

# Bivariate least squares linear regression: towards a unified analytic formalism.

## II. Extreme structural models

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### **Abstract**

Concerning bivariate least squares linear regression, the classical results obtained for extreme structural models in earlier attempts [14, 10] are reviewed using a new formalism in terms of deviation (matrix) traces which, for homoscedastic data, reduce to usual quantities leaving aside an unessential (but dimensional) multiplicative factor. Within the framework of classical error models, the dependent variable relates to the independent variable according to a variant of the usual additive model. The classes of linear models considered are regression lines in the limit of uncorrelated errors in  $X$  and in  $Y$ . The following models are considered in detail: (Y) errors in  $X$  negligible (ideally null) with respect to errors in  $Y$ ; (X) errors in  $Y$  negligible (ideally null) with respect to errors in  $X$ ; (C) oblique regression; (O) orthogonal regression; (R) reduced major-axis regression; (B) bisector regression. For homoscedastic data, the results are taken from earlier attempts and rewritten using a more compact notation. For heteroscedastic data, the results are inferred from a procedure related to functional models [23, 7]. An example of astronomical application is considered, concerning the  $[\text{O}/\text{H}]-[\text{Fe}/\text{H}]$  empirical relations deduced from five samples related to different stars and/or different methods of oxygen abundance determination. For low-dispersion samples and assigned methods, different regression models yield results which are

in agreement within the errors ( $\mp\sigma$ ) for both heteroscedastic and homoscedastic data, while the contrary holds for large-dispersion samples. In any case, samples related to different methods produce discrepant results, due to the presence of (still undetected) systematic errors, which implies no definitive statement can be made at present. Asymptotic expressions approximate regression line slope and intercept variance estimators, for normal residuals, to a better extent with respect to earlier attempts. Related fractional discrepancies are not exceeding a few percent for low-dispersion data, which grows up to about 10% for large-dispersion data. An extension of the formalism to generic structural models is left to further investigation.

keywords: bivariate regression; linear regression; least squares regression;

## 1 Introduction

Linear regression is a fundamental and frequently used statistical tool in almost all branches of science, among which astronomy. The related problem is twofold: regression line slope and intercept estimators are expressed involving minimizing or maximizing some function of the data; on the other hand, regression line slope and intercept variance estimators are expressed requiring knowledge of the error distributions of the data. The complexity mainly arises from the occurrence of intrinsic dispersion in addition to the dispersion related to the measurement processes (hereafter quoted as instrumental dispersion), where the distribution corresponding to the former can be different from the distribution corresponding to the latter i.e. non Gaussian (non normal).

In statistics, problems where the true points have fixed but unknown coordinates are called functional regression models, while problems where the true points have random (i.e. obeying their own intrinsic distribution) and unknown coordinates are called structural regression models. Accordingly, functional regression models may be conceived as structural regression models where the intrinsic dispersion is negligible (ideally null) with respect to the instrumental dispersion. Conversely, structural regression models where the instrumental dispersion is negligible (ideally null) with respect to the intrinsic dispersion, can be defined as extreme structural models [7]. A distinction between functional and structural modelling is currently preferred, where the former can be affected by intrinsic scatter but with no or only min-

imal assumptions on related distributions, while the latter implies (usually parametric) models are placed on the above mentioned distributions. For further details refer to specific textbooks e.g., [8] Chap. 2, §2.1. In addition, models where the instrumental dispersion is the same from point to point for each variable, are called homoscedastic models, while models where the instrumental dispersion is (in general) different from point to point, are called heteroscedastic models. Similarly, related data are denoted as homoscedastic and heteroscedastic, respectively.

In general, problems where the true points lie precisely on an expected line relate to functional regression models, while problems where the true points are (intrinsically) scattered about an expected line relate to structural regression models [10, 11].

Bivariate least squares linear regression related to heteroscedastic functional models with uncorrelated and correlated errors, following Gaussian distributions, were analysed and formulated in two classical papers [23, 25], where regression line slope and intercept variance estimators are determined using the method of partial differentiation [25]. On the contrary, the method of moments estimator is used to this aim in later attempts e.g., [12] Chap. 1, §1.3.2, Eq. (1.3.7), [10].

Bivariate least squares linear regression related to extreme structural models, where the instrumental dispersion is negligible (ideally null) with respect to intrinsic dispersion, was exhaustively treated in two classical papers [14, 10] and extended to generic structural models in a later attempt [1].

The above mentioned papers provide the simplest description of linear regression. In reality, biases and additional effects must be taken into consideration, which implies much more complicated description and formulation, as it can be seen in specific monographies e.g., [12, 8, 4]. Restricting to the astronomical literature, a recent investigation [15] is particularly relevant in that it is the first example (in the field under discussion) where linear regression is considered following the modern (since about half a century ago) approach based on likelihoods rather than the old (up to about a century ago) least-squares approach. More specifically, a hierarchical measurement error model is set up therein, the complicated likelihood is written down, and a variety of minimum least-squares and Bayesian solutions are shown, which can treat functional, structural, multivariate, truncated and censored measurement error regression problems.

Even in dealing with the simplest homoscedastic (or heteroscedastic) func-

tional and structural models, still no unified analytic formalism has been developed (to the knowledge of the author) where (i) structural heteroscedastic models with instrumental and intrinsic dispersion of comparable order in both variables, are considered; (ii) previous results are recovered in the limit of dominant instrumental dispersion; and (iii) previous results are recovered in the limit of dominant intrinsic dispersion. A related formulation may be useful also for computational methods, in the sense that both the general case and limiting situations can be described by a single numerical code.

A first step towards a unified analytic formalism of bivariate least squares linear regression involving functional models was performed in an earlier attempt [7], where the least-squares approach developed in two classical papers [23, 25] was reviewed and reformulated by definition and use of deviation (matrix) traces. The current investigation aims at making a second step along the same direction, in dealing with extreme structural models.

More specifically, the results found in two classical papers [14, 10] shall be reformulated in terms of deviation traces for homoscedastic models, and extended to the general case of heteroscedastic models by analogy with their counterparts related to functional models, within the framework of classical error models where the dependent variable relates to the independent variable according to a variant of the classical additive error model.

In this view, homoscedastic structural models are conceived as models where both the instrumental and the intrinsic dispersion are the same from point to point. Conversely, models where the instrumental and/or the intrinsic dispersion are (in general) different from point to point, are conceived as heteroscedastic structural models.

Regression line slope and intercept estimators, and related variance estimators, are expressed in terms of deviation traces for different homoscedastic models [14, 10] in section 2, where an extension to corresponding heteroscedastic models is also performed, and both normal and non normal residuals are considered. An example of astronomical application is outlined in section 3. The discussion is presented in section 4. Finally, the conclusion is shown in section 5. Some points are developed with more detail in the Appendix. An extension of the formalism to generic structural models is left to further investigation.

## 2 Least-squares fitting of a straight line

### 2.1 General considerations

Attention shall be restricted to the classical problem of least-squares fitting of a straight line, where both variables are measured with errors. Without loss of generality, structural models can be conceived as related to an ideal situation where the variables obey a linear relation<sup>1</sup>, as:

$$y_i^* = ax_i^* + b \quad ; \quad 1 \leq i \leq n \quad ; \quad (1)$$

in connection with true points,  $\mathbf{P}_i^* \equiv (x_i^*, y_i^*)$ ,  $1 \leq i \leq n$ . The occurrence of random (measure independent) processes makes true points shift outside or along the ideal straight line, inferred from Eq. (1), towards actual points,  $\mathbf{P}_{Si} \equiv (x_{Si}, y_{Si})$ . The occurrence of measurement processes makes the actual points shift towards the observed points,  $\mathbf{P}_i \equiv (X_i, Y_i)$ .

In this view, the least squares fitting of a straight line is conceptually similar for functional (in absence of intrinsic scatter) and structural (in presence of intrinsic scatter) models: “What is the best line fitting to a sample of observed points,  $\mathbf{P}_i$ ,  $1 \leq i \leq n$ ?” It is worth noticing the correspondence between true points,  $\mathbf{P}_i^*$ , and observed points,  $\mathbf{P}_i$ , is not one-to-one unless it is assumed all points are shifted along the same direction. More specifically, two observed points,  $\mathbf{P}_i, \mathbf{P}_j$ , with equal coordinates,  $(X_i, Y_i) = (X_j, Y_j)$ , relate to true points,  $\mathbf{P}_i^*, \mathbf{P}_j^*$ , with (in general) different coordinates,  $(x_i^*, y_i^*) \neq (x_j^*, y_j^*)$ , both in presence and in absence of intrinsic scatter. The least-square estimator and the loss function have the same formal expression for functional and structural models, but in the latter case the “statistical distances” e.g., [12] Chap. 1, §1.3.3, depend on the total (instrumental + intrinsic) scatter.

