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# Linear regression of TL data

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## Introduction

Recently, Rendell (1985) has presented a comparison of five approaches to linear regression of TL signals versus applied dose. The fifth approach apparently represents the one used at S.F.U., but it is titled and summarized incorrectly. This note presents the technique we use, outlines how it differs from the other four, and states why we believe the latter are inappropriate.

## Background

The history of attempts to develop rigorous techniques for linear regression has been outlined by York (1966). He proceeded to develop an exact solution to the generalized problem, following the initial approach of Deming (1943). York showed that because experimental uncertainties in the values of the variables X and Y will vary from point to point, the most general approach requires solving, iteratively, a recursive "cubic" equation in the parameter b (slope). This recursive equation (his equation 20) he called the "least squares cubic".

In application it is necessary to assign uncertainties to each $X_i$ and $Y_i$, uncertainties which may vary from point to point. In practice this assignment is usually done by choosing weights w(Xi) and w(Yi) that are inversely proportional to the variances in the respective variables. This, and other special cases of the generalized equations of 1966 are discussed and illustrated graphically in a short paper by York (1967). In a later publication, York (1969) developed a generalized solution of this "least squares cubic" for the case of uncertainties in X and Y that are correlated.

In the general case one may, therefore, have considerable mathematical complexity. In TL work this complexity is fortunately absent, because there is no evident correlation between the uncertainties in the TL signal and those in the applied dose. Furthermore, random uncertainties in the applied dose may be negligible; this will be true if random errors in both the dose rate and irradiation times are insignificant. There remains the question of how to determine the variances in the TL intensities. One could measure these; however, since a rather large number of (>10) sample discs would need to be measured for each point, this approach is somewhat impractical. Instead, we argue that TL intensity variations are due to variations in the amount or distribution of matter on the sample disc, or are due to intrinsic brightness variations of sample grains. In these cases one would expect the variance of the TL intensity to be proportional to the square of the TL intensity.

## Analysis of TL Data

Our approach is thus based on the following criteria:

(i) any random errors in the laboratory irradiation doses are insignificant,
(ii) uncertainties in the TL intensities are the same percentage of the intensity for all data points,
(iii) values for both the equivalent dose ($D_{eq}$) and its uncertainty are required.

These three criteria dictate the use of the following equations, derived from York (1966), where Y is applied dose and X is the TL signal:

$$Y = a + bX \qquad (1)$$

where $a = D_{eq}$,

$$a = \bar{Y} - b\bar{X} \quad , \qquad b = \frac{\sum w(X_i)V_i^2}{\sum w(X_i)U_iV_i} \quad ,$$

$$\bar{X} = \frac{\sum w(X_i)X_i}{\sum w(X_i)} \quad , \qquad \bar{Y} = \frac{\sum w(X_i)Y_i}{\sum w(X_i)} \quad ,$$

$U_i = X_i - \bar{X}$ and $V_i = Y_i - \bar{Y}$.

The variances of a and b are given by

$$\sigma_a^2 = \sigma_b^2 \cdot \frac{\sum w(X_i)X_i^2}{\sum w(X_i)} \qquad \text{and}$$

$$\sigma_b^2 = \frac{1}{n-2} \cdot \frac{\sum w(X_i)(bU_i - V_i)^2}{\sum w(X_i)U_i^2} \quad .$$

All sums are from i = 1 to n, where n is the number of data points. For a constant percent error p, the weighting factors are given by $w(X_i) = (pX_i)^{-2}$, but since p cancels out of all expressions, we use $w(X_i) = X_i^{-2}$.

It is not strictly correct to state, as Rendell does, that this approach treats dose as the dependent variable. The TL signal is still the dependent variable, but the requirements of weighting and error calculation necessitate a change from the usual notation. Rendell also states our equations for U and V incorrectly.

## Discussion

None of the first four approached as described by Rendell meet the criteria stated at the beginning of the previous section and, therefore, we believe they are invalid. In particular, none of them provide an uncertainty in the equivalent dose, and the first three use inappropriate weighting factors.

Application of our method to the set of data given by Rendell yields $D_{eq} = 10.95 \pm 1.12$ and a slope of $2.07 \pm 0.15$ (this is to be compared with the reciprocal of the slopes in her table). The large uncertainty in $D_{eq}$ is expected because of the large extrapolation. In practice, we prefer to avoid the use of linear regression for such data and to apply a larger range of doses, even if it becomes necessary to use sublinear regressions (higher order polynomials or saturating exponentials). However, that is another issue and will not be discussed here.

