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1 A modification of the arcsine-log calibration curve for analysing soil test

value - relative yield relationships*

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13

14 Abstract. This article aims to discuss the arcsine-log calibration curve (ALCC) method 15 designed for the Better Fertiliser Decisions for Cropping Systems (BFDC) to calibrate 16 relationships between relative yield (RY) and soil test value (STV). Its main advantage is 17 estimating confidence limits of the critical value (CSTV). Nevertheless, intervals for 95% 18 confidence level are often too wide, and authors suggest to reduce the confidence level to 70% 19 in order to achieve narrower estimates. Still, this method can be further improved by modifying 20 specific procedures. For this purpose, several datasets belonging to the BFDC were used. For 21 any confidence level, estimates with the modified-ALCC procedures were always more 22 accurate as compared with the original-ALCC. The overestimation of confidence limits with the 23 original-ALCC was inversely related to the correlation coefficient of the dataset, which might 24 allow a relatively simple and reliable correction of previous estimates. In addition, since the 25 method is based on the correlation between STV and RY, the importance to test it for 26 significance it is emphasized in order to support the hypothesis of a relationship. Then, the 27 modified-ALCC approach could also allow a more reliable comparison of datasets by slopes of 28 the bivariate linear relationship between transformed variables.

29

30 Additional keywords: bivariate model: correlation: standardized major axis regression.

31 Introduction

When developing fertilizer recommendation models based on 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 fertilization 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 RY, as the dependent one. Mathematical functions used to describe this relationship may be linear-plateau, quadratic-plateau or exponential (Mistcherlich) among others (Mallarino and Blackmer, 1992; Colwell, 1963).

39

40 The most widely method used for fitting regression models, the ordinary least squares (LS) 41 approach, assumes that only the dependent variable (e.g. RY) is random while the explanatory 42 or regressor variable (e.g. STV) is considered as fixed and error-free. This approach is 43 especially valid for cases in which the explanatory variable is truly fixed, such as fertiliser rate. 44 However, when this variable is not controlled by the researcher, as happens with STV, 45 researchers normally still consider it as fixed. In this sense, it has been pointed out that LS 46 regression is frequently abused in soil research (Webster, 1997). When the underlying 47 relationship is bivariate it should be described as such and not as a predictive one. As well as 48 crop yield, the STV represents an "observed" dimension of the experiments, and comes from a 49 population that has a reference distribution and thus, an error component. Therefore, a joint 50 distribution of both variables called "bivariate" should be also considered, which its simplest 51 case is the "bivariate normal" (Legendre and Legendre, 1998).

52

53 Furthermore, calibrating RY vs STV often shows problems related to normality and 54 homogeneity of variance. This means a lack of statistical robustness of LS regression to 55 answer questions of interest (Kutner et al., 2005). Neither RY nor STV follow normal

56 distribution, and thus, variable transformation is usually recommended (Webster, 2001). 57 However, the most common situation is transforming only the dependent variable (RY), while 58 keeping original units in the explanatory variable, and thus, the solution results partial. On the 59 other hand, if the nutrient under study is the only limitation to the crop growth, is expected that 60 high levels of STV may result in larger and also less variable yields each time. This behaviour 61 results in a dependence of RY variance on STV values when RY is the dependent variable. 62 Weighted regression is usually applied, but not always brings a solution (Motulsky and 63 Christopoulos, 2004).

64

65 On the other hand, an innovative approach has been recently proposed by Dyson and Convers 66 (2013) for calibrating soil tests aimed at recommending crop fertilization. The ALCC (Arcsine 67 Logarithm Calibration Curve) method has been developed for determining CSTVs for nitrogen 68 (N), phosphorus (P), potassium (K) and sulfur (S) and response of various grain crops in 69 Australia (Anderson et al. 2013:. Bell et al. 2013a; 2013b; 2013c; Brennan and Bell, 2013). As 70 opposed to most commonly used calibrating methodologies, the ALCC method: (i) transforms 71 both variables involved in the relationship (i.e. RY and STV), and (ii) reverses the axes (i.e. fit 72 STV vs. RY) to estimate not only the CSTV for a given RY level but also its confidence interval 73 (CI).

