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A modification of the arcsine–log calibration curve for analysing soil test value–relative yield relationships

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Abstract. This article aims to discuss the arcsine–log calibration curve (ALCC) method designed for the Better Fertiliser Decisions for Cropping Systems (BFDC) to calibrate relationships between relative yield (RY) and soil test value (STV). Its main advantage lies in estimating confidence limits of the critical value (CSTV). Nevertheless, intervals for 95% confidence level are often too wide, and authors suggest a reduction in the confidence level to 70% in order to achieve narrower estimates. Still, this method can be further improved by modifying specific procedures. For this purpose, several datasets belonging to the BFDC were used. For any confidence level, estimates with the modified ALCC procedures were always more accurate than the original ALCC. The overestimation of confidence limits with the original ALCC was inversely related to the correlation coefficient of the dataset, which might allow a relatively simple and reliable correction of previous estimates. In addition, because the method is based on the correlation between STV and RY, the importance to test it for significance is emphasised in order to support the hypothesis of a relationship. Then, the modified ALCC approach could also allow a more reliable comparison of datasets by slopes of the bivariate linear relationship between transformed variables.

Additional keywords: bivariate model, correlation, standardised major axis regression.

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Introduction

When developing fertiliser-recommendation models based on soil test value (STV), the most usual goal is to identify a critical value or range of a soil fertility variable for a given level of crop yield under which response to fertilisation is most likely. The most common approach is to fit a regression line between crop yield and STV, the latter as the independent variable and the crop yield, many times expressed as relative yield (RY), as the dependent one. Mathematical functions used to describe this relationship may be linear-plateau, quadratic-plateau or exponential (Mitscherlich) among others (Colwell 1963; Mallarino and Blackmer 1992).

The most widely method used for fitting regression models, the ordinary least-squares (LS) approach, assumes that only the dependent variable (e.g. RY) is random, whereas the explanatory or regressor variable (e.g. STV) is considered as fixed and error-free. This approach is especially valid for cases in which the explanatory variable is truly fixed, such as fertiliser rate. However, when this variable is not controlled by the researcher, as happens with STV, researchers normally still consider it as fixed. In this sense, it has been pointed out that LS regression is frequently abused in soil research (Webster 1997). When the underlying relationship is bivariate, it should be described as such and not as a predictive one. As well as crop yield, the STV represents an 'observed' dimension of the experiments, and comes from a population that has a reference distribution and, thus, an error component. Therefore, a joint distribution of both variables called 'bivariate' should be also considered, which in its simplest case is the 'bivariate normal' (Legendre and Legendre 1998).

Furthermore, calibrating RY *v.* STV often shows problems related to normality and homogeneity of variance. This means a lack of statistical robustness of LS regression to answer questions of interest (Kutner *et al.* 2005). Neither RY nor STV follow normal distribution, and thus, variable transformation is usually recommended (Webster 2001). However, the most common situation is to transform only the dependent variable (RY), while keeping original units in the explanatory variable, and thus, the solution results are partial. On the other hand, if the nutrient under study is the only limitation to the crop growth, it is expected that high levels of STV may result in larger and less variable yields each time. This behaviour results in a dependence of RY variance on STV values when RY is the dependent variable. Weighted regression is usually applied, but it does not always brings a solution (Motulsky and Christopoulos 2004).

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On the other hand, an innovative approach has been proposed by Dyson and Conyers (2013) for calibrating soil tests aimed at recommending crop fertilisation. The ALCC (arcsine–logarithm calibration curve) method has been developed for determining confidence limits of the critical value (CSTVs) for nitrogen (N), phosphorus (P), potassium (K) and sulfur (S) and response of various grain crops in Australia (Anderson *et al.* 2013; Bell *et al.* 2013*a*, 2013*b*, 2013*c*; Brennan and Bell 2013; Speirs *et al.* 2013). As opposed to most of the commonly used calibrating methodologies, the ALCC method: (*i*) transforms both variables involved in the relationship (i.e. RY and STV), and (*ii*) reverses the axes (i.e. fit STV *v.* RY) to estimate not only the CSTV for a given RY level but also its confidence interval (CI).

In the original study (Dyson and Conyers 2013), the authors highlighted that estimations of CI in the original methodology were often too wide for making reliable recommendations and comparisons between datasets. Therefore, they suggested that the CI be reduced from 95% ($P = 0.05$) to 70% ($P = 0.30$) in some comparisons (Dyson and Conyers 2013; Watmuff *et al.* 2013). However, a detailed review of the original ALCC method suggests that, by modifying specific procedures, it is possible to achieve more accurate estimates of CSTVs without reducing the level of confidence.