Finally, it should be apparent from our comments and from York's work that it is not useful to invoke values of "correlation coefficients" to describe the quality of data sets. This data correlation coefficient (r in Rendell) supplies little or no useful information about the quality of the regression. What is useful, however, is a "goodness-of-fit" parameter, such as described by York (1969) (his $[S/(n-2)]^{1/2}$ parameter). This and analogous goodness-of-fit parameters (see also Brooks et al 1972) are used routinely in the assessment of isochrons in radioisotopic dating. Unfortunately, its utility depends on an independent knowledge of the uncertainties in each TL observation. Such a state of knowledge does not yet exist in TL work because the variablility of TL signals is dominated by unspecified grain-to-grain or disc-to-disc differences.

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## Reviewer's Comments

As the authors point out, there are some inaccuracies in Rendell's description of their method. They should have an opportunity to correct them, and to state the assumptions on which their method is based. However, since the scope of a newsletter such as 'Ancient TL' does not allow detailed justification of the method, it is clear that many readers will require to consult York's original paper in order to understand the rationale behind the method and to assess its usefulness. For example, one potentially confusing aspect is the formulation of the line, equation (1). Here Y looks like the dependent variable - hence the original mistake by Rendell. In fact if (1) is turned around to $X = -a+1/bY$, then the estimate for b is just the inverse of the usual weighted least squares estimate for 1/b in the regression of X on Y. In view of this it is difficult to see, without access to York's paper, how the error estimates have been derived, and in what respect the approach differs from the standard 'X on Y' case (in their notation).

A further point to note is that N. Debenham's method, summarised as approach four in Rendell, does provide a measure of the uncertainty in D, given by the (asymmetric) intercepts of the one-sigma hyperbolic confidence bands for the regression of X on Y (in their notation). Readers could be given the (incorrect) impression that York's method is the only one meeting the criteria stated in the paper.

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# Extrapolation errors in linear regression

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The use of various regression techniques to fit TL-dose data (in the linear region) to a straight line was recently discussed by Rendell (1985). Variation covering a range of about 6% was found among the intercepts on the abscissa. On the other hand, the errors arising from the extrapolation itself are rather larger and may well make the differences among regression techniques unimportant, at least until much more precise data are at hand.

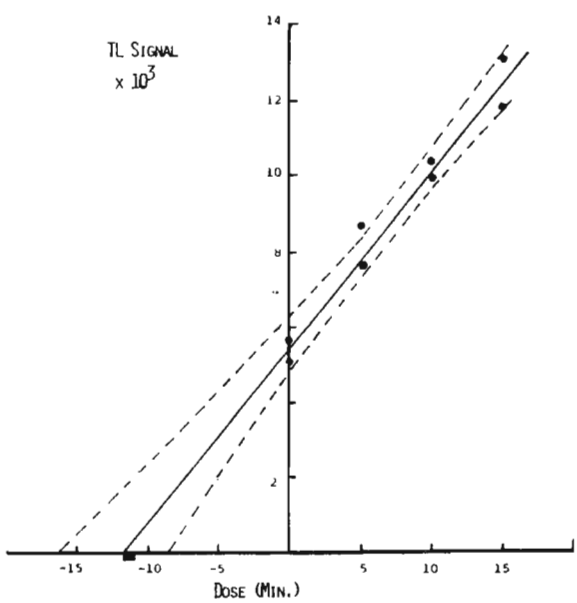


*Figure 1* *Uncertainty in extrapolated Estimated Dose from TL data of Rendell (1985). Points are Rendell's data; solid line is simple linear regression line; dashed lines define 95% confidence band. The short heavy portion of the abscissa around -11 min. represents the spread of intercepts found by Rendell for various regression techniques.*

For illustration I have plotted the table of data given by Rendell in her paper in figure 1. The intersection of the confidence band with the x-axis gives the uncertainty in the intercept at the 95% confidence level. Numerically the intercept and its uncertainty are expressed by:

$$x_0 = -11.63 \begin{matrix} -3.14 \\ +4.51 \end{matrix} \quad \text{or} \quad \begin{matrix} +27\% \\ -39\% \end{matrix}$$

The statistical uncertainty is much larger than the spread in intercepts found by Rendell. Actually it is not necessary to calculate the confidence band as such. Mandel (1964) gives equations (eqn. 12.20 - 12.25, p. 281) for the confidence limits of the intercept on a specific horizontal line, in this case the x-axis.