74

In the original study (Dyson and Conyers, 2013), 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 to reduce the confidence level 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 it is possible to achieve more accurate estimates of CSTVs without reducing the level of confidence by
 modifying specific procedures.

82

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

88

89 Materials and Methods

- 90 Data sources and analysis
- 91 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'.

- 99
- 100

101

FIG 1

Dataset #2. A second dataset was also defined using the *BFCD Interrogator Database* in order
 to make specific comparisons of parameters using the original and the modified ALCC method.

104 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'.

108

109 Dataset #3. A third dataset was built for a comparison of standard errors (SE) of the CSTV 110 estimator. For this purpose, 60 datasets of STV and RY were used. They were gathered from 111 (i) the BFCD Interrogator Database (23) (NSW DPI, 2012), and (ii) published and unpublished 112 grain crop fertilisation experiments in the Pampean Region of Argentina (37) including several 113 crop-nutrient combinations (wheat, maize, and soybean crops, and N, P, S, and Zn). This 114 Dataset #3 was defined using specific variables from each of the 60 datasets (n=60): (i) 115 correlation coefficient (r_{xy}) , (ii) SE of CSTV estimator using the original-ALLC method, and (iii) 116 SE of CSTV estimator using the modified-ALLC method.

117

All datasets were tabulated and processed in a Microsoft Excel ® 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).

123

124 Procedures of the modified-ALCC

A total of 9 steps are needed, each one 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 they could vary depending on the software version and language. Steps #1 to #3 of the modified-ALCC are basically the same as the original-ALCC method (Dyson and Conyers, 2013). Specific differences are detailed in the Results andDiscussion section.

- 131 **1.** Transform variables. This will simplify the relationship between variables as a simple
 132 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, cmol_c/kg, among others.
- b. Arcsine of the square root for the RY, hereinafter X (=ASIN(SQRT(RY_i/100))).
 The original RY units must be always expressed with respect to a maximum
 yield (observed or estimated), see Dyson & Conyers (2013) for additional
 details.
- 1402. Center the X variable, with respect to the RY level for which you want to estimate the141CSTV (=ASIN(SQRT(RY_i/100))-ASIN(SQRT(RY_{goal}/100))). For example, for a142RY_{goal}=90% we need to subtract, from each value of X, the corresponding143arcsine $\sqrt{(90/100)} = 1.249$.
- 144
 3. Estimate the Pearson correlation coefficient (r_{xy}), between X (centered) and Y
 145 (=PEARSON(X_{values}, Y_{values}). Since the methodology is based on "correlation" between
 146 variables, it is advisable to test this coefficient for significance before the next steps.
- 147 **4.** Estimate the average means of centered X (=AVERAGE(X_{values})) and Y 148 (=AVERAGE(Y_{values})). They represent coordinates of the data ellipse centroid ($\overline{X}, \overline{Y}$), 149 where all possible regressions pass through.
- 150 5. Estimate a linear regression (Eqn. 1) between X and Y values (Fig. 2) using the
 151 ordinary least squares (LS) approach.
- 152 $\hat{Y}_{iLS} = \hat{\alpha}_{LS} + \hat{\beta}_{LS} * X_i \tag{1}$

153 Where, \hat{Y}_{iLS} are the fitted LS values of ln(STV) and X_i are the observed (and centered) 154 X values (see Step #2).