The objectives of this study were: (*i*) to evaluate changes in procedures of the ALCC method in order to obtain CSTVs with narrower CI; (*ii*) to test the reliability of the shape of STV–RY relationships based on a simple linear parameter; and (*iii*) to discuss the importance of testing the correlation coefficient for significance in order to support the hypothesis of a relationship between variables.

Materials and methods

Data sources and analyses

Datasets were gathered from several sources.

Dataset 1

The first dataset was obtained from the *BFCD Interrogator Database* (NSW DPI 2012). It was intentionally the same as Dyson and Conyers (2013) described in their paper, belonging to the National Soil Fertility Program (NSFP) from 1968–72 (Fig. 1). The follow filters in the *BFDC Interrogator* were applied to obtain this dataset: *Nutrient* = 'P', *Farming System* = 'dryland', *From Year* = '1968', *To Year* = '1972', *State* = 'Victoria', *Season* = 'winter', *Crop* = 'cereal wheat', *Australian Soil Class* = 'All', *Soil Test and sample depth* = 'P Colwell mg/kg at 0–10 cm', *Trial quality* = 'A trials only'.

Dataset 2

A second dataset was also defined by using the *BFCD Interrogator Database* in order to make specific comparisons of parameters using the original and the modified ALCC methods. This dataset was obtained through the follow filters: *Nutrient* = 'P', *Farming System* = 'dryland', *From Year* = 'All', *To Year* = 'All', *State* = 'All', *Season* = 'winter', *Crop* = 'cereal wheat', *Australian Soil Class* = 'Vertosol Black + Vertosol Grey', *Soil Test and sample depth* = 'P Colwell mg/kg at 0–10 cm'.

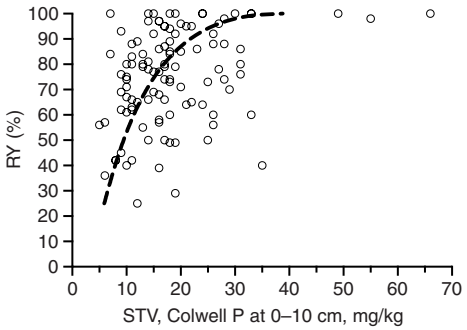

Fig. 1. Scatter-plot of relative yield (RY, %) and soil test value (STV, Colwell P at 0–10 cm, mg/kg) for dataset 1: 107 experiments from the National Soil Fertility Program (1968–72) in Victoria (107 class A trials). Data were gathered from the *BFDC Interrogator* database following previous descriptions given by Dyson and Conyers (2013). Dashed line represents the fitted calibration curve by the arcsine–log calibration curve (ALCC) approach (back-transformed from a linear regression between transformed variables (Fig. 2).

Dataset 3

A third dataset was built for a comparison of standard errors (SE) of the CSTV estimator. For this purpose, 60 datasets of STV and RY were used. They were gathered from (*i*) the *BFCD Interrogator Database* (23) (NSW DPI 2012); and (*ii*) published and unpublished grain crop fertilisation experiments in the Pampean Region of Argentina (37) including several crop–nutrient combinations (wheat, maize and soybean crops, and N, P, S and zinc (Zn)). Dataset 3 was defined by using specific variables from each of the 60 datasets ($n = 60$): (*i*) correlation coefficient (r_{xy}), (*ii*) SE of CSTV estimator by using the original-ALLC method, and (*iii*) SE of CSTV estimator by using the modified ALLC method.

All datasets were tabulated and processed in a Microsoft Excel (Microsoft Corp., Redmond, WA, USA) environment in order to make all comparisons. Analyses of obtained linear models were also checked in the R software environment using packages *Smatr v3.4-3* (Warton *et al.* 2012) and *Stats* v3.2.4 (R Core Team 2016). All figures were made with the GraphPad Prism software v7.0a for MacOSx (GraphPad Software Inc. 2016).

Procedures of the modified ALCC

Nine steps are needed; each can be performed with a common spreadsheet in Microsoft Excel or similar. Essential commands for applying in a common spreadsheet are included in parentheses. Note that they could vary depending on the software version and language. Steps 1–3 of the modified ALCC are essentially the same as the original ALCC method (Dyson and Conyers 2013). Specific differences are detailed in the *Results and discussion*.