The observed points and the actual points are related as:

$$Z_i = z_{Si} + (\xi_{F_z})_i \quad ; \quad Z = X, Y \quad ; \quad z = x, y \quad ; \quad 1 \leq i \leq n \quad ; \quad (2)$$

where  $(\xi_{F_x})_i, (\xi_{F_y})_i$ , are the instrumental (i.e. due to the instrumental scatter) errors on  $x_{Si}, y_{Si}$ , respectively, assumed to obey Gaussian distributions with null expectation values and known variances,  $[(\sigma_{xx})_F]_i, [(\sigma_{yy})_F]_i$ , and covariance,  $[(\sigma_{xy})_F]_i$ .

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<sup>1</sup>The Italian convention shall be adopted here, according to which the slope and the intercept of a straight line on the Cartesian plane, are denoted as  $a, b$ , respectively.

The actual points and the true points on the ideal straight line are related as:

$$z_{Si} = z_i^* + (\xi_{S_z})_i ; \quad z = x, y; \quad 1 \leq i \leq n ; \quad (3)$$

where  $(\xi_{S_x})_i, (\xi_{S_y})_i$ , are the intrinsic (i.e. due to the intrinsic scatter) errors on  $x_i^*, y_i^*$ , respectively, assumed to obey specified distributions with null expectation values and finite variances,  $[(\sigma_{xx})_S]_i, [(\sigma_{yy})_S]_i$ , and covariance,  $[(\sigma_{xy})_S]_i$ .

The observed points and the true points on the ideal straight line are related as:

$$Z_i = z_i^* + \xi_{z_i} ; \quad Z = X, Y; \quad z = x, y ; \quad 1 \leq i \leq n ; \quad (4)$$

where the (instrumental + intrinsic) errors,  $\xi_{x_i}, \xi_{y_i}$ , are defined as:

$$\xi_{z_i} = (\xi_{F_z})_i + (\xi_{S_z})_i ; \quad z = x, y ; \quad 1 \leq i \leq n ; \quad (5)$$

which obey specified distributions with null expectation values and finite variances,  $(\sigma_{xx})_i, (\sigma_{yy})_i$ , and covariance,  $(\sigma_{xy})_i$ . The further restriction that  $(\xi_{F_z})_i, (\xi_{S_z})_i, z = x, y, 1 \leq i \leq n$ , are independent, implies the relation [1]:

$$(\sigma_{zz})_i = [(\sigma_{zz})_F]_i + [(\sigma_{zz})_S]_i ; \quad (\sigma_{xy})_i = [(\sigma_{xy})_F]_i + [(\sigma_{xy})_S]_i ; \quad (6)$$

where the intrinsic covariance matrixes are unknown and must be assigned or estimated, which will be supposed in the following.

Then the error model is defined by Eqs. (1)-(6), where both instrumental errors,  $(\xi_{F_z})_i$ , and intrinsic errors,  $(\xi_{S_z})_i$ , are assumed to be independent of true values,  $z_i^*$ , for given instrumental covariance matrixes,  $(\Sigma_F)_i = \|[ (\sigma_{xy})_F ]_i \|$ , intrinsic covariance matrixes,  $(\Sigma_S)_i = \|[ (\sigma_{xy})_S ]_i \|$ , respectively, and (total) covariance matrixes,  $\Sigma_i = \|[ (\sigma_{xy})_i ] \|$ , hence  $\Sigma_i = (\Sigma_F)_i + (\Sigma_S)_i, 1 \leq i \leq n$ . It may be considered as a variant of the classical additive error model e.g., [1], [8] Chap. 1, §1.2, Chap. 3, §3.2.1, [15, 16], [4] Chap. 4, §4.3.

In the case under discussion, the regression estimator minimizes the loss function, defined as the sum (over the  $n$  observations) of squared residuals e.g., [25], or statistical distances of the observed points,  $P_i \equiv (X_i, Y_i)$ , from the estimated line in the unknown parameters,  $a, b, x_1, \dots, x_n$ , e.g., [12] Chap. 1, §1.3.3. Under restrictive assumptions, the regression estimator is the functional maximum likelihood estimator e.g., [8] Chap. 3, §3.4.2.

The coordinates,  $(x_i, y_i)$ , may be conceived as the adjusted values of related observations,  $(X_i, Y_i)$ , on the estimated regression line [23, 25] and, in addition, as estimators of the coordinates,  $(x_i^*, y_i^*)$ , on the true regression line i.e. the ideal straight line. The line of adjustment,  $\overline{P_i \hat{P}_i}$  e.g., [25], may be conceived as an estimator of the statistical distance,  $\overline{P_i P_i^*}$  e.g., [12] Chap. 1, §1.3.3, where  $\hat{P}_i(x_i, y_i)$  is the adjusted point on the estimated regression line, which implies the relation:

$$y_i = \hat{a}x_i + \hat{b} \quad ; \quad 1 \leq i \leq n \quad ; \quad (7)$$

where, in general, estimators are denoted by hats, and  $P_i^*(x_i^*, y_i^*)$  is the true point on the ideal straight line, Eq. (1).

To the knowledge of the author, only classical error models are considered for astronomical applications, and for this reason different error models such as Berkson models and mixture error models e.g., [8] Chap. 3, Sect. 3.2, shall not be dealt with in the current attempt. From this point on, investigation shall be limited to extreme structural models and least-squares regression estimators for the following reasons. First, they are important models in their own right, furnishing an approximation to real world situations. Second, a careful examination of these simple models helps for understanding the theoretical underpinnings of methods for other models of greater complexity such as hierarchical models e.g., [15, 16].

## 2.2 Extreme structural models

With regard to extreme structural models, bivariate least squares linear regression were analysed in two classical papers in the special case of oblique regression i.e. constant variance ratio,  $(\sigma_{yy})_i/(\sigma_{xx})_i = c^2$ ,  $1 \leq i \leq n$ , and constant correlation coefficients,  $r_i = r$ ,  $1 \leq i \leq n$ . More specifically, orthogonal ( $c^2 = 1$ ) and oblique regression were analysed in the earlier [14] and in the latter [10] paper, respectively. In absence of additional information, homoscedastic models are used [14] unless the intrinsic dispersion is estimated [1], from which related weights may be determined and the least squares estimator together with the loss function may be expressed for both homoscedastic and heteroscedastic models [1, 16].

The (dimensionless) squared weighted residuals can be defined as in the

case of functional models [25]:

$$(\tilde{R}_i)^2 = \frac{w_{x_i}(X_i - x_i)^2 + w_{y_i}(Y_i - y_i)^2 - 2r_i\sqrt{w_{x_i}w_{y_i}}(X_i - x_i)(Y_i - y_i)}{1 - r_i^2} ; \quad (8a)$$

$$r_i = \frac{(\sigma_{xy})_i}{[(\sigma_{xx})_i(\sigma_{yy})_i]^{1/2}} ; \quad |r_i| \leq 1 ; \quad 1 \leq i \leq n ; \quad (8b)$$

where  $w_{x_i}$ ,  $w_{y_i}$ , are the weights of the various measurements (or observations) and  $r_i$  the correlation coefficients. The terms,  $w_{x_i}(X_i - x_i)^2$ ,  $w_{y_i}(Y_i - y_i)^2$ ,  $r_i$ ,  $1 \leq i \leq n$ , are dimensionless by definition. An equivalent formulation in matrix formalism can be found in specific textbooks, where weighted true residuals are conceived as (dimensionless) “statistical distances” from data points to related points on the regression line e.g., [12] Chap. 1, §1.3.3, Eq. (1.3.16).

Accordingly, the least-squares regression estimator and the loss function can be expressed as in the case of functional models [7] but the weights,  $w_{x_i}$ ,  $w_{y_i}$ , and the correlation coefficients,  $r_i$ , are related to intrinsic scatter instead of instrumental scatter. Then the regression line slope and intercept estimators take the same formal expression with respect to their counterparts related to functional models, while (in general) the contrary holds for regression line slope and intercept variance estimators.

