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Luminescence dating, single-grain dose distribution

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Abstract

The graphical display of single-grain or single-aliquot equivalent dose values can be accomplished in various ways, of which the radial plot provides an effective means of assessing all of the salient information at a glance. After an initial visual inspection of the distribution, one or more statistical "age models" can be used to estimate the equivalent dose for the population of grains (or aliquots) related most closely to the event of interest. Such models should be supported by well-established statistical theory, but the choice of model depends fundamentally on the scientific context of each sample and on the purpose of the investigation.

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Title: Luminescence Dating, Single Grain Dose Distribution

Synonyms: Single Grain Equivalent Dose Distribution; Single Grain D_e Distribution

Definition: A single grain dose distribution refers to the spread in measured dose values (and their associated uncertainties) for individual mineral grains in luminescence dating; usually these are independent dose estimates for tens to hundreds of single grains from the same sample.

Main Text:

Introduction

In luminescence dating, an estimate is made of the equivalent dose for a single grain or for a group of mineral grains, the latter commonly referred to as an 'aliquot'. The equivalent dose (expressed in grays, Gy) corresponds to the radiation energy absorbed by a mineral grain since it was last exposed to sunlight ('bleached') or was last heated to a high temperature, but this only holds true for an aliquot if each and every grain on the aliquot had been bleached or heated to the same, sufficient extent. For this reason, a single grain is the smallest meaningful unit of analysis in luminescence dating, because each grain in a sample may, in principle, have had a different bleaching, heating or post-depositional history.

An equivalent dose estimate for a single grain, or for a single aliquot composed of multiple grains, is obtained experimentally, so it has an associated uncertainty. The uncertainty is usually expressed as the standard error, at the 1-sigma (1σ) or 68% confidence interval. The estimate of uncertainty is as important as the estimate of the equivalent dose itself and this is especially true for single grains, because the size of the uncertainty can vary greatly from grain to grain. A set of bivariate observations (of equivalent dose and standard error) are, therefore, commonly obtained for each sample, and the distribution of these observed values should be examined before calculating the burial age of the sample, or some other event of interest.

As a general note of caution, it is important to ensure that the quoted standard error encapsulates all of the measurement uncertainties associated with estimation of the equivalent dose. For single grains, the standard error includes uncertainties associated with photon counting statistics, instrumental reproducibility, mathematical fitting of the dose-response curve to the measured luminescence data, and corrections for any spatial heterogeneity in the laboratory beta sources. Equivalent dose values might appear more scattered than is actually the case if the standard errors are underestimated, whereas dose distributions may look misleadingly homogeneous if the standard errors are overestimated.

Graphical displays of equivalent dose distributions

Researchers often wish to plot the distribution of equivalent dose estimates, and there are several means of doing so. Galbraith and Roberts (2012) review some of the most popular approaches to displaying equivalent dose values.

Frequency distributions

A commonly used form of data display is the histogram. This requires equivalent dose values to be sorted into 'bins' of some fixed size and then the number of observations summed for each bin to generate a frequency distribution. In Fig. 1, the bottom left-hand plot is a histogram of the

equivalent dose values for 120 aliquots composed of sand-sized quartz grains from a fluvial sample. Most values cluster between 20 and 30 Gy, with a few smaller values and some much larger ones. The distribution appears to be asymmetric and positively skewed.

Despite their apparent simplicity, however, histograms present various problems of implementation and interpretation. The bin size, for example, is an arbitrary choice, so the shape of the histogram can be affected by the choice of bin size. Furthermore, equivalent dose histograms include information about the distribution of the 'true' doses (that is, the doses that would have been observed if we could do so without measurement error) and the distribution of the standard errors, among other things.

In Fig. 1, the chosen bin size is 5 Gy. This is larger than the standard errors for most of the equivalent dose estimates, which are displayed in the top left-hand plot. The combination of these two plots is useful, as it allows the reader to see the distribution of equivalent doses and the size of their standard errors, which is not something that can be judged from the histogram alone. The standard errors of this sample show an interesting feature that is typical of many luminescence samples: the size of the uncertainty increases with the size of the equivalent dose. Because of this, larger equivalent dose values will tend to scatter more in a histogram than smaller values and thereby create a positive skew, regardless of the bleaching and burial history of the grains.

To compensate for this effect, it is useful to take the natural logarithm of each equivalent dose value and to express the standard error as the relative standard error (that is, the standard error in Gy divided the equivalent dose in Gy). Logarithmic transformations are commonplace in statistics and exploit the fact that the relative standard error of an estimate is approximately equal to the absolute standard error of its natural logarithm.