1. Transform variables. This will simplify the relationship between variables as a simple linear equation. Transformations are:

(*a*) Natural logarithm for the STV, hereinafter Y (= LN(STV_i)). The method does work independently of STV units, which normally are expressed in kg/ha, mg/kg, among others.

(*b*) Arcsine of the square root for the RY, hereinafter X (= ASIN (SQRT(RY_i/100))). The estimations of RY must be made with respect to a maximum yield (observed or estimated) as the non-deficient situation. For further details, see Dyson and Conyers (2013).

2. Center the X variable, with respect to the RY level for which you want to estimate the CSTV (= ASIN(SQRT (RY_i/100)) – ASIN(SQRT(RY_{goal}/100))). For example, for an RY_{goal} = 90%, we need to subtract, from each value of X, the corresponding arcsine$\sqrt{(90/100)} = 1.249$.
3. Estimate the Pearson correlation coefficient (r_{xy}), between X (centred) and Y (= PEARSON(X_{values}, Y_{values}). Because the methodology is based on 'correlation' between variables, it is advisable to test this coefficient for significance before the next steps. See *Testing correlation significance* for details.
4. Estimate the average means of centred X (= AVERAGE (X_{values})) and Y (= AVERAGE(Y_{values})). They represent coordinates of the data ellipse centroid ($\bar{X}, \bar{Y}$), through which all possible regressions pass through.
5. Estimate a linear regression (Eqn 1) between X and Y values (Fig. 2) by using the ordinary LS approach:

$$\hat{Y}_{i\mathrm{LS}} = \hat{\alpha}_{\mathrm{LS}} + \hat{\beta}_{\mathrm{LS}} * X_i \quad (1)$$

where $\hat{Y}_{i\mathrm{LS}}$ are the fitted LS values of ln(STV) and X_i are the observed (and centred) X values (see step 2).

6. Estimate the bivariate equation between X and Y. This step consists in rotating the LS regression (Eqn 1) about the centroid of the data ellipse (step 4). The equation of interest is called standardised major axis (SMA), which describes a structural or bivariate relationship between variables based on correlation. There is specific software for fitting this type of regression (Warton *et al.* 2012). However, the most direct and simplest method is to use a mathematical property that relates slopes of LS and SMA regressions (Eqn 2) (Legendre and Legendre 1998). Thus, because all possible regressions of any data ellipse pass through the centroid coordinates ($\bar{X}, \bar{Y}$) (Eqn 3), we can estimate the SMA intercept ($\hat{\alpha}_{\mathrm{SMA}}$) by Eqn 4. Finally, we obtain the complete SMA equation, which for the example application is shown in Fig. 2*b*. Note that Eqn 2 is not plausible when r_{xy} = 0, so it is recommended to test the correlation for significance first (see *Testing correlation significance* section):

$$\hat{\beta}_{\mathrm{SMA}} = \frac{\hat{\beta}_{\mathrm{LS}}}{r_{xy}} \text{ when } r_{xy} \neq 0 \quad (2)$$

$$\bar{Y} = \hat{\alpha}_{\mathrm{SMA}} + \hat{\beta}_{\mathrm{SMA}} * \bar{X} \quad (3)$$

$$\hat{\alpha}_{\mathrm{SMA}} = \bar{Y} - \left[\left(\frac{\hat{\beta}_{\mathrm{LS}}}{r_{xy}} \right) * \bar{X} \right] \quad (4)$$

7. Estimate the CSTV. We must consider the model when X = 0. As in this example, the X values are centred on RY = 90%, the intercept represents the $CSTV_{90\%}$. Because the estimator ($\hat{\alpha}_{\mathrm{SMA}}$) is expressed in logarithmic units (Eqn 5), it is necessary to back-transform it to its original units (Eqn 6, = EXP($\hat{\alpha}_{\mathrm{SMA}}$)):

$$\hat{\alpha}_{\mathrm{SMA}} = \ln(\mathrm{CSTV}_{90}) \quad (5)$$

$$\mathrm{CSTV}_{90} = e^{(\hat{\alpha}_{\mathrm{SMA}})} \quad (6)$$

8. Estimate the confidence interval (CI) of the CSTV. To estimate the confidence limits of the CSTV, we must use Eqns 7 and 8, which have been described as the most appropriate to estimate the CI of intercept for SMA regression (Warton *et al.* 2006). Therefore, a CI with 95% of confidence level equals approximately (depending on the