Classical results on extreme structural models [14, 10] are restricted to oblique regression for homoscedastic data with constant correlation coefficients ( $w_{x_i} = w_x$ ,  $w_{y_i} = w_y$ ,  $r_i = r$ ,  $1 \leq i \leq n$ ). In the following subsections, the above mentioned results extended to heteroscedastic data shall be expressed in terms of weighted deviation (matrix) traces [7]:

$$\tilde{Q}_{pq} = \sum_{i=1}^n Q_i(w_{x_i}, w_{y_i}, r_i)(X_i - \tilde{X})^p(Y_i - \tilde{Y})^q ; \quad (9)$$

$$\tilde{Q}_{00} = \sum_{i=1}^n Q_i(w_{x_i}, w_{y_i}, r_i) = n\bar{Q} ; \quad (10)$$

where  $\tilde{Q}_{pq}$  are the (weighted) pure ( $p = 0$  and/or  $q = 0$ ) and mixed ( $p > 0$  and  $q > 0$ ) deviation traces, and  $\tilde{X}$ ,  $\tilde{Y}$ , are weighted means:

$$\tilde{Z} = \frac{\sum_{i=1}^n W_i Z_i}{\sum_{i=1}^n W_i} ; \quad Z = X, Y ; \quad (11)$$



$$W_i = \frac{w_{x_i} \Omega_i^2}{1 + a^2 \Omega_i^2 - 2ar_i \Omega_i} ; \quad 1 \leq i \leq n ; \quad (12)$$

$$\Omega_i = \sqrt{\frac{w_{y_i}}{w_{x_i}}} ; \quad 1 \leq i \leq n ; \quad (13)$$

in the limit of homoscedastic data with equal correlation coefficients,  $w_{x_i} = w_x$ ,  $w_{y_i} = w_y$ ,  $r_i = r$ ,  $1 \leq i \leq n$ , which implies  $Q_i(w_{x_i}, w_{y_i}, r_i) = Q(w_x, w_y, r) = Q$ , Eqs. (9), (10), (11), (12), and (13) reduce to:

$$\tilde{Q}_{pq} = QS_{pq} ; \quad (14)$$

$$S_{pq} = \sum_{i=1}^n (X_i - \bar{X})^p (Y_i - \bar{Y})^q ; \quad (15)$$

$$\tilde{Q}_{00} = QS_{00} ; \quad (16)$$

$$S_{00} = n ; \quad (17)$$

$$\tilde{Z} = \bar{Z} ; \quad Z = X, Y ; \quad (18)$$

$$W_i = W = \frac{w_x \Omega^2}{1 + a^2 \Omega^2 - 2ar\Omega} ; \quad 1 \leq i \leq n ; \quad (19)$$

$$\Omega_i = \Omega = \sqrt{\frac{w_y}{w_x}} ; \quad 1 \leq i \leq n ; \quad (20)$$

where  $S_{pq}$  are the (unweighted) pure ( $p = 0$  and/or  $q = 0$ ) and mixed ( $p > 0$  and  $q > 0$ ) deviation traces.

Turning to the general case and using the weighted squared error loss function,  $T_{\tilde{R}} = \sum_{i=1}^n (\tilde{R}_i)^2$ , yields for regression line slope and intercept estimators the same expression with respect to functional models [7]. Accordingly, regression line slope and intercept estimators may be conceived similarly to state functions in thermodynamics: for an assigned true point,  $\mathbf{P}_i^* \equiv (x_i^*, y_i^*)$ , what is relevant is the related observed point,  $\mathbf{P}_i \equiv (X_i, Y_i)$ , regardless of the path followed via instrumental and/or intrinsic scatter. More specifically, the regression line intercept estimator obeys the equation e.g., [25, 7]:

$$\hat{b} = \tilde{Y} - \hat{a} \tilde{X} ; \quad (21)$$

which implies the ‘‘barycentre’’ of the data,  $\tilde{\mathbf{P}} \equiv (\tilde{X}, \tilde{Y})$ , lies on the estimated regression line, inferred from Eq. (7), and the regression line slope estimator is one among three real solutions of a pseudo cubic equation or two real solutions of a pseudo quadratic equation, where the coefficients are weakly

dependent on the unknown slope. For further details refer to earlier attempts [23, 25, 7]. The above mentioned equations have the same formal expression for functional and structural models, which also holds for the regression line slope and intercept estimators.

The regression line slope and intercept variance estimators for functional models, calculated using the method of partial differentiation e.g., [25] and the method of moments estimators e.g., [12] Chap. 1, §1.3.2, Eq. (1.3.7), yield, in general, different results [7]. The same is expected to hold, a fortiori, for structural models, for which the method of moments estimators and the  $\delta$ -method have been exploited in classical investigations e.g., [14, 10]. Accordingly, related results shall be considered and expressed in terms of unweighted deviation traces for homoscedastic data with equal correlation coefficients and extended in terms of weighted deviation traces for heteroscedastic data, with regard to a number of special cases considered in earlier attempts in the limit of uncorrelated errors in  $X$  and in  $Y$  [14, 10]. With this restriction, the pseudo cubic equation reduces to:

$$\tilde{V}_{20}a^3 - 2\tilde{V}_{11}a^2 - (\tilde{W}_{20} - \tilde{V}_{02})a + \tilde{W}_{11} = 0 \quad ; \quad (22)$$

where the deviation traces are defined by Eq. (9), via Eq. (12) and  $V_i = W_i^2/w_{x_i}$ . For further details refer to the parent paper [23] and to a recent attempt [7]. A formulation of Euclidean and statistical squared residual sum for homoscedastic and heteroscedastic data is expressed in A.

### 2.3 Errors in $X$ negligible with respect to errors in $Y$

In the limit of errors in  $X$  negligible with respect to errors in  $Y$ ,  $a^2(\sigma_{xx})_i \ll (\sigma_{yy})_i$ ,  $a(\sigma_{xy})_i \ll (\sigma_{yy})_i$ ,  $1 \leq i \leq n$ . Ideally,  $(\sigma_{xx})_i \rightarrow 0$ ,  $(\sigma_{xy})_i \rightarrow 0$ ,  $1 \leq i \leq n$ , which implies  $r_i \rightarrow 0$ ,  $w_{x_i} \rightarrow +\infty$ ,  $\Omega_i \rightarrow 0$ ,  $W_i \rightarrow w_{y_i}$ ,  $1 \leq i \leq n$ . Accordingly, the errors in  $X$  and in  $Y$  are uncorrelated.

For homoscedastic data,  $w_{x_i} = w_x$ ,  $w_{y_i} = w_y$ ,  $1 \leq i \leq n$ , the regression line slope and intercept estimators are [14, 7]:

$$\hat{a}_Y = \frac{S_{11}}{S_{20}} \quad ; \quad (23)$$

$$\hat{b}_Y = \bar{Y} - \hat{a}_Y \bar{X} \quad ; \quad (24)$$

where the index,  $Y$ , stands for OLS( $Y|X$ ) i.e. ordinary least square regression or, in general, WLS( $Y|X$ ) i.e. weighted least square regression of the depen-

dent variable,  $Y$ , against the independent variable,  $X$  [14]. Accordingly, related models shall be quoted as  $Y$  models.

The regression line slope and intercept variance estimators, in the special case of normal residuals may be calculated using different methods and/or models e.g., [12] Chap. 1, §1.3.2, Eq. (1.3.7), [10, 7]. The result is:

$$\begin{aligned} [(\hat{\sigma}_{\hat{a}_Y})_N]^2 &= \frac{(\hat{a}_Y)^2}{n-2} \left[ \frac{(n-2)R_Y}{\hat{a}_Y S_{11}} + \Theta(\hat{a}_Y, \hat{a}_Y, \hat{a}_X) \right] \\ &= \frac{(\hat{a}_Y)^2}{n-2} \left[ \frac{\hat{a}_X - \hat{a}_Y}{\hat{a}_Y} + \Theta(\hat{a}_Y, \hat{a}_Y, \hat{a}_X) \right] ; \end{aligned} \quad (25)$$

$$[(\hat{\sigma}_{\hat{b}_Y})_N]^2 = \left[ \frac{1}{\hat{a}_Y} \frac{S_{11}}{S_{00}} + (\bar{X})^2 \right] [(\hat{\sigma}_{\hat{a}_Y})_N]^2 - \frac{\hat{a}_Y}{n-2} \frac{S_{11}}{S_{00}} \Theta(\hat{a}_Y, \hat{a}_Y, \hat{a}_X) ; \quad (26)$$

where the index,  $N$ , denotes normal residuals,  $R$  is defined in A, and  $\hat{a}_X = S_{02}/S_{11}$ . The function,  $\Theta(\hat{a}_Y, \hat{a}_Y, \hat{a}_X)$ , is a special case of a more general function,  $\Theta(\hat{a}_C, \hat{a}_Y, \hat{a}_X)$  which, in turn, depends on the method and/or model used. For further details refer to B.

The regression line slope and intercept variance estimators, in the general case of non normal residuals may be calculated using the  $\delta$ -method [14]. The result is:

$$(\hat{\sigma}_{\hat{a}_Y})^2 = \frac{S_{22} + (\hat{a}_Y)^2 S_{40} - 2\hat{a}_Y S_{31}}{(S_{20})^2} ; \quad (27)$$

$$(\hat{\sigma}_{\hat{b}_Y})^2 = \frac{\hat{a}_Y}{n} \frac{\hat{a}_X - \hat{a}_Y}{\hat{a}_Y} \frac{S_{11}}{S_{00}} + (\bar{X})^2 (\hat{\sigma}_{\hat{a}_Y})^2 - \frac{2}{n} \bar{X} \hat{\sigma}_{\hat{b}_Y \hat{a}_Y} ; \quad (28)$$

$$\hat{\sigma}_{\hat{b}_Y \hat{a}_Y} = \frac{S_{12} + (\hat{a}_Y)^2 S_{30} - 2\hat{a}_Y S_{21}}{S_{20}} ; \quad (29)$$

where Eqs.(27)-(29) are equivalent to their counterparts expressed in the parent paper [14].

The application of the  $\delta$ -method provides asymptotic formulae which underestimate the true regression coefficient uncertainty in samples with low ( $n \lesssim 50$ ) or weakly correlated population [10]. In the special case of normal and data-independent residuals,  $\Theta(\hat{a}_Y, \hat{a}_Y, \hat{a}_X) \rightarrow 0$ , Eqs. (27), (28), must necessarily reduce to (25), (26), respectively, which implies an additional factor,  $n/(n-2)$ , in the first term on the right-hand side of Eqs. (27)-(29). For further details refer to C.