The two right-hand plots in Fig. 1 show the same data as in the left-hand column, but with the relative standard errors plotted in the top right-hand panel and the equivalent doses presented on a logarithmic scale. The relative standard errors do not increase with the size of the equivalent dose, and the equivalent dose distribution is much closer to normal (Gaussian) in shape. As the latter may be interpreted differently from the bottom left-hand histogram, it is worthwhile displaying data in different ways before drawing conclusions about the likely bleaching and burial history of a sample from its equivalent dose distribution.

Another form of the histogram, often referred to as a 'probability density function', is sometimes used in luminescence dating. Probability density functions have the appealing appearance of 'smoothed' histograms, but they suffer from many statistical shortcomings and their use is strongly discouraged (Galbraith, 1998, 2010; Galbraith and Roberts, 2012).

Radial plots

The preferred form of data display for equivalent dose values is the 'radial plot' (Galbraith, 1988; Galbraith et al., 1999; Galbraith and Roberts, 2012). This plot is particularly useful to display single-grain (and single-aliquot) dose distributions because both the equivalent dose value and its standard error are shown for each and every grain (or aliquot), and this allows a number of other features of the distribution to be discerned at the same time. Fig. 2 is a radial plot of the same data as shown in Fig. 1. Each of the open circles denotes the equivalent dose value and relative standard error for a single aliquot. The equivalent dose can be read by drawing a line from the zero-point on the 'standardised estimate' axis (on the left-hand side), through the data point of interest, to intersect the radial axis on the right-hand side. The point of intersection is the equivalent dose (D_e). The relative standard error on this estimate is read by drawing a vertical line from the same data point to intersect the horizontal axis at the bottom. The relative standard error is shown in % (that is,

as the standard error divided by the equivalent dose, multiplied by 100) and the 'precision' is the reciprocal of the relative standard error.

A benefit of displaying the data in this form is that the equivalent dose values measured with the highest precision (that is, the smallest relative standard errors) fall furthest to the right, whereas those measured with least precision lie furthest to the left. In addition to this self-sorting of values by precision, the use of the standardised estimate allows other aspects of the distribution to be conveniently assessed at a glance. The standardised estimate represents the unit standard deviation applicable to all of the data points. For each point, it is calculated as the equivalent dose minus a chosen reference value (such as the average equivalent dose for the entire distribution), divided by the relative standard error for that point. Accordingly, any band of width ± 2 units projecting from the standardised estimate axis will capture 95% of the points if they are statistically consistent at 2σ.

In Fig. 2, the equivalent doses are plotted on a log scale (as in the right-hand panels of Fig. 1), so the standardised estimates and relative standard errors are based on the log equivalent dose values. Clearly, no single band extending ± 2 units from the standardised estimate axis can capture 95% of the equivalent dose values, so there is some additional spread, which can be expressed in terms of the 'overdispersion'. The latter term is used to describe the scatter among the equivalent dose values over and above that due to the measurement error associated with each observation (Galbraith et al., 2005; Galbraith and Roberts, 2012). The data in Fig. 2 are overdispersed by 32.0 ± 2.3%, as calculated from the 'central age model' (see below). Two other noteworthy features of this distribution are visually apparent. First, there is a high density of data points consistent with equivalent dose values of 20 to 30 Gy, so the 'frequency' aspect of the histogram is inherent in the radial plot also. Second, the plot shows clearly the existence of three very high equivalent dose values and one very low value, each measured with reasonable precision (that is, a relative standard error of less than 10%).

The use of log values may not be appropriate for young samples that contain grains with equivalent dose values close to zero or negative dose estimates within error of zero. In such instances, the unlogged or modified log-transformed versions of the radial plot can be used (Arnold et al., 2009; Galbraith, 2010; Galbraith and Roberts, 2012). Example radial plots for samples deposited in a variety of contexts are provided by Jacobs and Roberts (2007) and Galbraith and Roberts (2012), the latter summarising the many appealing features of radial plots as follows:

- equivalent dose values can be viewed simultaneously with their standard errors;
- data are sorted automatically so that the equivalent dose values can be distinguished easily in terms of their relative precisions;
- any overdispersion can be identified at a glance; and
- patterns in the data, such as the clustering of equivalent dose values, the presence of outliers or the existence of multiple, discrete dose components (see below) can be recognised before calculating the sample age.