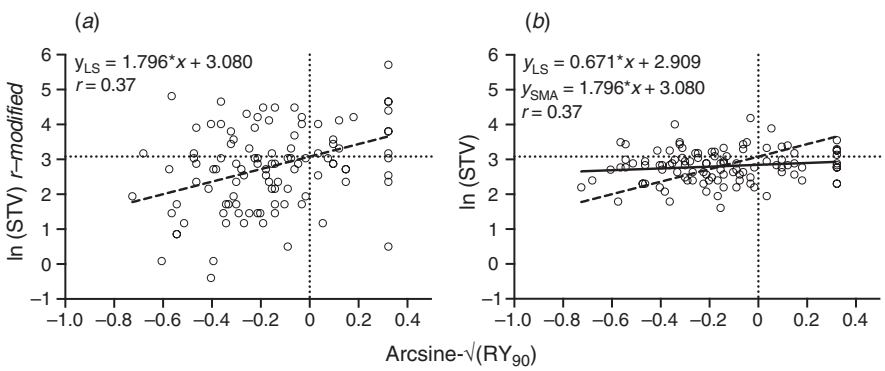

Fig. 2. Linear relationships between soil test value (STV, Colwell P at 0–10 cm) and wheat relative yield (RY) both as transformed variables of dataset 1. The same bivariate linear relationship (dotted lines) is derived from two different data ellipses: (*a*) ordinary least-squares (LS) regression of $Y_{r\text{-modified}}$ values (dotted line) for the original arcsine–log calibration curve (ALCC) (Dyson and Conyers 2013); (*b*) bivariate standardised major axis (SMA) regression (dotted line) for the modified ALCC, derived from the LS regression of ln(STV) (not *r*-modified) on the arcsine of square root of centred RY. In both cases, the intercept ($\hat{\alpha}$) of dashed lines represents the natural logarithm of CSTV.

sample size, n) ± 2SE, whereas a CI with 70% of confidence level equals approximately ± 1 SE. Equation 7 is:

$$SE\hat{\alpha}_{SMA} = \sqrt{\frac{\sum_{i=1}^{n}\left(y_i - \hat{y}_{iSMA}\right)^2}{n-2} * \left[\frac{1}{n} + \frac{\bar{x}^2}{\sum_{i=1}^{n}\left(x_i - x\right)^2}\right]}$$

$$= \sqrt{MSE * \left[\frac{1}{n} + \frac{\bar{x}^2}{SS_x}\right]} \quad (7)$$

where $SE\hat{\alpha}_{SMA}$ represents the standard error of the intercept, y_i are the observed Y values, $\hat{y}_{iSMA}$ are the fitted SMA values ($= \hat{\alpha}_{SMA} + \hat{\beta}_{SMA} * X_i$), n is the sample size, $n - 2$ is degrees of freedom (d.f.), MSE is the mean square error of the model (= (SUM(($y_i - \hat{y}_{iSMA}$)^2))/(d.f.)), and SS_x is the sum of squares of centred X values (= VAR.S(X_{values})*($n - 1$)). Equation 8 is:

$$CI_{\hat{\alpha}_{SMA}} = \hat{\alpha}_{SMA} \pm SE\hat{\alpha}_{SMA} * t_{\left(1-\frac{\alpha}{2};n-2\right)} \quad (8)$$

where $SE\hat{\alpha}_{SMA}$ represents the standard error of the intercept (Eqn 7), and t is the two-tailed Student-$t_{\frac{\alpha}{2}}$ value for an α significance level and $n - 2$ d.f. (= TINV(α, d.f.)).

9. Draw the curve. To fit a RY *v.* STV curve, we must solve the equation based on the ALCC method. The ALCC curve does not describe a causal relationship (predictive) but a bivariate relationship (back-transformed) instead. Fitted values of ln (STV) are obtained by the SMA linear equation (Eqn 9) and back-transformed STV values are obtained by Eqn 10. Finally, for the same range of fitted values with Eqn 9, we can also express the RY values (%) using the parameters of the bivariate relationship (Eqn 11) $\hat{\alpha}_{SMA}$ and $\hat{\beta}_{SMA}$, and the RY_{goal} for which we estimated the CSTV:

$$\hat{Y}_{iSMA}, \ln(STV) = \hat{\alpha}_{SMA} + \hat{\beta}_{SMA}$$

$$* \left[\arcsin\sqrt{\frac{RY_i}{100}} - \arcsin\sqrt{\frac{RY_{goal}}{100}}\right] \quad (9)$$

$$STV_{iSMA} = e^{\left[\ln\left(\hat{Y}_{iSMA}\right)\right]} \quad (10)$$

$$RY_{iSMA}, \% = 100 * \left\{\sin\left[\arcsin\left(\sqrt{\frac{RY_{goal}}{100}}\right) + \frac{\hat{Y}_{iSMA} - \hat{\alpha}_{SMA}}{\hat{\beta}_{SMA}}\right]\right\}^2 \quad (11)$$