- 155 6. Estimate the bivariate equation between X and Y. This step basically consists in 156 rotating the LS regression (Eqn. 1) about the centroid of the data ellipse (Step #4). The 157 equation of interest is called standardized major axis (SMA), which describes a 158 structural or bivariate relationship between variables based on correlation. There is 159 specific software for fitting this type of regression (Warton et al., 2012). However, the 160 most direct and simplest way is to use a mathematical property that relates slopes of LS 161 and SMA regressions (Eqn. 2) (Legendre and Legendre, 1998). Thus, since all possible regressions of any data ellipse pass through the centroid coordinates $(\overline{X}, \overline{Y})$ (**Eqn. 3**), 162 we can estimate the SMA intercept ($\hat{\alpha}_{SMA}$) by Eqn. 4. Finally, we obtain the complete 163 164 SMA equation, which for the example application is shown in Fig. 2B. Note that Eqn. 2 is not plausible when $r_{xy} = 0$, so correlation is recommended to be tested for 165 166 significance first (see "Testing correlation significance" section).
- 167
- 168

169

FIG 2

(2)

- 170 $\hat{\beta}_{SMA} = \frac{\hat{\beta}_{LS}}{r_{xy}}, \text{ when } r_{xy} \neq 0$
- 171

172
$$\bar{Y} = \hat{\alpha}_{SMA} + \hat{\beta}_{SMA} * \bar{X}$$
(3)

- 173
- 174 $\hat{\alpha}_{SMA} = \overline{Y} \left[\left(\frac{\widehat{\beta}_{LS}}{r_{xy}} \right) * \overline{X} \right]$ (4)

7. Estimate the CSTV. It has to be consider the model when X = 0. As in this example, the X values are centered on RY = 90%, the intercept represents the CSTV_{90%}. Since the estimator ($\hat{\alpha}_{SMA}$) is expressed in logarithmic units (**Eqn. 5**), it is necessary to backtransform it to its original units (**Eqn. 6**, =EXP($\hat{\alpha}_{SMA}$)).

180

$$\hat{\alpha}_{SMA} = ln(CSTV_{90}) \tag{5}$$

182

$$CSTV_{90} = e^{(\widehat{\alpha}_{SMA})}$$
(6)

184

8. Estimate the confidence interval (CI) of the CSTV. To estimate the confidence limits of the CSTV we must use **Eqn. 7** and **Eqn.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 sample size n) ± 2 standard errors (SE), while a CI with 70% of confidence level equals approximately ± 1 SE.

191

192
$$SE\hat{\alpha}_{SMA} = \sqrt{\frac{\sum_{i=1}^{n} (y_i - \hat{y}_{iSMA})^2}{n-2} * \left[\frac{1}{n} + \frac{\bar{x}^2}{\sum_{i=1}^{n} (x_i - \bar{x})^2}\right]} = \sqrt{MSE * \left[\frac{1}{n} + \frac{\bar{x}^2}{SS_x}\right]}$$
(7)

193 Where, $SE\hat{\alpha}_{SMA}$ represents the standard error of the intercept, y_i are the observed Y values, 194 \hat{y}_{iSMA} are the fitted SMA values (= $\hat{\alpha}_{SMA} + \hat{\beta}_{SMA} * X_i$), n is the sample size, n - 2 are 195 degrees of freedom (df), MSE represents the mean square error of the model (=(SUM(($y_i - \hat{y}_{iSMA})^2$))/(df)), and SS_x is the sum of squares of centered X values (=VAR.S(X_{values})*(n-1)).

198
$$CI_{\hat{\alpha}_{SMA}} = \hat{\alpha}_{SMA} \pm SE\hat{\alpha}_{SMA} * t_{\left(1 - \frac{\alpha}{2}; n - 2\right)}$$
(8)

199 Where, $SE\hat{\alpha}_{SMA}$ represents the standard error of the intercept (**Eqn. 7**), and *t* is the two-tailed 200 Student- $t_{\frac{\alpha}{2}}$ value for an α significance level and n - 2 df (=TINV(α , df)).