The expression of the regression line slope and intercept estimators and related variance estimators for normal residuals, Eqs. (23), (24), (25), (26),

coincide with their counterparts determined for Y models in classical and recent attempts e.g., [10] Eq. (4) therein in the limit  $c^2 = \sigma_{yy}/\sigma_{xx} \rightarrow +\infty$ , [17] Eqs. (3)-(7) therein.

For heteroscedastic data, the regression line slope and intercept estimators are [7]:

$$\hat{a}_Y = \frac{(\tilde{w}_y)_{11}}{(\tilde{w}_y)_{20}} ; \quad (30)$$

$$\hat{b}_Y = \tilde{Y} - \hat{a}_Y \tilde{X} ; \quad (31)$$

where the weighted means,  $\tilde{X}$  and  $\tilde{Y}$ , are defined by Eqs. (11)-(13).

For functional models, regression line slope and intercept variance estimators in the general case of heteroscedastic data reduce to their counterparts in the special case of homoscedastic data, as  $\{\hat{\sigma}_{\hat{a}_Y}[(\tilde{w}_y)_{pq}]\}^2 \rightarrow [\hat{\sigma}_{\hat{a}_Y}(w_y S_{pq})]^2$ ,  $\{\hat{\sigma}_{\hat{b}_Y}[(\tilde{w}_y)_{pq}]\}^2 \rightarrow [\hat{\sigma}_{\hat{b}_Y}(w_y S_{pq})]^2$ , via Eq. (9) where  $Q_i = (w_y)_i = w_y$ ,  $1 \leq i \leq n$ . For further details refer to an earlier attempt [7].

Under the assumption that the same holds for extreme structural models, Eqs. (25)-(29) take the general expression:

$$\begin{aligned} [(\hat{\sigma}_{\hat{a}_Y})_N]^2 &= \frac{(\hat{a}_Y)^2}{n-2} \left[ \frac{n-2}{n} \frac{R_Y}{\hat{a}_Y} \frac{(\tilde{w}_y)_{00}}{(\tilde{w}_y)_{11}} + \Theta(\hat{a}_Y, \hat{a}_Y, \hat{a}'_X) \right] \\ &= \frac{(\hat{a}_Y)^2}{n-2} \left[ \frac{\hat{a}'_X - \hat{a}_Y}{\hat{a}_Y} + \Theta(\hat{a}_Y, \hat{a}_Y, \hat{a}'_X) \right] ; \end{aligned} \quad (32)$$

$$[(\hat{\sigma}_{\hat{b}_Y})_N]^2 = \left[ \frac{1}{\hat{a}_Y} \frac{(\tilde{w}_y)_{11}}{(\tilde{w}_y)_{00}} + (\tilde{X})^2 \right] [(\hat{\sigma}_{\hat{a}_Y})_N]^2 - \frac{\hat{a}_Y}{n-2} \frac{(\tilde{w}_y)_{11}}{(\tilde{w}_y)_{00}} \Theta(\hat{a}_Y, \hat{a}_Y, \hat{a}'_X) ; \quad (33)$$

$$(\hat{\sigma}_{\hat{a}_Y})^2 = \frac{(\tilde{w}_y)_{00} (\tilde{w}_y)_{22} + (\hat{a}_Y)^2 (\tilde{w}_y)_{40} - 2\hat{a}_Y (\tilde{w}_y)_{31}}{n [(\tilde{w}_y)_{20}]^2} ; \quad (34)$$

$$(\hat{\sigma}_{\hat{b}_Y})^2 = \frac{\hat{a}_Y}{n} \frac{\hat{a}'_X - \hat{a}_Y}{\hat{a}_Y} \frac{(\tilde{w}_y)_{11}}{(\tilde{w}_y)_{00}} + (\tilde{X})^2 (\hat{\sigma}_{\hat{a}_Y})^2 - \frac{2}{n} \tilde{X} \hat{\sigma}_{\hat{b}_Y \hat{a}_Y} ; \quad (35)$$

$$\hat{\sigma}_{\hat{b}_Y \hat{a}_Y} = \frac{(\tilde{w}_y)_{12} + (\hat{a}_Y)^2 (\tilde{w}_y)_{30} - 2\hat{a}_Y (\tilde{w}_y)_{21}}{(\tilde{w}_y)_{20}} ; \quad (36)$$

where  $\hat{a}'_X = (\tilde{w}_y)_{02}/(\tilde{w}_y)_{11}$ ,  $R$  is defined in A and  $\Theta$  is expressed in terms of  $n(\tilde{w}_y)_{pq}/(\tilde{w}_y)_{00}$  instead of  $S_{pq}$ .

In the special case of normal and data-independent residuals,  $\Theta(\hat{a}_Y, \hat{a}_Y, \hat{a}'_X) \rightarrow 0$ , Eqs. (34), (35), must necessarily reduce to (32), (33), respectively, which implies an additional factor,  $n/(n-2)$ , in the first term on the right-hand side of Eqs. (34)-(36).

In absence of a rigorous proof, Eqs. (32)-(36) must be considered as approximate results.

## 2.4 Errors in $Y$ negligible with respect to errors in $X$

In the limit of errors in  $Y$  negligible with respect to errors in  $X$ ,  $(\sigma_{yy})_i \ll a^2(\sigma_{xx})_i$ ,  $(\sigma_{xy})_i \ll a(\sigma_{xx})_i$ ,  $1 \leq i \leq n$ . Ideally,  $(\sigma_{yy})_i \rightarrow 0$ ,  $(\sigma_{xy})_i \rightarrow 0$ ,  $1 \leq i \leq n$ , which implies  $r_i \rightarrow 0$ ,  $w_{y_i} \rightarrow +\infty$ ,  $\Omega_i \rightarrow +\infty$ ,  $W_i \rightarrow w_{x_i}$ ,  $1 \leq i \leq n$ . Accordingly, the errors in  $X$  and in  $Y$  are uncorrelated. As outlined in an earlier paper [7], the model under discussion can be related to the inverse regression, which has a large associate literature e.g., [18, 13, 19, 2, 17].

For homoscedastic data,  $w_{x_i} = w_x$ ,  $w_{y_i} = w_y$ ,  $1 \leq i \leq n$ , the regression line slope and intercept estimators are ([14, 7]:

$$\hat{a}_X = \frac{S_{02}}{S_{11}} ; \quad (37)$$

$$\hat{b}_X = \bar{Y} - \hat{a}_X \bar{X} ; \quad (38)$$

where the index, X, stands for OLS(X|Y) i.e. ordinary least square regression or, in general, WLS(X|Y) i.e. weighted least square regression of the dependent variable,  $X$ , against the independent variable,  $Y$  [14]. Accordingly, related models shall be quoted as X models.

The regression line slope and intercept variance estimators, in the special case of normal residuals may be calculated using different methods and/or models e.g., [12] Chap. 1, §1.3.2, Eq. (1.3.7), [10, 7]. The result is:

$$\begin{aligned} [(\hat{\sigma}_{\hat{a}_X})_N]^2 &= \frac{(\hat{a}_X)^2}{n-2} \left[ \frac{(n-2)R_X}{\hat{a}_X S_{11}} + \Theta(\hat{a}_X, \hat{a}_Y, \hat{a}_X) \right] \\ &= \frac{(\hat{a}_X)^2}{n-2} \left[ \frac{\hat{a}_X - \hat{a}_Y}{\hat{a}_Y} + \Theta(\hat{a}_X, \hat{a}_Y, \hat{a}_X) \right] ; \end{aligned} \quad (39)$$

$$[(\hat{\sigma}_{\hat{b}_X})_N]^2 = \left[ \frac{1}{\hat{a}_X} \frac{S_{11}}{S_{00}} + (\bar{X})^2 \right] [(\hat{\sigma}_{\hat{a}_X})_N]^2 - \frac{\hat{a}_X}{n-2} \frac{S_{11}}{S_{00}} \Theta(\hat{a}_X, \hat{a}_Y, \hat{a}_X) ; \quad (40)$$

where the index, N, denotes normal residuals,  $R$  is defined in A, and  $\hat{a}_Y = S_{11}/S_{20}$ . The function,  $\Theta(\hat{a}_X, \hat{a}_Y, \hat{a}_X)$ , is a special case of a more general function,  $\Theta(\hat{a}_C, \hat{a}_Y, \hat{a}_X)$  which, in turn, depends on the method and/or model used. For further details refer to B.