Results and discussion

Confidence intervals of CSTVs

Because both variables are inexact, Dyson and Conyers (2013) emphasise finding a 'major axis equation' of the data ellipse. However, the way they reach it has an impact on the error size of the model. In order to get the major axis equation (in this case a standardised major axis), they apply a second transformation of the already transformed ln(STV). This step is designated as the '*r*-modification procedure', but the specific equation used for this second transformation is not described in detail in the paper. The equation is described in the Eqn 12 (C. B. Dyson, pers. comm.). This second transformation produces a new variable ($Y_{r\text{-modified}}$), which has a wider range of values than the original one (Y). Then, by LS regression of $Y_{r\text{-modified}}$ values on X (Eqn 13), they reach the structural relationship of interest. Even though the mean values of intercept ($\hat{\alpha}_{LSr}$) and slope ($\hat{\beta}_{LSr}$) parameters are correct, the *r*-modification procedure generates an unnecessary error overestimation of the model, and thus affects the precision when estimating the CI of CSTV.

$$Y_{i-r\ \text{modified}} = \bar{Y} + \left(\frac{Y_i - \bar{Y}}{r_{xy}}\right) \quad (12)$$

$$\hat{Y}_{iLSr} = \hat{\alpha}_{LSr} + \hat{\beta}_{LSr} * X_i \quad (13)$$

where $\hat{Y}_{iLSr}$ are the fitted *r*-modified values of ln(STV) and X_i are the observed X values (centred).

In cases with wide $CI_{95\%}$ for CSTV, Dyson and Conyers (2013) suggest also to estimate the CSTV with a lower confidence level ($CI_{70\%}$) in order to achieve narrower estimates, especially for the *BFDC Interrogator* (Conyers *et al.* 2013; Watmuff *et al.* 2013). However, this issue of wide CI of CSTVs is a consequence of the *r*-modification procedure, which generates a 'wider in *Y*' data ellipse (Fig. 2). The regression of $Y_{r\text{-modified}}$ values on X is not actually based on the 'true data ellipse', where the bivariate major axis regressions are based on (Jolicoeur 1990; Sokal and Rohlf 1995; Warton *et al.* 2006). In this sense, we suggest this procedure be modified to obtain the bivariate relationship of interest between transformed variables without the error overestimation.

Instead of using the *r*-modification of Y values, we propose to use a bivariate approach called 'standardised major axis regression (SMA)'. This approach is not a prediction of Y depending on X as usual. It is based on representing in one dimension—or axis—data that vary in two dimensions, which could be called a bivariate relationship (Warton *et al.* 2006). The model assumptions are the same as usual: independency, normal distribution of error and homoscedasticity. Transformation seems to play an important role for fulfilling the last two assumptions, which is exemplified for dataset 1 (Fig. 3). In addition, correlation between variables, and whether data follow a distribution that approximates a bivariate normal, should be checked.

In the case of interest (describing a relationship between RY and STV), there are three main characteristics that determine the usefulness of the SMA approach: (*i*) RY and STV represent two observed variables or dimensions of the same experiments; (*ii*) standardisation allows the use of variables that do not have comparable scales of measure; and (*iii*) the independence from any causal relationship between variables means that the X–Y direction of regression is functional to the objectives of the researcher.

With the SMA regression approach, we can estimate exactly the same equation as the original ALCC algorithm but avoiding the CI overestimation of the intercept parameter ($\hat{\alpha}$), which is the CSTV estimator (Fig. 2). Consequently, keeping the same level of confidence (e.g. 95%), the CIs of the modified ALCC algorithm are always more accurate than the original ALCC. For dataset 1, the SMA equation shows more accurate estimates of the intercept ($\hat{\alpha}_{SMA}$; $CI_{95\%}$ = 2.963–3.198) compared with the LS regression

of $Y_{r\text{-modified}}$ values used by the original ALCC method ($\hat{\alpha}_{LS_r}$; $CI_{95\%} = 2.819–3.341$). These results are also observed for dataset 2, with CSTV estimates 30.3–61.4% more accurate for the modified ALCC than the original ALCC algorithm (Table 1).