201

9. Draw the curve. To fit a RY vs 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.

209

210
$$\hat{Y}_{iSMA}, \ ln(STV) = \hat{\alpha}_{SMA} + \hat{\beta}_{SMA} * \left[arcsine \sqrt{\frac{RY}{100}} - arcsine \sqrt{\frac{RY_{goal}}{100}} \right]$$
(9)

211

212
$$STV_{iSMA} = e^{\left[\hat{Y}_{iSMA}\right]}$$
(10)

213

214
$$RY(\%) = 100 * \left\{ sin\left[arcsine\left(\sqrt{\frac{RY_{goal}}{100}}\right) + \frac{\hat{Y}_{iSMA} - \hat{\alpha}_{SMA}}{\hat{\beta}_{SMA}} \right] \right\}^2$$
(11)

215

216 **Results and Discussion**

217 Confidence intervals of CSTVs

Since both variables are inexact, Dyson and Conyers (2013) make focus in 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 standardized major 221 axis), they apply a second transformation of the already transformed In(STV). This step is 222 designated as the "r-modification procedure", but the specific equation used for this second 223 transformation is not properly described in the paper. The equation is described in the Eqn. 12 224 (Dyson, pers. comm.). This second transformation produces a new variable (Y_{r-modified}) which has a wider range of values than the original one (Y). Then by a LS regression of $Y_{r-modified}$ 225 226 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" 227 228 procedure" generates an unnecessary error overestimation of the model, and thus affects the 229 precision when estimating the CI of CSTV.

230

231
$$Y_{i-r \ modified} = \overline{Y} + \left(\frac{Y_i - \overline{Y}}{r_{xy}}\right)$$
(12)

232

233

234
$$\hat{Y}_{iLSr} = \hat{\alpha}_{LSr} + \hat{\beta}_{LSr} * X_i$$
(13)

Where, \hat{Y}_{iLSr} are the fitted r-modified values of ln(STV) and X_i are the observed X values (centered).

236

In cases with wide $CI_{95\%}$ for CSTV, Dyson and Conyers (2013) suggests to also 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 lies on the r-modification procedure which generates a "wider in Y" data ellipse (**Fig. 2**). Regression of *Y*_{*r*-modified} values on X is not actually based on the "true data ellipse", where the bivariate major axis equations are based on (Jolicoeur, 1990; Sokal and Rohlf, 1995; Warton et al., 2006). In this sense, we suggest to modify this procedure to obtain the bivariate relationship of interest between transformed variables without the error overestimation.

246

247 Instead of using the *r*-modification of Y values, we propose to use a bivariate approach called 248 'standardized major axis regression (SMA)'. This approach is not a prediction of Y depending 249 on X as usual. It is based on representing in one dimension -or axis- data that varies in two 250 dimensions, which could be called as a bivariate relationship (Warton et al., 2006). The model 251 assumptions are the same as usual: independency, normal distribution of error and 252 homoscedasticity. Transformation seems to play an important role for fulfilling the last two 253 assumptions, which is exemplified for Dataset #1 (Fig. 3). In addition, correlation between 254 variables and whether data follow a distribution that approximates a bivariate normal or not 255 should be checked out.

256

In the particular 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) standardization allows using variables that do not have comparable scales of measure, and (iii) the independence from any causal relationship between variables, then the X:Y direction of SMA regression is functional to the objectives of the researcher.