Age models for equivalent dose distributions

After a visual inspection of the equivalent dose distribution, it is common for researchers to then estimate the equivalent dose for the population of grains (or aliquots) related most closely to the event of interest. This may be the burial time of the most fully bleached grains in the sample, or the last time that the grains were heated to a high temperature. In sediment dating, the value often sought is the equivalent dose corresponding to the most recent bleaching event. But if a sample had been disturbed after burial and become contaminated by younger or older intrusive grains, then it is useful to be able to identify and exclude these grains before calculating the sample age.

To allow for these and other possibilities requires a range of models based on sound statistical principles. Several parametric models, developed originally for fission track dating (Galbraith and Green, 1990; Galbraith and Laslett, 1993), have been adapted for luminescence data and are now in widespread use. Galbraith and Roberts (2012) review these different 'age models', although it should be borne in mind that they are rarely applied to ages per se in luminescence dating. Instead, these models are applied to equivalent dose values, because the information required to determine single-grain ages – namely, the environmental dose rate specific to each grain – is not generally known. At present, the same (sample mean) dose rate is usually employed for all grains, while research continues into methods of measuring and modelling grain-specific dose rates.

A critical element of any decision-making process involving statistical models is sample context. This should dictate which, if any, of the models may be the most appropriate for the sample of interest. On the basis of its depositional context, for example, one could ask if a sample is likely to have been fully or incompletely bleached at the time of deposition. Similarly, one could consider if there is any independent evidence that the stratigraphic integrity of the site has been compromised, perhaps resulting in post-depositional disturbance of the sample? In short, statistical models should not be applied without first taking into account the archaeological or geological context of a sample, stratigraphic considerations, and other relevant information, such as independent age control (Galbraith et al., 2005; Galbraith and Roberts, 2012).

Common and central age models

These two models represent the most straightforward case in luminescence dating: one in which the 'average' equivalent dose is the quantity of interest. This may be a useful value to estimate for samples composed of grains that have been well bleached before deposition, exposed to the same environmental dose rate after burial, and remained unaffected by any processes of post-depositional sediment mixing. The equations for the common and central age models are given in Galbraith et al. (1999) and Galbraith and Roberts (2012), together with worked examples in the former. The two models are identical insofar as they both weight each equivalent dose by the inverse square of its standard error, which is a standard statistical method of averaging values with differing precisions. A major difference, however, is that the central age model also calculates – and explicitly includes in the standard error – the extent of any overdispersion among the equivalent dose values. If there is zero overdispersion (that is, all of the spread among the equivalent doses can be accounted for by the individual measurement uncertainties alone), then the central age model reduces to the common age model. But even for samples that are known or are thought to have been fully bleached at deposition, overdispersion values of 10–20% are commonplace (Galbraith et al., 2005; Jacobs and Roberts, 2007; Arnold and Roberts, 2009), so the central age model is usually the more appropriate of the pair.

As illustrated by the two lower plots in Fig. 1, log equivalent doses typically produce a much closer approximation to a normal (Gaussian) distribution than do their unlogged counterparts. This is due to the size of the absolute standard error increasing in concert with the equivalent dose (see top left-hand panel), a common feature of many luminescence samples. For this reason, the most widely used form of the central age model utilises log equivalent dose values and the relative standard errors; the resulting model estimate of equivalent dose approximates the geometric mean. If the measured equivalent doses are zero or negative, as can occur with some young samples and with modern samples, then log transformations are not applicable and the unlogged version of the central age model could be used instead (Arnold et al., 2009).

Minimum age models

The assumption of complete bleaching before deposition and lack of disturbance thereafter will not be true for many samples. For example, sediment grains transported underwater may not be fully bleached, and some deposits may be subject to bioturbation or human disturbance. In such cases,

the ‘average’ equivalent dose will be of little interest. For samples that are thought to contain some grains that were fully bleached before deposition and others that were only partially bleached, the minimum age model can provide a useful means of estimating the equivalent dose associated with the subset of well bleached grains. Details of this model are given in Galbraith et al. (1999) and Galbraith and Roberts (2012). Alternative approaches that are philosophically similar to the minimum age model are rarely based on well-established statistical principles, so the statistical properties of the resulting equivalent dose and uncertainty estimates are ambiguous, at best.