The regression line slope and intercept variance estimators, in the general case of non normal residuals may be calculated using the  $\delta$ -method [14]. The result is:

$$(\hat{\sigma}_{\hat{a}_X})^2 = \frac{S_{04} + (\hat{a}_X)^2 S_{22} - 2\hat{a}_X S_{13}}{(S_{11})^2} ; \quad (41)$$

$$(\hat{\sigma}_{\hat{b}_X})^2 = \frac{\hat{a}_X \hat{a}_X - \hat{a}_Y \frac{S_{11}}{S_{00}}}{n} + (\bar{X})^2 (\hat{\sigma}_{\hat{a}_X})^2 - \frac{2}{n} \bar{X} \hat{\sigma}_{\hat{b}_X \hat{a}_X} ; \quad (42)$$

$$\hat{\sigma}_{\hat{b}_X \hat{a}_X} = \frac{S_{03} + (\hat{a}_X)^2 S_{21} - 2\hat{a}_X S_{12}}{S_{11}} ; \quad (43)$$

where Eqs.(41)-(43) are equivalent to their counterparts expressed in the parent paper [14].

The application of the  $\delta$ -method provides asymptotic formulae which underestimate the true regression coefficient uncertainty in samples with low ( $n \lesssim 50$ ) or weakly correlated population [10]. In the special case of normal and data-independent residuals,  $\Theta(\hat{a}_X, \hat{a}_Y, \hat{a}_X) \rightarrow 0$ , Eqs. (41), (42), must necessarily reduce to (39), (40), respectively, which implies an additional factor,  $n/(n-2)$ , in the first term on the right-hand side of Eqs. (41)-(43). For further details refer to C.

For heteroscedastic data, the regression line slope and intercept estimators are [7]:

$$\hat{a}_X = \frac{(\tilde{w}_x)_{02}}{(\tilde{w}_x)_{11}} ; \quad (44)$$

$$\hat{b}_X = \tilde{Y} - \hat{a}_X \tilde{X} ; \quad (45)$$

where the weighted means,  $\tilde{X}$  and  $\tilde{Y}$ , are defined by Eqs. (11)-(13).

For functional models, regression line slope and intercept variance estimators in the general case of heteroscedastic data reduce to their counterparts in the special case of homoscedastic data, as  $\{\hat{\sigma}_{\hat{a}_X}[(\tilde{w}_x)_{pq}]\}^2 \rightarrow [\hat{\sigma}_{\hat{a}_X}(w_x S_{pq})]^2$ ,  $\{\hat{\sigma}_{\hat{b}_X}[(\tilde{w}_x)_{pq}]\}^2 \rightarrow [\hat{\sigma}_{\hat{b}_X}(w_x S_{pq})]^2$ , via Eq. (9) where  $Q_i = (w_x)_i = w_x$ ,  $1 \leq i \leq n$ . For further details refer to an earlier attempt [7].

Under the assumption that the same holds for extreme structural models, Eqs. (39)-(43) take the general expression:

$$[(\hat{\sigma}_{\hat{a}_X})_N]^2 = \frac{(\hat{a}_X)^2}{n-2} \left[ \frac{n-2}{n} \frac{R_X}{\hat{a}_X} \frac{(\tilde{w}_x)_{00}}{(\tilde{w}_x)_{11}} + \Theta(\hat{a}_X, \hat{a}'_Y, \hat{a}_X) \right]$$

$$= \frac{(\hat{a}_X)^2}{n-2} \left[ \frac{\hat{a}_X - \hat{a}'_Y}{\hat{a}'_Y} + \Theta(\hat{a}_X, \hat{a}'_Y, \hat{a}_X) \right] ; \quad (46)$$

$$[(\hat{\sigma}_{\hat{b}_X})_N]^2 = \left[ \frac{1}{\hat{a}_X} \frac{(\tilde{w}_x)_{11}}{(\tilde{w}_x)_{00}} + (\tilde{X})^2 \right] [(\hat{\sigma}_{\hat{a}_X})_N]^2 - \frac{\hat{a}_X}{n-2} \frac{(\tilde{w}_x)_{11}}{(\tilde{w}_x)_{00}} \Theta(\hat{a}_X, \hat{a}'_Y, \hat{a}_X) ; \quad (47)$$

$$(\hat{\sigma}_{\hat{a}_X})^2 = \frac{(\tilde{w}_x)_{00} (\tilde{w}_x)_{04} + (\hat{a}_X)^2 (\tilde{w}_x)_{22} - 2\hat{a}_X (\tilde{w}_x)_{13}}{n [(\tilde{w}_x)_{11}]^2} ; \quad (48)$$

$$(\hat{\sigma}_{\hat{b}_X})^2 = \frac{\hat{a}_X \hat{a}_X - \hat{a}'_Y}{n \hat{a}'_Y} \frac{(\tilde{w}_x)_{11}}{(\tilde{w}_x)_{00}} + (\tilde{X})^2 (\hat{\sigma}_{\hat{a}_X})^2 - \frac{2}{n} \tilde{X} \hat{\sigma}_{\hat{b}_X \hat{a}_X} ; \quad (49)$$

$$\hat{\sigma}_{\hat{b}_X \hat{a}_X} = \frac{(\tilde{w}_x)_{03} + (\hat{a}_X)^2 (\tilde{w}_x)_{21} - 2\hat{a}_X (\tilde{w}_x)_{12}}{(\tilde{w}_x)_{11}} ; \quad (50)$$

where  $\hat{a}'_Y = (\tilde{w}_x)_{11}/(\tilde{w}_x)_{20}$ ,  $R$  is defined in A, and  $\Theta$  is formulated in terms of  $n(\tilde{w}_x)_{pq}/(\tilde{w}_x)_{00}$  instead of  $S_{pq}$ .

In the special case of normal and data-independent residuals,  $\Theta(\hat{a}_X, \hat{a}'_Y, \hat{a}_X) \rightarrow 0$ , Eqs. (48), (49), must necessarily reduce to (46), (47), respectively, which implies an additional factor,  $n/(n-2)$ , in the first term on the right-hand side of Eqs. (48)-(50).

In absence of a rigorous proof, Eqs. (46)-(50) must be considered as approximate results.

## 2.5 Oblique regression

In the limit of constant  $y$  to  $x$  variance ratios and constant correlation coefficients, the following relations hold:

$$\frac{(\sigma_{yy})_i}{(\sigma_{xx})_i} = c^2 ; \quad \frac{w_{x_i}}{w_{y_i}} = \Omega_i^{-2} = c^2 ; \quad \frac{(\sigma_{xy})_i}{(\sigma_{xx})_i} = r_i c = rc ; \quad 1 \leq i \leq n ; \quad (51)$$

$$W_i = \frac{w_{x_i}}{a^2 + c^2 - 2rac} ; \quad 1 \leq i \leq n ; \quad \frac{(\tilde{w}_y)_{pq}}{(\tilde{w}_y)_{rs}} = \frac{(\tilde{w}_x)_{pq}}{(\tilde{w}_x)_{rs}} ; \quad (52)$$

where the weights are assumed to be inversely proportional to related variances,  $w_{z_i} \propto 1/(\sigma_{zz})_i$ ,  $z = x, y$ , as usually done e.g., [10]. By definition,  $c$  has the dimensions of a slope, which highly simplifies dimension checks throughout equations, and for this reason it has been favoured with respect to different choices exploited in earlier attempts e.g., [23], [12] Chap. 1, §1.3, [10].

It is worth noticing that Eq. (51) holds for both homoscedastic and heteroscedastic data. It can be seen that the lines of adjustment are oriented

along the same direction [24] but are perpendicular to the regression line only in the special case of orthogonal regression,  $c^2 = 1$  e.g., [8] Chap. 3, §3.4.2. Accordingly, the term “oblique regression” has been preferred with respect to “generalized orthogonal regression” used in an earlier attempt [7].

The variance ratio,  $c^2$ , may be expressed in terms of instrumental and intrinsic variance ratios,  $c_F^2$ , and  $c_S^2$ , respectively, as:

$$c^2 = \frac{[(\sigma_{xx})_i]_F}{(\sigma_{xx})_i} c_F^2 + \frac{[(\sigma_{xx})_i]_S}{(\sigma_{xx})_i} c_S^2 ; \quad 1 \leq i \leq n ; \quad (53a)$$

$$c_F^2 = \frac{[(\sigma_{yy})_i]_F}{[(\sigma_{xx})_i]_F} ; \quad c_S^2 = \frac{[(\sigma_{yy})_i]_S}{[(\sigma_{xx})_i]_S} ; \quad 1 \leq i \leq n ; \quad (53b)$$

where  $c_F^2 = c_S^2$  implies  $c_F^2 = c_S^2 = c^2$ ;  $c^2 \rightarrow c_F^2$  for functional models,  $[(\sigma_{zz})_i]_S \ll [(\sigma_{zz})_i]_F$ ,  $z = x, y$ ,  $1 \leq i \leq n$ ;  $c^2 \rightarrow c_S^2$  for extreme structural models,  $[(\sigma_{zz})_i]_F \ll [(\sigma_{zz})_i]_S$ ,  $z = x, y$ ,  $1 \leq i \leq n$ .