- 263
- 264
- 265

<u>FIG 3.</u>

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

269	Cls of the modified-ALCC algorithm are always more accurate than the original-ALCC. For the
270	Dataset #1, the SMA equation shows more accurate estimates of the intercept (\hat{a}_{SMA} ,
271	$CI_{95\%}$ =2.963-3.198) as compared with the LS regression of $Y_{r-modified}$ values used by the original-
272	ALCC method ($\hat{\alpha}_{LS_r}$; Cl _{95%} =2.819-3.341). These results are also observed for Dataset #2, with
273	CSTV estimaties from +30.3% to +61.4% more accurate for the modified-ALCC as compared
274	to the original-ALCC algorithm (Table 1).
275	
276	TABLE 1
277	
278	Based on a 60 datasets comparison (Dataset #3), we also observed that the overestimation of
279	the SE $\hat{\alpha}$ (Eqn. 14) was inversely proportional to the correlation coefficient (r _{xy}) of a dataset
280	(Fig. 4). For the analysed cases (n=60), the overestimation varied from +10.6% to +222.5% for
281	datasets with r_{xy} of 0.245 and 0.875, respectively. This inverse relationship is explained by the
282	r-modification procedure which retransforms the $ln(STV)$ values based on the r_{xy} coefficient
283	(Eqn. 12). However, the relationship described in Fig. 4 might also allow a relatively simple
284	and reliable (r^2 =0.99) correction of previous estimations based on the original-ALCC algorithm
285	(e.g. for the <i>BFDC Interrogator</i>) just using the "r _{xy} " coefficient of the dataset and Eqn. 8 .
286	$SE\hat{\alpha}_{overestimation}(\%) = 100 * \left(\frac{SE\hat{\alpha}_{original} - SE\hat{\alpha}_{modified}}{SE\hat{\alpha}_{modified}}\right) $ (14)
287	
288	FIG 4
289	
290	Testing SMA slopes
291	Since the ALCC curve (back-transformed) comes from a bivariate linear relationship, the SMA
292	slope ($\hat{\beta}_{SMA}$) can also be compared among datasets (Fig. 5A and 5B). It might be considered

as an index of the ALCC curvature (**Fig. 5C** and **5D**). Following **Eqn. 10** -back-transformed in terms of RY-, a greater $\hat{\beta}_{SMA}$ results in a less steep curve. In contrast, a smaller $\hat{\beta}_{SMA}$ results in a steeper curve. This behaviour was observed in Dataset #2 for wheat RY related to soil Colwell-P level at 0-10 cm, where Vertosol Black soils showed a greater $\hat{\beta}_{SMA}$ $(\hat{\beta}_{Black-CI95\%}=2.671-3.370)$ as compared to Vertosol Grey soils $(\hat{\beta}_{Grey-CI95\%}=1.610-2.333)$ which also means different fitted ALCC curve shapes (**Fig. 5**).

- 299
- 300
- 301

FIG 5

302 Dyson and Convers (2013) proposed an estimation of the average slope (and its SE) from 50% 303 to 80% of RY as the deficient zone of the curve. However, the formula is not specified for users 304 who want to apply the technique. Moreover, even if detailed, the comparison of slopes of SMA 305 regressions does not follow the same formula as the LS regression, as Dyson and Convers 306 (2013) followed after the *r-modification* procedure. In fact, as well as for intercept, the LS regression of Y_{r-modified} values also overestimates the error of the slope ($\hat{\beta}_{SMA}$) as compared to 307 308 the true SMA approach (Fig. 2). For the Dataset #1, the modified-ALCC approach showed a 309 62.6% more accurate estimation for the slope ($\hat{\beta}_{SMA}$, Cl_{95%}=1.502-2.147) as compared with the 310 original-ALCC method ($\hat{\beta}_{LS_{r}}$, Cl_{95%}=0.933-2.659).

311

The SMA regressions have been used to study allometric relationships where the slope $\hat{\beta}_{SMA}$ is the main parameter of interest (Warton et al., 2002). The confidence interval for the $\hat{\beta}_{SMA}$ can be estimated at a predetermined confidence level, and checked whether a value of interest lies inside or outside the confidence limits. The formula to compute CI for SMA is different compared to 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 others, the importance of testing the correlation for significance is discussed below.

321

322
$$CI_{\hat{\beta}_{SMA}} = \hat{\beta}_{SMA} * \left(\sqrt{(\beta+1)} \pm \sqrt{\beta}\right), \text{ where } \beta = \frac{t^2 * 1 - r_{XY}^2}{n-2}$$
 (15)

323 Where, $\hat{\beta}_{SMA}$ represents the slope value, r_{xy} is the correlation coefficient of dataset, t represents a two-324 tailed Student's $t_{\frac{\alpha}{2}}$ value for an α significance level, and n - 2 are degrees of freedom.