It should be noted that where several runs are made at each dose and the means used to form the linear plot, the uncertainty in the intercept must reflect not only the scatter of the mean values about the regression line but also the uncertainty in the means. Note also the use of the 95% confidence interval for the intercept. When comparing a statistical with a systematic error, it is advisable to use a realistic confidence level for the former.

Improvement (reduction in the statistical uncertainty) can be brought about by increasing the precision of the data, the number of runs at each dose, and the number and range of doses. Because we can usually afford only a limited number of runs overall, the judicious distribution of these over the range of doses is an important question. These infuences can readily be seen using a simplified version of Mandel's eqn. 12.25. We may calculate the intervals $\Delta x$ between the confidence limits for the intercept and expand it in terms containing $\hat{V}(\delta)$, the standard deviation *(? variance, Rev'r)* of the data points about the regression line. Only the leading term makes an appreciable contribution:

$$\Delta x = \frac{2\bar{y}\, t_c}{\hat{\beta}^2} \left[\hat{V}(\delta) / \sum_p n_p (x_p - \bar{x})^2\right]^{1/2}$$

The quantities $t_c$ (the critical value of student's t) and $\beta$ (the slope of the regression line) are not at our disposal, and $\sqrt{\hat{V}(\delta)}$ reflects the precision of the data, which we know we must optimize. We are left with the ratio $\bar{y} / \sqrt{\sum_p n_p (x_p - \bar{x})^2}$ to manipulate to achieve minimum error in the extrapolation, in which $\bar{x}$ and $\bar{y}$ are the mean values, the subscript p indicates the dose, and $n_p$ is the number of values at the pth dose.

The sum $\sum_p n_p (x_p - \bar{x})^2$ can be maximized by maximizing the range of doses, and suggests putting greatest weight at the ends of the range. The average $\bar{y}$ can be minimized by making most of the runs at zero dose.

These conclusions can easily be made quantitative and practical for the special case in which we are confident of the linearity of the data. Then only two doses are required, zero and the largest possible within the linear range. Setting the total number of runs we can afford equal to

$$N = n_1 + n_3 \tag{2a}$$

where $n_1$ is the number of zero-dose and $n_3$ the number of maximum-dose runs (let $n_2 = 0$ for the moment), we can minimize the ratio $\bar{y} / \sqrt{\sum_p n_p(x_p - \bar{x})^2}$ with respect to $n_1$, holding N constant. The result is the remarkably simple prescription

$$\frac{n_1}{n_3} = \frac{y_3}{y_1} \tag{2b}$$

Equation 1 may be further manipulated, using eqns. (2a) and (2b), to yield a value for the total number of runs needed to yield a predetermined precision level in the intercept:

$$N = \frac{4k(1 + k)t_c^2}{R^2} \tag{3}$$

where R is the ratio,

$$R = (\Delta x / 2x_0) \; / \; (\sigma / y_1),$$

with $\sigma$ the standard deviation of the TL value for a single run and

$$k = \frac{x_0}{x_3 - x_1} = \frac{\text{Intercept}}{\text{Maximum Laboratory Dose}}$$

We note that $t_c$ depends upon N so eqn. 3 is solved comparing $N/t_c^2$ to values derived from statistical tables. Eqn. 3 is plotted in fig. 2 for several values of R for 95% confidence intervals.

To obtain the intercept with maximum efficiency, the maximum range of doses within which linearity is expected to hold is chosen and a few runs made at each end to yield a trial intercept and estimate of $\sigma$. These data are used to calculate k and R, after selection of the desired precision for the intercept. With k and R, a figure such as fig. 2, which is appropriate for a 95% confidence level, can be consulted to obtain N, the minimum total number of runs needed, and these divided between zero and maximum laboratory dose according to eqn. 2b. The value for N obtained from fig. 2 is a minimum. In practice, the number of runs at maximum dose should not be less than 3.

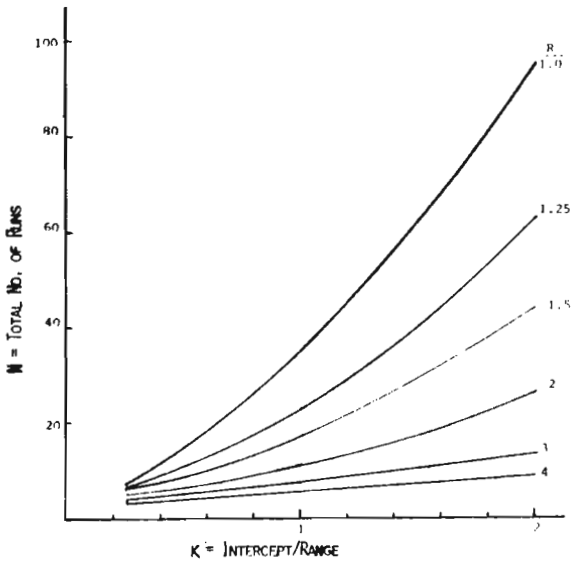


*Figure 2*
*Total number N of runs needed to obtain a given error in the intercept. R is the ratio of ($\Delta x/2x_0$) to ($\sigma/y_1$) where $\Delta x$ is the 95% confidence interval in the intercept $x_0$, $\Delta$ the standard deviation for replication of a single run, and $y_1$ the NTL.*