The most widely used version of the minimum age model assumes that the log equivalent doses form a truncated normal distribution, with the lower truncation point corresponding to the average log dose of the subset of fully bleached grains. This assumed distribution is one of several that could be made, but it is convenient to assume a normal distribution in the absence of independent support for another type. The minimum age model was originally developed with 4 adjustable parameters, but it has been shown that data sets with small numbers of equivalent dose values or less dispersed distributions are often fitted better using a 3-parameter model, in which the lower truncation point equals the mean of a normal distribution. As with the central age model, the unlogged version of the minimum age model may be more appropriate for samples with zero or negative measured equivalent doses (Arnold et al., 2009).

When implementing the minimum age model, allowance needs to be made for the extent of inherent overdispersion among the equivalent dose values of the subset of fully bleached grains. That is, well bleached samples commonly exhibit some amount of overdispersion in their equivalent dose values, so an estimate of this overdispersion should be added to the relative standard error of each equivalent dose before running the model. This estimate could be obtained from a well bleached sample of the same mineral that is similar in age and derived from the same source. In the absence of independent data, one could conduct a sensitivity test of the model using overdispersion values of 10% and 20%, for example.

Minimum age models have been tested in numerical simulations and in comparisons against independently-dated Holocene samples from a variety of geomorphic settings (Olley et al., 2004; Arnold et al., 2009). The latter studies utilised single grains of quartz, but the minimum age model can also be applied to single aliquots with one additional caveat: the estimate of the minimum dose may still be larger than the equivalent dose of the most recently bleached grains unless at least one aliquot consists entirely of fully bleached grains. For aliquots composed of relatively few fully bleached grains, the minimum dose may be much too large and single-grain analysis may be required to obtain an accurate estimate of depositional age.

Finite mixture model

For some samples, neither the mean nor minimum estimates of equivalent dose may correspond to the event of interest. This may be so for deposits affected by bioturbation or for sites disturbed by human activities, both of which may result in mixing of grains between units of different ages. In such circumstances, the finite mixture model may be able to discern the existence of multiple, discrete components in a single-grain equivalent dose distribution (Roberts et al., 2000; Galbraith and Roberts, 2012).

In the finite mixture model, the log equivalent doses for single grains are assumed to represent a mixture of discrete populations, each of which is normally distributed with the same relative overdispersion. The extent of overdispersion is one of the parameters in the model, as is the number of discrete populations. In practice, the model is run by initially fixing the number of components at 2, and then inserting some reasonable overdispersion values (such as 10%, 15% and 20%). The number of fitted components is then increased to 3, using the same overdispersion values as previously, and so on. The model uses maximum likelihood to estimate the mean equivalent dose

and standard error for each fitted component, and the proportion of grains in each component. When the number of components is set at 1, the finite mixture model is mathematically identical to the central age model.

The goodness-of-fit of the model to the data can be assessed using the Bayes Information Criterion (BIC), which takes into account the maximum likelihood estimates and the number of fitted components; the smallest BIC indicates the minimum number of components needed to explain the dose distribution. It is important to also check that the model estimates are sensible and to compare them with the distribution of equivalent doses on a radial plot, as no model should be used as a 'black box'. Straightforward explanations and worked examples of the finite mixture model fitting procedure are given in David et al. (2007) and Jacobs et al. (2008).

For 2- and 3-component mixtures of single grains that were bleached and then given known laboratory doses, the model could successfully recover the correct number of discrete components, their relative proportions and the corresponding equivalent dose values, provided the overdispersion parameter was small, known or similar for each component (Roberts et al., 2000; Jacobs et al., 2006). But the finite mixture model may be unable to identify discrete components in more complex equivalent dose distributions, such as those associated with heterogeneously bleached grains that have been mingled subsequently. The model should also not be applied to the equivalent dose distributions of multi-grain aliquots, even for those consisting of very few grains. If aliquots contain luminescent grains from more than one parent population, then 'phantom' components with intermediate doses can easily be generated – that is, equivalent dose components not present in any of the single-grain parent populations (Arnold and Roberts, 2009).

Summary or conclusions:
The graphical display of single-grain or single-aliquot equivalent dose values can be accomplished in various ways, of which the radial plot provides an effective means of assessing all of the salient information at a glance. After an initial visual inspection of the distribution, one or more statistical 'age models' can be used to estimate the equivalent dose for the population of grains (or aliquots) related most closely to the event of interest. Such models should be supported by well-established statistical theory, but the choice of model depends fundamentally on the scientific context of each sample and on the purpose of the investigation (Galbraith and Roberts, 2012).