325

326 Testing correlation significance

327 A criterion to exclude a dataset based only on its correlation strength was established by 328 Dyson and Convers (2013). In the BFDC Interrogator, estimations will not be fitted if a dataset 329 has an r_{xy} <0.2. Despite this criterion is 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 330 331 order to determine if a relationship between variables is supported (McArdle, 1988). A 332 relationship could be weak but significant or could be strong and yet not significant, where the 333 sample size (n) might play a key role. For large sample sizes it is easy to achieve significance 334 and one should also consider the strength of correlation to determine whether the relationship 335 explains very much or not. Conversely, for small sample sizes it could be easy to produce a 336 strong correlation by chance and one should also consider its significance to keep from 337 rejecting a true null hypothesis. Additionally, as discussed above, the SMA slope is only 338 meaningful when r_{xy} is different from zero (Eqn. 2). Therefore, it is advisable to evaluate not 339 only the correlation strength but also its significance for a better interpretation of data. Since 340 correlation between STV and RY is normally expected be positive (rxy>0), the commands to

test it in a spreadsheet is =TDIST(t_r , df, 1), where t_r is the t-statistic (**Eqn. 16**) and df are degrees of freedom.

343
$$t_r = \frac{r_{xy} * \sqrt{n-2}}{\sqrt{r_{xy}^2}}$$
 (16)

344

345 **Conclusions**

The ALCC algorithm is an interesting approach for estimating CSTVs, which cope with problems usually faced when using traditional regression methods for calibrating soil tests 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 add complexity), it 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.

353

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359

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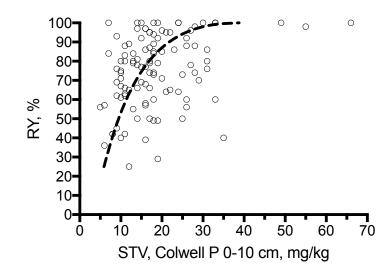


Fig. 1. Scatter plot of relative yield (RY, %) and soil test value (STV, Colwell P at 0-10 cm, mg/kg) for Dataset #1 -107 experiments from the National Soil Fertility Program (NSFP, 1968-72) in Victoria (107 class A trials)-. Data was gathered from the BFDC Interrogator database following previous descriptions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

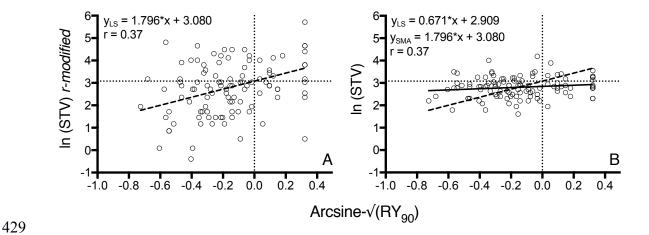


Fig. 2. Linear relationships between STV (Colwell P, 0-10cm) and wheat relative yield (RY) both as transformed variables of Dataset #1. The same structural linear relationship (dotted lines) is derived from two different data ellipses (A and B). A: ordinary least-squares (LS) regression of $Y_{r-modified}$ values (dotted line) for the original ALCC (Dyson and Conyers, 2013). B: bivariate standardized major axis (SMA) regression (dotted line) for the modified ALCC, derived from the LS regression of ln(STV) *–not rmodified-* on the arcsine of square root of centered RY. In both cases, the intercept ($\hat{\alpha}$) of dashed lines represents the natural logarithm of CSTV.

