paper, the emphasis being on *rapid* publication; reviewers are encouraged to make a brief written comment for publication at the end of the paper. Where a contribution is judged not to meet an adequate standard without substantial modification, the author will be advised that the contribution is not suitable for publication. Articles that are not considered to be of sufficient interest may also be rejected.

Procedures

- Articles should be submitted to an appropriate member of the Reviewing Panel or Editorial Board, chosen on the basis of the subject matter, but who is not in any of the authors' laboratories
- Articles should not normally exceed the equivalent of 5000 words inclusive of diagrams, tables and references. Greater space will be appropriate for certain topics; for these the Editor should first be consulted.
 - Short notes and letters are also invited. These should not exceed two printed pages in Ancient TL, including diagrams, tables and references (equivalent to ~1400 words of text).
- 3. Diagrams and labels should be ready for direct reproduction and not normally exceed 12 cm wide by 10 cm high. Where possible, high quality electronic versions of figures should be submitted. Separate figure captions should be supplied. Inappropriately scaled drawings and labels will be returned for alteration.
- 4. Authors are asked to submit the paper, including diagrams, to the Reviewer and a duplicate copy to the Editor.

 The final version of the text must be submitted to the Editor electronically using a standard format (Microsoft Word for PC is currently used for producing Ancient TL). Electronic copies of Diagrams and Tables should also be submitted.
- 5. Upon receipt of an article, the Editor will send an acknowledgement to the author. If the Reviewer is unable to deal with the contribution within **4 weeks** he/she will inform the author and advise the Editor.

Requirements under various situations

When agreement concerning an article has been reached:

The Editor should receive a copy of the final version of the paper, both as hard copy and electronically. The Reviewer should send their final decision, including comments for publication if any, to the Editor.

If the article has not been rejected, but agreement on its final form cannot be reached or where there are protracted delays in the reviewing process:

The Editor may request an assessment from the Reviewer and responsibility passes to the Editor.

If the article is rejected:

The Editor and author receive notification from the Reviewer, with an indication of the reason for rejection.

Thesis abstracts are to be sent to the Editor and in principle do not need reviewing. However, authors are requested to make sure that the English is correct before submission. Thesis abstracts should not exceed 750 words, and figures and tables are not accepted.

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