The impact of this treatment may be illustrated again using Rendell's data, preserving the linear regression and the uncertainty in the data. Let us set $\Delta x/x_0$, the relative 95% confidence interval, at 40%, or ± 20%. The pooled standard deviation of the intensity data is 0.372 and $y_1$ = 5.229, leading to R = 2.8. The intercept and range are nearly equal, or k ~ 1. Consulting fig. 2, we find the minimum number of runs needed, N, to be 8, the same as the actual number. The ratio ($y_3/y_1$) of maximum dose/zero intensities is 2.29. If we concentrate all of the runs at zero dose and the maximum dose, and set $n_1$ = 6, $n_3$ = 2, we obtain a value for $\Delta x$ = 4.9 min. compared to 7.1 min. for the uniform distribution across the 4 doses in the original data. This is a substantial reduction in error. Much of the reduction is already accomplished ($\Delta x$ = 5.3 min) by dividing the runs equally between just the two doses zero and maximum.

It must be emphasized that this simple prescription can be used only when we have already proved the linearity of the data. To do that obviously requires runs in the middle of the range, as well as at the ends. Since it seems probable that the major departure from linearity arises from a quadratic term (e.g., the next term in the expansion of the exponential in a saturating curve), the most efficient test for curvature can be made using several (say $n_2 = [n_1 + n_3]/2$) runs exactly in the middle of the range (at $[x_1 + x_3]/2$). An appropriate test is to examine the F-statistic

$$F = \frac{\hat{V}(\delta)}{V_R}$$

where $V_R$ is the replication variance of the data (the variance of the runs at each dose, pooled over all runs). If F exceeds the critical value at the confidence level chosen (e.g. 5%) for the degrees of freedom appropriate to $\hat{V}(\delta)$ (N-2) and $V_R$ (N-1), curvature is probably present.

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Note A fuller report may be obtained from the author.

**P.R. Reviewed by Morven Leese and accepted after revisions.**

# TL Networks

## European Network on "Thermoluminescence Applied to Archaeology"

At a conference of European ministers responsible for research, convened by the Council of Europe and held in Paris, September 1984, the ministers declared their desire to intensify scientific and technological research in Europe by strengthening existing networks of co-operation and promoting the establishment of new networks where required.

In order to comply with this declaration the Council of Europe group PACT (Physical and Chemical Techniques Applied to Archaeology), established in 1975, decided that its subgroups including that on TL dating should be transformed into networks.

To review the situation in TL dating PACT organized a European workshop on "Thermoluminescence in Archaeology" in Ravello, Italy May 29 - 31. 1986 and invited the European TL workers to participate. It was recognized at the meeting that the TL community already has an informal world-wide network operating through regular meetings and its newletter Ancient TL, and that the emphasis of research has now shifted to sediment dating.

It was decided to leave the scientific and technological aspects to the existing network and to recommend the establishment of a European network on "Thermoluminescence applied to Archaeology" in order to promote the application of TL for archaeological dating.

The European network should include representative archaeologists from the European countries and scientists from European TL laboratories engaged in dating materials of archaeological interest. The next meeting is planned to take place in the beginning of 1987 and progress will be reported at the TL Specialist Seminar in Cambridge, July 1987.

Vagn Mejdahl
Ian Bailiff

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Compiled by Ann Wintle

## Erratum

Paleographical and stratigraphical references from TL properties of Saalian and Weichselian loess of N.W. Europe. Balescu et al. AnTL 4(i).

In the Reviewer's comments a line was unfortunately omitted: The second paragraph should have read;

In respect of the latter use, a number of questions arise. As no bleaching curves are presented, overbleaching may have occurred. Wintle (1985) has suggested that dose-dependent sensitivity changes may occur when a sample is exposed to light, but whether such dose dependent changes would survive significant overbleaching is presently unknown. Investigation of sensitivity changes in the samples in the present study might provide an answer to this question.