Based on a comparison of 60 datasets (dataset 3), we also observed that the overestimation of the $SE\hat{\alpha}$ (Eqn 14) was inversely proportional to the correlation coefficient (r_{xy}) of a dataset (Fig. 4). For the analysed cases ($n = 60$), the overestimation varied from 10.6% to 222.5% for datasets with r_{xy} of 0.245 and 0.875, respectively. This inverse relationship is explained by the *r*-modification procedure, which retransforms the ln(STV) values based on the r_{xy} coefficient (Eqn 12). However, the relationship described in Fig. 4 might also allow a relatively simple and reliable ($r^2 = 0.99$) correction of previous estimations based on the original ALCC algorithm (e.g. for the *BFDC Interrogator*) just by using the r_{xy} coefficient of the dataset and Eqn 8. Equation 14 is:

$$SE\hat{\alpha}_{overestimation}(\%) = 100 * \left(\frac{SE\hat{\alpha}_{original} - SE\hat{\alpha}_{modified}}{SE\hat{\alpha}_{modified}} \right) \quad (14)$$

Testing SMA slopes

Because the ALCC curve (back-transformed) comes from a bivariate linear relationship, the SMA slope ($\hat{\beta}_{SMA}$) can also be compared among datasets (Fig. 5*a*, *b*). It might be considered an index of the ALCC curvature (Fig. 5*c*, *d*). Following Eqn 10, back-transformed in terms of RY, a greater $\hat{\beta}_{SMA}$ results in a less steep curve. By contrast, a smaller $\hat{\beta}_{SMA}$ results in a steeper curve. This behaviour was observed in dataset 2 for wheat RY

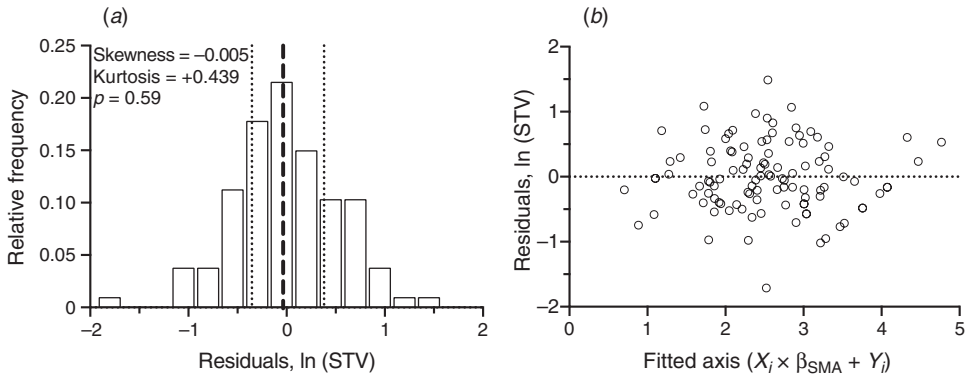

Fig. 3. Residual distribution for testing normality (*a*) and homoscedasticity (*b*) for the standardised major axis (SMA) regression model of transformed variables applying the modified arcsine–log calibration curve (ALCC) methodology of dataset 1 (Fig. 2*b*). STV, Soil test value. The skewness and kurtosis values indicate the level of asymmetry and bias of dataset. Vertical dotted lines indicate percentiles 25, 50 (median) and 75 of distribution. Significance of the D'Agostino–Pearson normality test is indicated with the *P*-value (D'Agostino *et al*. 1990). Homogeneity of variances of SMA regression is tested visually against the fitted axis as described by Warton *et al*. (2006).

Table 1. Comparison of confidence limits of critical soil test value (CSTV) estimates using the modified arcsine–log calibration curve (ALCC) and the original ALCC methods at two levels of confidence (95% and 70%)

Calculations were made for soil Colwell-P at 0–10 cm (mg/kg) at three levels of wheat relative yield (RY: 80%, 90% and 95%). Data was gathered from the *BFDC Interrogator* database (dataset 2)