For homoscedastic data,  $w_{x_i} = w_x$ ,  $w_{y_i} = w_y$ ,  $1 \leq i \leq n$ , the regression line slope and intercept estimators are [10, 7]:

$$\begin{aligned} \hat{a}_C &= \frac{S_{02} - c^2 S_{20}}{2S_{11}} \left\{ 1 \mp \left[ 1 + c^2 \left( \frac{S_{02} - c^2 S_{20}}{2S_{11}} \right)^{-2} \right]^{1/2} \right\} \\ &= \frac{\hat{a}_X \hat{a}_Y - c^2}{2\hat{a}_Y} \left\{ 1 \mp \left[ 1 + c^2 \left( \frac{\hat{a}_X \hat{a}_Y - c^2}{2\hat{a}_Y} \right)^{-2} \right]^{1/2} \right\} ; \end{aligned} \quad (54)$$

$$\hat{b}_C = \bar{Y} - \hat{a}_C \bar{X} ; \quad (55)$$

where the index, C, denotes oblique regression,  $\hat{a}_Y = S_{11}/S_{20}$ ,  $\hat{a}_X = S_{02}/S_{11}$ , and the double sign corresponds to the solutions of a second-degree equation, where the parasite solution must be disregarded. Accordingly, related models shall be quoted as C models or O models in the special case of orthogonal regression ( $c^2 = 1$ ). For further details refer to an earlier attempt [7].

The regression line slope and intercept variance estimators, in the special case of normal residuals may be calculated using different methods and/or models e.g., [12] Chap. 1, §1.3.2, Eq. (1.3.7), [10, 7]. The result is:

$$\begin{aligned} [(\hat{\sigma}_{\hat{a}_C})_N]^2 &= \frac{(\hat{a}_C)^2}{n-2} \left[ \frac{(n-2)R_C}{\hat{a}_C S_{11}} + \Theta(\hat{a}_C, \hat{a}_Y, \hat{a}_X) \right] \\ &= \frac{(\hat{a}_C)^2}{n-2} \left[ \frac{\hat{a}_X - \hat{a}_C}{\hat{a}_C} + \frac{\hat{a}_C - \hat{a}_Y}{\hat{a}_Y} + \Theta(\hat{a}_C, \hat{a}_Y, \hat{a}_X) \right] ; \end{aligned} \quad (56)$$



Table 1: Explicit expression of the function,  $\Theta(\hat{a}_C, \hat{a}_Y, \hat{a}_X)$ , appearing in the slope and intercept variance estimator formula for oblique regression, Eq. (56) and (57), respectively, according to different methods and/or models. Symbol captions:  $A_{UV} = \hat{a}_U/\hat{a}_V - 1$ ;  $(U,V) = (X,C), (C,Y)$ . Method captions: AFD - asymptotic formula determination; MME - method of moments estimators; LSE - least squares estimation; MPD - method of partial differentiation. Model captions: F - functional; S - structural; E - extreme structural. Case captions: HM - homoscedastic; HT - heteroscedastic.

$\Theta(\hat{a}_C, \hat{a}_Y, \hat{a}_X)$	method	model	case	source
0	AFD	E	HM	[11]
$A_{XC}A_{CY} + \frac{(A_{CY})^2}{n-1}$	MME	E	HM	[10]
$A_{XC}A_{CY} + \frac{(A_{CY})^2}{n-1}$	MME	S	HM	[12]
$\frac{A_{XC}A_{CY}}{n-1} + \left(\frac{A_{CY}}{n-1}\right)^2$	LSE	E	HM	[11]
$2A_{XC}A_{CY}$	MPD	F	HT	[7]

$$[(\hat{\sigma}_{\hat{b}_C})_N]^2 = \left[ \frac{1}{\hat{a}_C} \frac{S_{11}}{S_{00}} + (\bar{X})^2 \right] [(\hat{\sigma}_{\hat{a}_C})_N]^2 - \frac{\hat{a}_C}{n-2} \frac{S_{11}}{S_{00}} \Theta(\hat{a}_C, \hat{a}_Y, \hat{a}_X) ; \quad (57)$$

where  $R$  is defined in A and  $\Theta$  depends on the method and/or model used, as shown in Table 1. For a formal demonstration, see B. The extreme situations,  $a_C \rightarrow a_Y$ ,  $a_C \rightarrow a_X$ , are directly inferred from Table 1 as  $\Theta(a_Y, a_Y, a_X) = 0$ ,  $\Theta(a_X, a_Y, a_X) = 0$ , respectively, in all cases. More specifically, the former relation rigorously holds while the latter has to be restricted to large ( $n \gg 1$ , ideally  $n \rightarrow +\infty$ ) samples when appropriate. In general,  $\Theta$  can be neglected with respect to the remaining terms in the asymptotic expressions of Eqs. (56) and (57). If the residuals are independent of the data,  $\Theta$  also vanishes regardless of the sample population. For further details refer to B and C.

The regression line slope and intercept variance estimators, in the general case of non normal residuals, may be calculated using the  $\delta$ -method [14, 10]. The result is:

$$(\hat{\sigma}_{\hat{a}_C})^2 = (\hat{a}_C)^2 \frac{c^4 (\hat{\sigma}_{\hat{a}_Y})^2 + (\hat{a}_Y)^4 (\hat{\sigma}_{\hat{a}_X})^2 + 2(\hat{a}_Y)^2 c^2 \hat{\sigma}_{\hat{a}_Y \hat{a}_X}}{(\hat{a}_Y)^2 [4(\hat{a}_Y)^2 c^2 + (\hat{a}_Y \hat{a}_X - c^2)^2]} ; \quad (58)$$

$$(\hat{\sigma}_{\hat{b}_C})^2 = \frac{\hat{a}_C}{n} \left[ \frac{\hat{a}_X - \hat{a}_C}{\hat{a}_C} + \frac{\hat{a}_C - \hat{a}_Y}{\hat{a}_Y} \right] \frac{S_{11}}{S_{00}} + (\bar{X})^2 (\hat{\sigma}_{\hat{a}_C})^2$$

$$-\frac{2}{n}\bar{X}(\hat{\sigma}_{\hat{b}_Y\hat{a}_C} + \hat{\sigma}_{\hat{b}_X\hat{a}_C}) ; \quad (59)$$

$$\hat{\sigma}_{\hat{a}_Y\hat{a}_X} = \frac{S_{13} + \hat{a}_Y\hat{a}_X S_{31} - (\hat{a}_Y + \hat{a}_X)S_{22}}{S_{20}S_{11}} ; \quad (60)$$

$$\hat{\sigma}_{\hat{b}_Y\hat{a}_C} = \frac{\hat{a}_C c^2}{\hat{a}_Y [4(\hat{a}_Y)^2 c^2 + (\hat{a}_Y\hat{a}_X - c^2)]^{1/2}} \frac{S_{12} + \hat{a}_Y\hat{a}_C S_{30} - (\hat{a}_Y + \hat{a}_C)S_{21}}{S_{20}} ; \quad (61)$$

$$\hat{\sigma}_{\hat{b}_X\hat{a}_C} = \frac{\hat{a}_C\hat{a}_Y}{[4(\hat{a}_Y)^2 c^2 + (\hat{a}_Y\hat{a}_X - c^2)]^{1/2}} \frac{S_{03} + \hat{a}_X\hat{a}_C S_{21} - (\hat{a}_X + \hat{a}_C)S_{12}}{S_{11}} ; \quad (62)$$

where Eqs. (58) and (59) in the special case,  $c^2 = 1$ , are equivalent to their counterparts expressed in the parent paper [14] provided absolute values appearing therein are removed. For a formal discussion refer to D. In addition, Eq. (58) is equivalent to its counterpart expressed in the parent paper [11].

The dependence on the variance ratio,  $c^2$ , in Eqs. (58), (61), (62), may be eliminated via Eq. (142), B. The result is:

$$(\hat{\sigma}_{\hat{a}_C})^2 = (\hat{a}_C)^2 \times \frac{(\hat{a}_C)^4 (A_{XC})^2 (\hat{\sigma}_{\hat{a}_Y})^2 + (\hat{a}_Y)^4 (A_{CY})^2 (\hat{\sigma}_{\hat{a}_X})^2 + 2(\hat{a}_Y)^2 (\hat{a}_C)^2 A_{XC} A_{CY} \hat{\sigma}_{\hat{a}_Y\hat{a}_X}}{(\hat{a}_Y)^2 \{4(\hat{a}_Y)^2 (\hat{a}_C)^2 A_{XC} A_{CY} + [\hat{a}_Y\hat{a}_X A_{CY} - (\hat{a}_C)^2 A_{XC}]^2\}} ; \quad (63)$$

$$\hat{\sigma}_{\hat{b}_Y\hat{a}_C} = \frac{(\hat{a}_C)^3 A_{XC}}{\hat{a}_Y \{4(\hat{a}_Y)^2 (\hat{a}_C)^2 A_{XC} A_{CY} + [\hat{a}_Y\hat{a}_X A_{CY} - (\hat{a}_C)^2 A_{XC}]^2\}^{1/2}} \times \frac{S_{12} + \hat{a}_Y\hat{a}_C S_{30} - (\hat{a}_Y + \hat{a}_C)S_{21}}{S_{20}} ; \quad (64)$$

$$\hat{\sigma}_{\hat{b}_X\hat{a}_C} = \frac{\hat{a}_C\hat{a}_Y A_{CY}}{\{4(\hat{a}_Y)^2 (\hat{a}_C)^2 A_{XC} A_{CY} + [\hat{a}_Y\hat{a}_X A_{CY} - (\hat{a}_C)^2 A_{XC}]^2\}^{1/2}} \times \frac{S_{03} + \hat{a}_X\hat{a}_C S_{21} - (\hat{a}_X + \hat{a}_C)S_{12}}{S_{11}} ; \quad (65)$$

$$A_{UV} = \frac{\hat{a}_U}{\hat{a}_V} - 1 ; \quad (U, V) = (X, C), (C, Y), (X, Y) ; \quad (66)$$

in terms of slope estimators, variance slope estimators, and deviation traces.