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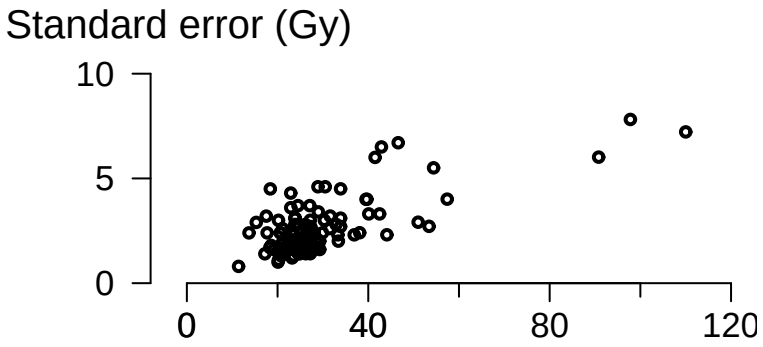
Cross-references: Luminescence Dating; Luminescence Dating, Uncertainties and Age Range

Figure captions:

Fig. 1 Histograms of equivalent dose values and scatter plots of their standard errors for 120 single aliquots of a fluvial sample. The plots in the left-hand column use a linear scale for the equivalent dose and show the absolute standard errors in Gy. The right-hand panels use a logarithmic scale for the equivalent dose (that is, equal divisions of log dose) and show the relative standard errors in %. (From Galbraith and Roberts, 2012)

Fig. 2 A radial plot of the same data as displayed in Fig. 1. The equivalent dose values are plotted on a log scale and the relative standard errors (in %) are indicated on the horizontal axis. (From Galbraith and Roberts, 2012)


Standard error (Gy)
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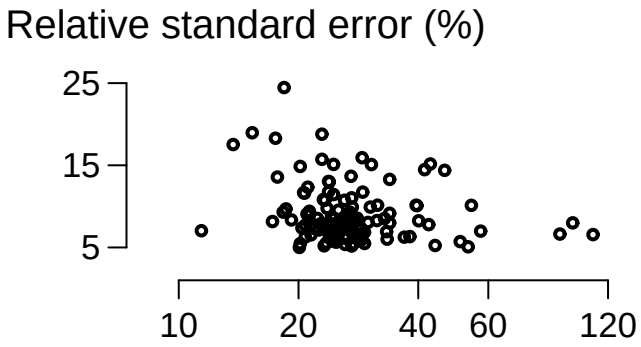
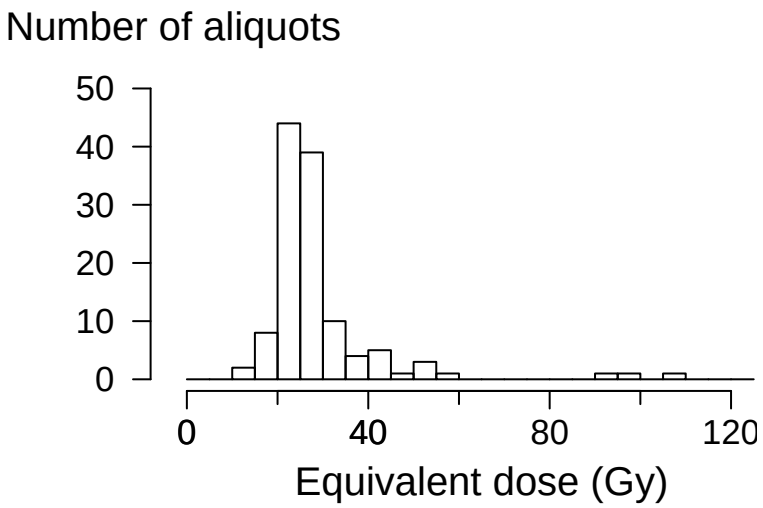
5
0
0
40
80
120