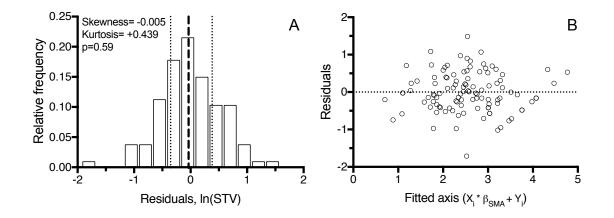


Fig. 3. Residual distribution for testing normality (A) and homoscedasticity (B) for the SMA regression model of transformed variables applying the modified-ALCC methodology of Dataset #1 (Fig. 2 B). The Skewness and Kurtosis values indicate the level of asymmetry and bias of dataset. Vertical dotted 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).

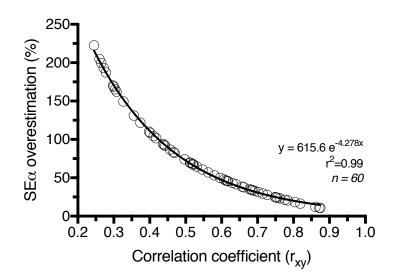
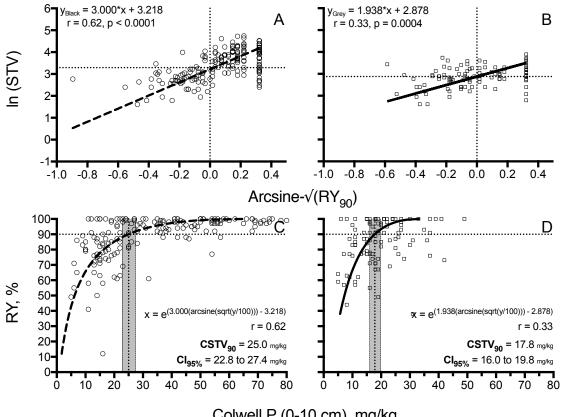


Fig. 4. Relationship between the correlation coefficient (r_{xy}) of a dataset and the relative overestimation of the standard error of the intercept (SE) using the original-ALCC method in comparison to the modified-ALCC (**Eqn. 14**). The overestimation is related to the r-modification procedure that the original-ALCC algorithm requires to estimate the bivariate equation of interest (standardized major axis). A total of 60 datasets with different r_{xy} were used (Dataset #3).





Colwell P (0-10 cm), mg/kg

454 Fig. 5. Relationships between wheat relative yield and soil Colwell P concentration (0-10 cm, mg/kg) for 455 two soil types in Australia (Dataset #2). Data was gathered from the BFDC Interrogator filtering by P 456 response trials in cereal wheat under dryland conditions in Vertosol Black (A and C, n=180) and Vertosol 457 Grey soils (B and D, n=103). A and B show the bivariate linear regressions (standardized major axis) 458 between transformed variables, while C and D show the same relationships, back-transformed to the 459 original units. Critical values (CSTV) and their confidence intervals (CI, grey vertical strips) were 460 estimated for 90% of RY with a 95% confidence level.

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466 **Table 1.** Comparison of confidence limits of critical soil test values (CSTV) estimates using the modified-467 ALCC and the original-ALCC methods at two levels of confidence (95% and 70%). Calculations were 468 made for soil Colwell-P at 0-10 cm (mg/kg) at three levels of wheat relative yield (RY 80%, 90% and 469 95%). Data was gathered from the BFDC Interrogator database (Dataset #2).

		80% RY		90% RY		95% RY	
Vertosol Grey	CSTV	13.5		17.8		21.4	
(n = 103, r = 0.33)		Lower	Upper	Lower	Upper	Lower	Upper
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
Vertosol Black	CSTV	16.3		25.0		33.3	
(n = 180, r = 0.62)							
(11 = 100, 1 = 0.02)		Lower	Upper	Lower	Upper	Lower	Upper
	Modified	Lower 14.5	Upper 18.4	Lower 22.8	Upper 27.4	Lower 30.5	Upper 36.4
95% Confidence	Modified Original		•••				
		14.5	18.4	22.8	27.4	30.5	36.4
	Modified		•••				