The application of the  $\delta$ -method provides asymptotic formulae which underestimate the true regression coefficient uncertainty in samples with low ( $n \lesssim 50$ ) or weakly correlated population [10]. In the special case of normal and data-independent residuals,  $\Theta(\hat{a}_C, \hat{a}_Y, \hat{a}_X) \rightarrow 0$ , Eqs. (58), (59), must necessarily reduce to (56), (57), respectively, which implies an additional factor,  $n/(n-2)$ , in the first term on the right-hand side of Eqs. (27), (41), and (59)-(62). For further details refer to C.

For heteroscedastic data, the regression line slope and intercept estimators are [7]:

$$\begin{aligned}\hat{a}_C &= \frac{(\tilde{w}_x)_{02} - c^2(\tilde{w}_x)_{20}}{2(\tilde{w}_x)_{11}} \left\{ 1 \mp \left[ 1 + c^2 \left( \frac{(\tilde{w}_x)_{02} - c^2(\tilde{w}_x)_{20}}{2(\tilde{w}_x)_{11}} \right)^{-2} \right]^{1/2} \right\} \\ &= \frac{\hat{a}_X \hat{a}'_Y - c^2}{2\hat{a}'_Y} \left\{ 1 \mp \left[ 1 + c^2 \left( \frac{\hat{a}_X \hat{a}'_Y - c^2}{2\hat{a}'_Y} \right)^{-2} \right]^{1/2} \right\} ;\end{aligned}\quad (67)$$

$$\hat{b}_C = \tilde{Y} - \hat{a}_C \tilde{X} ; \quad (68)$$

where  $\hat{a}'_Y = (\tilde{w}_x)_{11}/(\tilde{w}_x)_{20}$ ;  $\hat{a}_X = (\tilde{w}_x)_{02}/(\tilde{w}_x)_{11}$ ; and the weighted means,  $\tilde{X}$ ,  $\tilde{Y}$ , are defined by Eqs. (11)-(13).

For functional models, regression line slope and intercept variance estimators in the general case of heteroscedastic data reduce to their counterparts in the special case of homoscedastic data, as  $\{\hat{\sigma}_{\hat{a}_C}[(\tilde{w}_x)_{pq}]\}^2 \rightarrow [\hat{\sigma}_{\hat{a}_C}(w_x S_{pq})]^2$ ,  $\{\hat{\sigma}_{\hat{b}_C}[(\tilde{w}_x)_{pq}]\}^2 \rightarrow [\hat{\sigma}_{\hat{b}_C}(w_x S_{pq})]^2$ , via Eq. (9) where  $Q_i = (w_x)_i = w_x$ ,  $1 \leq i \leq n$ . For further details refer to an earlier attempt [7].

Under the assumption that the same holds for extreme structural models, Eqs. (56)-(65) take the general expression:

$$\begin{aligned}[(\hat{\sigma}_{\hat{a}_C})_N]^2 &= \frac{(\hat{a}_C)^2}{n-2} \left[ \frac{n-2}{n} \frac{R_C}{\hat{a}_C} \frac{(\tilde{w}_x)_{00}}{(\tilde{w}_x)_{11}} + \Theta(\hat{a}_C, \hat{a}'_Y, \hat{a}_X) \right] \\ &= \frac{(\hat{a}_C)^2}{n-2} \left[ \frac{\hat{a}_X - \hat{a}_C}{\hat{a}_C} + \frac{\hat{a}_C - \hat{a}'_Y}{\hat{a}'_Y} + \Theta(\hat{a}_C, \hat{a}'_Y, \hat{a}_X) \right] ;\end{aligned}\quad (69)$$

$$[(\hat{\sigma}_{\hat{b}_C})_N]^2 = \left[ \frac{1}{\hat{a}_C} \frac{(\tilde{w}_x)_{11}}{(\tilde{w}_x)_{00}} + (\tilde{X})^2 \right] [(\hat{\sigma}_{\hat{a}_C})_N]^2 - \frac{\hat{a}_C}{n-2} \frac{(\tilde{w}_x)_{11}}{(\tilde{w}_x)_{00}} \Theta(\hat{a}_C, \hat{a}'_Y, \hat{a}_X) ; \quad (70)$$

$$(\hat{\sigma}_{\hat{a}_C})^2 = (\hat{a}_C)^2 \frac{c^4 (\hat{\sigma}_{\hat{a}_Y})^2 + (\hat{a}_Y)^4 (\hat{\sigma}_{\hat{a}_X})^2 + 2(\hat{a}_Y)^2 c^2 \hat{\sigma}_{\hat{a}_Y \hat{a}_X}}{(\hat{a}_Y)^2 [4(\hat{a}_Y)^2 c^2 + (\hat{a}_Y \hat{a}_X - c^2)^2]} ; \quad (71)$$

$$\begin{aligned}(\hat{\sigma}_{\hat{b}_C})^2 &= \frac{\hat{a}_C}{n} \left[ \frac{\hat{a}_X - \hat{a}_C}{\hat{a}_C} + \frac{\hat{a}_C - \hat{a}'_Y}{\hat{a}'_Y} \right] \frac{(\tilde{w}_x)_{11}}{(\tilde{w}_x)_{00}} + (\tilde{X})^2 (\hat{\sigma}_{\hat{a}'_C})^2 \\ &\quad - \frac{2}{n} \tilde{X} (\hat{\sigma}_{\hat{b}_Y \hat{a}_C} + \hat{\sigma}_{\hat{b}_X \hat{a}_C}) ;\end{aligned}\quad (72)$$

$$\hat{\sigma}_{\hat{a}_Y \hat{a}_X} = \frac{(\tilde{w}_x)_{00} (\tilde{w}_x)_{13} + \hat{a}_Y \hat{a}_X (\tilde{w}_x)_{31} - (\hat{a}_Y + \hat{a}_X) (\tilde{w}_x)_{22}}{n (\tilde{w}_x)_{20} (\tilde{w}_x)_{11}} ; \quad (73)$$

$$\hat{\sigma}_{\hat{b}_Y \hat{a}_C} = \frac{\hat{a}_C c^2}{\hat{a}_Y [4(\hat{a}_Y)^2 c^2 + (\hat{a}_Y \hat{a}_X - c^2)]^{1/2}}$$

$$\times \frac{(\tilde{w}_x)_{12} + \hat{a}_Y \hat{a}_C (\tilde{w}_x)_{30} - (\hat{a}_Y + \hat{a}_C) (\tilde{w}_x)_{21}}{(\tilde{w}_x)_{20}} ; \quad (74)$$

$$\hat{\sigma}_{\hat{b}_X \hat{a}_C} = \frac{\hat{a}_C \hat{a}_Y}{[4(\hat{a}_Y)^2 c^2 + (\hat{a}_Y \hat{a}_X - c^2)^2]^{1/2}} \times \frac{(\tilde{w}_x)_{03} + \hat{a}_X \hat{a}_C (\tilde{w}_x)_{21} - (\hat{a}_X + \hat{a}_C) (\tilde{w}_x)_{12}}{(\tilde{w}_x)_{11}} ; \quad (75)$$

$$(\hat{\sigma}_{\hat{a}_C})^2 = (\hat{a}_C)^2 \times \frac{(\hat{a}_C)^4 (A_{XC})^2 (\hat{\sigma}_{\hat{a}_Y})^2 + (\hat{a}_Y)^4 (A_{CY'})^2 (\hat{\sigma}_{\hat{a}_X})^2 + 2(\hat{a}_Y)^2 (\hat{a}_C)^2 A_{XC} A_{CY'} \hat{\sigma}_{\hat{a}_Y \hat{a}_X}}{(\hat{a}_Y)^2 \{4(\hat{a}_Y)^2 (\hat{a}_C)^2 A_{XC} A_{CY'} + [\hat{a}_Y \hat{a}_X A_{CY'} - (\hat{a}_C)^2 A_{XC}]^2\}} ; \quad (76)$$