		80% RY		90% RY		95% RY	
		Lower	Upper	Lower	Upper	Lower	Upper
		Grey Vertosol ($n = 103$, $r_{xy} = 0.33$)					
	CSTV:	13.5		17.8		21.4	
95% Confidence	Modified	11.9	15.3	16.0	19.8	19.1	24.1
	Original	9.9	18.3	13.6	23.2	16.0	28.7
70% Confidence	Modified	12.7	14.4	16.8	18.8	20.1	22.8
	Original	11.5	15.9	15.4	20.5	18.4	25.0
		Black Vertosol ($n = 180$, $r_{xy} = 0.62$)					
	CSTV:	16.3		25.0		33.3	
95% Confidence	Modified	14.5	18.4	22.8	27.4	30.5	36.4
	Original	13.7	19.4	21.9	28.5	29.3	37.9
70% Confidence	Modified	15.3	17.3	23.8	26.2	31.8	34.9
	Original	14.9	17.9	23.3	26.8	31.1	35.7

related to soil Colwell-P level at 0–10 cm, where Black Vertosol soils showed a greater $\hat{\beta}_{SMA}$ ($\hat{\beta}_{Black-CI95\%} = 2.671 - 3.370$) than Grey Vertosol soils ($\hat{\beta}_{Grey-CI95\%} = 1.610 - 2.333$), which also means different fitted ALCC curve shapes (Fig. 5).

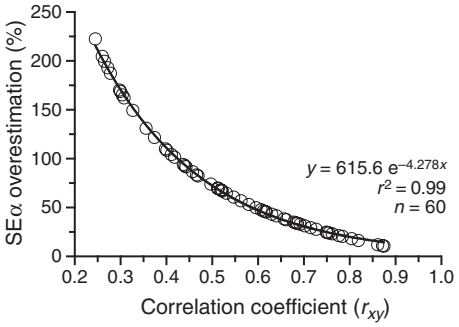

Fig. 4. Relationship between the correlation coefficient (r_{xy}) of a dataset and the relative overestimation of the standard error of the intercept (SE), using the original arcsine–log calibration curve (ALCC) method compared with the modified ALCC (Eqn 14). The overestimation is related to the *r*-modification procedure that the original ALCC algorithm requires to estimate the bivariate equation of interest (standardised major axis). In total, 60 datasets with different r_{xy} were used (dataset 3).

Dyson and Conyers (2013) proposed an estimation of the average slope (and its SE) from 50% to 80% of RY as the deficient zone of the curve. However, the formula is not specified for users who wish to apply the technique. Moreover, even if detailed, the comparison of slopes of SMA regressions does not follow the same formula as the LS regression, as Dyson and Conyers (2013) followed with the *r*-modification procedure. In fact, as well as for the intercept, the $\hat{Y}_{LSr}$ regression (Eqn 13) also overestimates the error of the slope ($\hat{\beta}_{LSr}$) compared with the SMA approach ($\hat{\beta}_{SMA}$, Fig. 2). For dataset 1, the modified ALCC approach showed a 62.6% more accurate estimation for the slope ($\hat{\beta}_{SMA}$; $CI_{95\%} = 1.502–2.147$) than the original ALCC method ($\hat{\beta}_{LSr}$; $CI_{95\%} = 0.933–2.659$).

The SMA regressions have been used to study allometric relationships where the slope $\hat{\beta}_{SMA}$ is the main parameter of interest (Warton and Weber 2002). The confidence interval for the $\hat{\beta}_{SMA}$ can be estimated at a predetermined confidence level, and checked for whether a value of interest lies inside or outside the confidence limits. The formula to compute CI for SMA is different from the LS regression (Eqn 15) (Jolicoeur and Mosimann 1968; Jolicoeur 1990; Sokal and Rohlf 1995). A peculiarity of SMA regression is that the slope cannot be tested for significance (Legendre and Legendre 1998). This is a trivial case because $\hat{\beta}_{SMA}$ (Eqn 2) cannot be zero unless the standard deviation of Y (s_y) is equal to zero. For this reason, among