Relative standard error (%)
25
15
5
10
20
40
60
120


Number of aliquots
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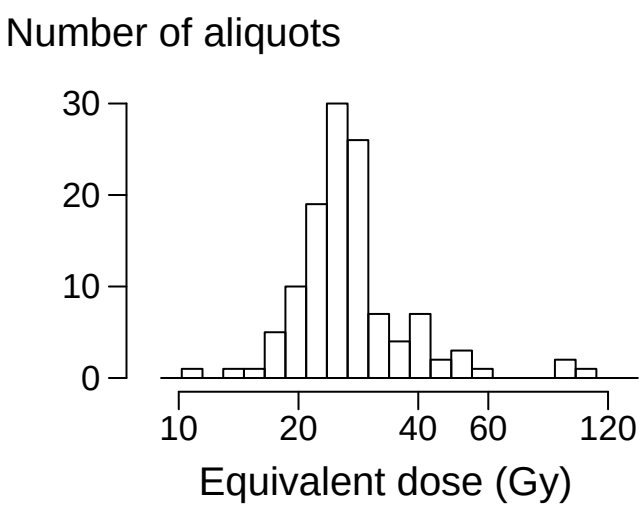
0
40
80
120
Equivalent dose (Gy)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20
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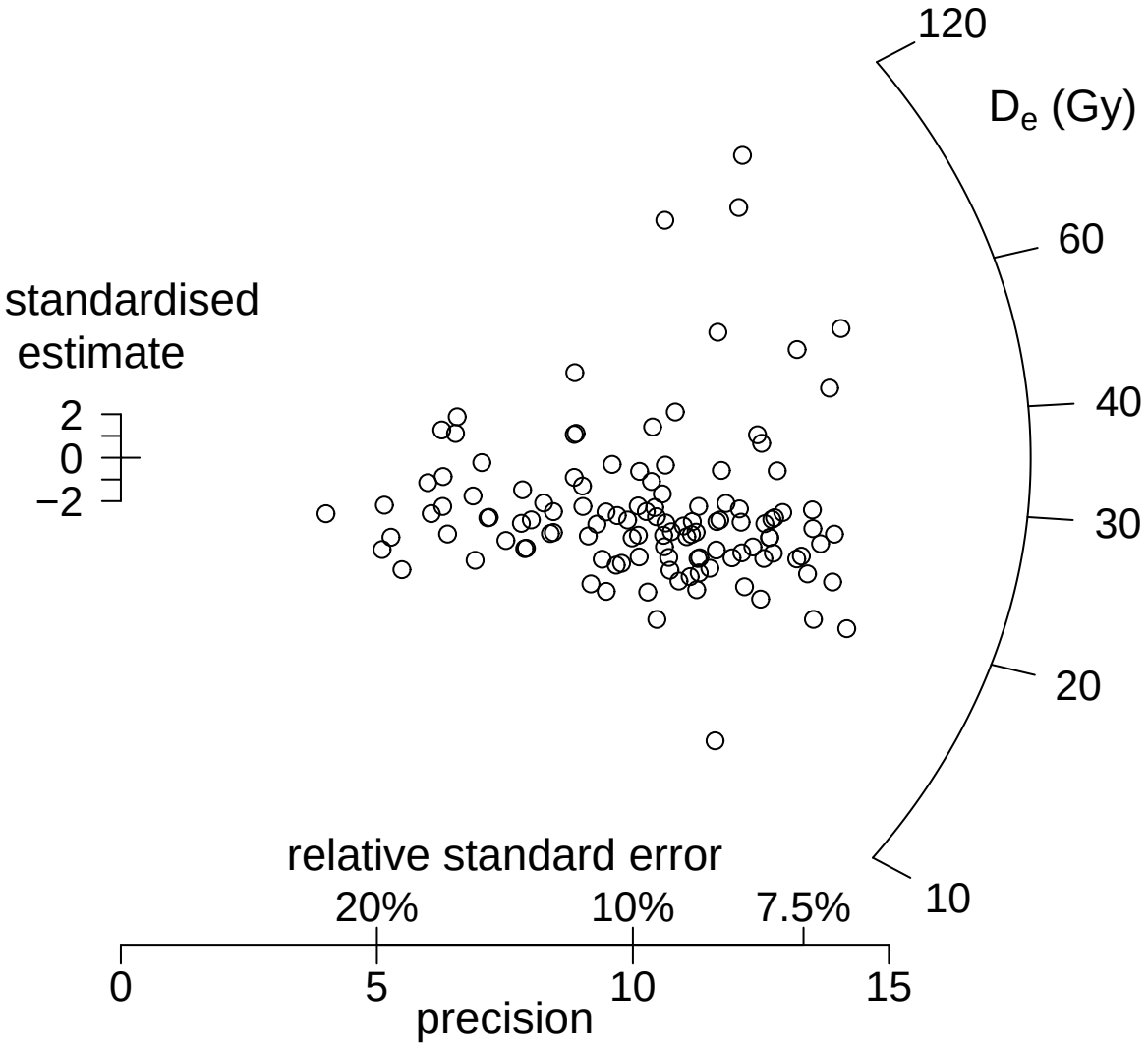
0
10
20
40
60
120
Equivalent dose (Gy)


120
D_e (Gy)
60
40
30
20
10
standardised
estimate
2
0
−2
relative standard error
20%
10%
7.5%
0
5
10
15
precision