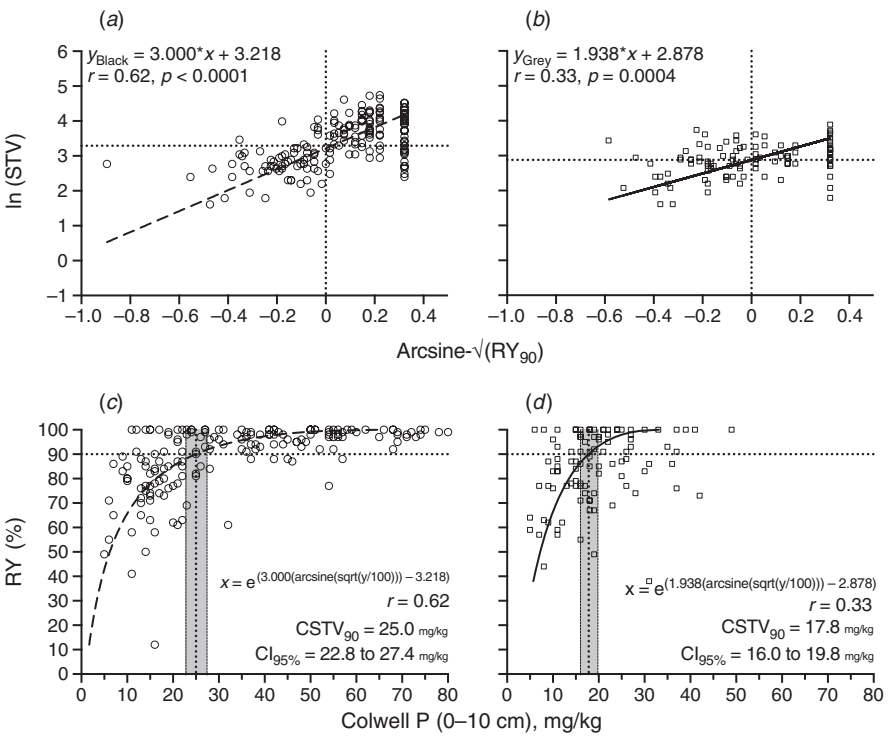

Fig. 5. Relationships between wheat relative yield (RY) and soil test value (STV; Colwell P concentration at 0–10 cm) for two soil types in Australia (dataset 2). Data were gathered from the *BFDC Interrogator* filtering by P-response trials in cereal wheat under dryland conditions in (*a*, *c*) Black Vertosol ($n = 180$) and (*b*, *d*) Grey Vertosol soils ($n = 103$). (*a*, *b*) Bivariate linear regressions (standardised major axis) between transformed variables; (*b*, *d*) the same relationships, back-transformed to the original units. Critical values (CSTV) and their confidence intervals (CI, grey vertical strips) were estimated for 90% of RY with a 95% confidence level.

others, the importance of testing the correlation for significance is discussed below. Equation 15 is:

$$CI_{\hat{\beta}_{SMA}} = \hat{\beta}_{SMA} * \left(\sqrt{(\beta + 1)} \pm \sqrt{\beta} \right), \text{where } \beta = \frac{t^2 * 1 - {r_{xy}}^2}{n - 2} \quad (15)$$

where $\hat{\beta}_{SMA}$ represents the slope value, r_{xy} is the correlation coefficient of the dataset, Y represents a two-tailed Student's $t_{\frac{\alpha}{2}}$ value for an α significance level, and $n-2$ is degrees of freedom.

Testing correlation significance

A criterion to exclude a dataset based only on its correlation strength was established by Dyson and Conyers (2013). In the *BFDC Interrogator*, estimations will not be fitted if a dataset has an r_{xy} <0.2. Despite this criterion being reasonably valid, it could not be enough for potential users of the method. The significance of the correlation coefficient r_{xy} should be tested first in order to determine if a relationship between variables is supported (McArdle 1988). A relationship could be weak but significant or could be strong and yet not significant, where the sample size (n) might play a key role. For large sample sizes, it is easy to achieve significance, and so one should consider the strength of correlation to determine whether the relationship explains very much, or not. Conversely, for small sample sizes, it could be easy to produce a strong correlation by chance and one should consider its significance to prevent rejecting a true null hypothesis. Additionally, as discussed above, the SMA slope is only meaningful when r_{xy} is different from zero (Eqn 2). Therefore, it is advisable to evaluate not only the correlation strength but also its significance for a better interpretation of data. Because correlation between STV and RY is normally expected to be positive (r_{xy} >0), the command to test it in a spreadsheet is = TDIST(t_r, df, 1), where t_r is the t-statistic (Eqn 16) and df is degrees of freedom:

$$t_r = \frac{r_{xy} * \sqrt{n-2}}{\sqrt{r_{xy}^2}} \quad (16)$$

Conclusions

The ALCC algorithm is an interesting approach for estimating CSTVs, which copes with problems usually faced when using traditional regression methods for calibrating soil test data (i.e. lack of normality and homoscedasticity, both variables measured with error). The modified ALCC method described in this paper, even when it requires some additional steps (and probably adds complexity), also incorporates comparative advantages over the original ALCC method. Based on the SMA regression, it produces more accurate estimates of CSTVs and their confidence intervals, as well as more reliable comparisons between datasets.

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