$$\hat{\sigma}_{\hat{b}_Y \hat{a}_C} = \frac{(\hat{a}_C)^3 A_{XC}}{\hat{a}_Y \{4(\hat{a}_Y)^2 (\hat{a}_C)^2 A_{XC} A_{CY'} + [(\hat{a}_Y \hat{a}_X A_{CY'} - (\hat{a}_C)^2 A_{XC}]^2\}^{1/2}} \times \frac{(\tilde{w}_x)_{12} + \hat{a}_Y \hat{a}_C (\tilde{w}_x)_{30} - (\hat{a}_Y + \hat{a}_C) (\tilde{w}_x)_{21}}{(\tilde{w}_x)_{20}} ; \quad (77)$$

$$\hat{\sigma}_{\hat{b}_X \hat{a}_C} = \frac{\hat{a}_C \hat{a}_Y A_{CY'}}{\{4(\hat{a}_Y)^2 (\hat{a}_C)^2 A_{XC} A_{CY'} + [(\hat{a}_Y \hat{a}_X A_{CY'} - (\hat{a}_C)^2 A_{XC}]^2\}^{1/2}} \times \frac{(\tilde{w}_x)_{03} + \hat{a}_X \hat{a}_C (\tilde{w}_x)_{21} - (\hat{a}_X + \hat{a}_C) (\tilde{w}_x)_{12}}{(\tilde{w}_x)_{11}} ; \quad (78)$$

and, in addition:

$$(\hat{\sigma}_{\hat{a}'_C})^2 = (\hat{a}_C)^2 \frac{c^4 (\hat{\sigma}_{\hat{a}'_Y})^2 + (\hat{a}_Y)^4 (\hat{\sigma}_{\hat{a}_X})^2 + 2(\hat{a}_Y)^2 c^2 \hat{\sigma}_{\hat{a}_Y \hat{a}_X}}{(\hat{a}_Y)^2 [4(\hat{a}_Y)^2 c^2 + (\hat{a}_Y \hat{a}_X - c^2)^2]} ; \quad (79)$$

$$(\hat{\sigma}_{\hat{a}'_Y})^2 = \frac{(\tilde{w}_x)_{00} (\tilde{w}_x)_{22} + (\hat{a}_Y)^2 (\tilde{w}_x)_{40} - 2\hat{a}_Y (\tilde{w}_x)_{31}}{n [(\tilde{w}_x)_{20}]^2} ; \quad (80)$$

where  $\hat{a}_Y = (\tilde{w}_y)_{11}/(\tilde{w}_y)_{20}$ ;  $\hat{a}'_Y = (\tilde{w}_x)_{11}/(\tilde{w}_x)_{20}$ ;  $\hat{a}_X = (\tilde{w}_x)_{02}/(\tilde{w}_x)_{11}$ ;  $A_{CY'} = \hat{a}_C/\hat{a}'_Y - 1$ ;  $R$  is defined in A, and  $\Theta$  is formulated in terms of  $n(\tilde{w}_x)_{pq}/(\tilde{w}_x)_{00}$  instead of  $S_{pq}$ .

In the special case of normal and data-independent residuals,  $\Theta(\hat{a}_C, \hat{a}'_Y, \hat{a}_X) \rightarrow 0$ , Eqs. (71), (72), must necessarily reduce to (69), (70), respectively, which implies an additional factor,  $n/(n-2)$ , in the first term on the right-hand side of Eqs. (34), (48), and (72)-(75).

In absence of a rigorous proof, Eqs. (69)-(75) must be considered as approximate results.

## 2.6 Reduced major-axis regression

The reduced major-axis regression may be considered as a special case

of oblique regression, where  $c^2 = a_X a_Y$ . Accordingly, Eqs. (51) and (52) also hold.

For homoscedastic data,  $w_{x_i} = w_x$ ,  $w_{y_i} = w_y$ ,  $1 \leq i \leq n$ , the regression line slope and intercept estimators, via Eqs. (54) and (55) are:

$$\hat{a}_R = \mp \sqrt{\frac{S_{02}}{S_{20}}} = \mp \sqrt{\hat{a}_X \hat{a}_Y} ; \quad (81)$$

$$\hat{b}_R = \bar{Y} - \hat{a}_R \bar{X} ; \quad (82)$$

where the index, R, denotes reduced major-axis regression,  $\hat{a}_Y = S_{11}/S_{20}$ ;  $\hat{a}_X = S_{02}/S_{11}$ ; and the double sign corresponds to the solutions of the square root, where the parasite solution must be disregarded. Accordingly, related models shall be quoted as R models. For further details refer to an earlier attempt [7].

The regression line slope and intercept variance estimators may be directly inferred from Eqs. (56), (57), for normal residuals, in the limit,  $\hat{a}_C \rightarrow \hat{a}_R = \sqrt{\hat{a}_X \hat{a}_Y}$ . The result is:

$$\begin{aligned} [(\hat{\sigma}_{\hat{a}_R})_N]^2 &= \frac{(\hat{a}_R)^2}{n-2} \left[ \frac{(n-2)R_R}{\hat{a}_R S_{11}} + \Theta(\hat{a}_R, \hat{a}_Y, \hat{a}_X) \right] \\ &= \frac{(\hat{a}_R)^2}{n-2} \left[ \frac{\hat{a}_X - \hat{a}_R}{\hat{a}_R} + \frac{\hat{a}_R - \hat{a}_Y}{\hat{a}_Y} + \Theta(\hat{a}_R, \hat{a}_Y, \hat{a}_X) \right] ; \end{aligned} \quad (83)$$

$$[(\hat{\sigma}_{\hat{b}_R})_N]^2 = \left[ \frac{1}{\hat{a}_R} \frac{S_{11}}{S_{00}} + (\bar{X})^2 \right] [(\hat{\sigma}_{\hat{a}_R})_N]^2 - \frac{\hat{a}_R}{n-2} \frac{S_{11}}{S_{00}} \Theta(\hat{a}_R, \hat{a}_Y, \hat{a}_X) ; \quad (84)$$

and for non normal residuals the application of the  $\delta$ -method yields [14]:

$$(\hat{\sigma}_{\hat{a}_R})^2 = (\hat{a}_R)^2 \left[ \frac{1}{4} \frac{(\hat{\sigma}_{\hat{a}_Y})^2}{(\hat{a}_Y)^2} + \frac{1}{4} \frac{(\hat{\sigma}_{\hat{a}_X})^2}{(\hat{a}_X)^2} + \frac{1}{2} \frac{\hat{\sigma}_{\hat{a}_Y \hat{a}_X}}{\hat{a}_Y \hat{a}_X} \right] ; \quad (85)$$

$$\begin{aligned} (\hat{\sigma}_{\hat{b}_R})^2 &= \frac{\hat{a}_R}{n} \left[ \frac{\hat{a}_X - \hat{a}_R}{\hat{a}_R} + \frac{\hat{a}_R - \hat{a}_Y}{\hat{a}_Y} \right] \frac{S_{11}}{S_{00}} + (\bar{X})^2 (\hat{\sigma}_{\hat{a}_R})^2 \\ &\quad - \frac{2}{n} \bar{X} (\hat{\sigma}_{\hat{b}_Y \hat{a}_R} + \hat{\sigma}_{\hat{b}_X \hat{a}_R}) ; \end{aligned} \quad (86)$$

$$\hat{\sigma}_{\hat{b}_Y \hat{a}_R} = \frac{1}{2} \left( \frac{\hat{a}_X}{\hat{a}_Y} \right)^{1/2} \frac{S_{12} + \hat{a}_Y \hat{a}_R S_{30} - (\hat{a}_Y + \hat{a}_R) S_{21}}{S_{20}} ; \quad (87)$$

$$\hat{\sigma}_{\hat{b}_X \hat{a}_R} = \frac{1}{2} \left( \frac{\hat{a}_Y}{\hat{a}_X} \right)^{1/2} \frac{S_{03} + \hat{a}_X \hat{a}_R S_{21} - (\hat{a}_X + \hat{a}_R) S_{12}}{S_{11}} ; \quad (88)$$

where  $\hat{\sigma}_{\hat{a}_Y \hat{a}_X}$  is defined by Eq. (60) and Eqs. (85), (86), are equivalent to their counterparts expressed in the parent paper [14]. For further details refer to D.

The extension of the above results to heteroscedastic data via Eqs. (81)-(88) reads:

$$\hat{a}_R = \mp \sqrt{\frac{(\tilde{w}_x)_{02}}{(\tilde{w}_x)_{20}}} = \mp \sqrt{\hat{a}_X \hat{a}'_Y} ; \quad (89)$$

$$\hat{b}_R = \tilde{Y} - \hat{a}_R \tilde{X} ; \quad (90)$$

$$\begin{aligned} [(\hat{\sigma}_{\hat{a}_R})_N]^2 &= \frac{(\hat{a}_R)^2}{n-2} \left[ \frac{n-2}{n} \frac{R_R (\tilde{w}_x)_{00}}{\hat{a}_R (\tilde{w}_x)_{11}} + \Theta(\hat{a}_R, \hat{a}'_Y, \hat{a}_X) \right] \\ &= \frac{(\hat{a}_R)^2}{n-2} \left[ \frac{\hat{a}_X - \hat{a}_R}{\hat{a}_R} + \frac{\hat{a}_R - \hat{a}'_Y}{\hat{a}'_Y} + \Theta(\hat{a}_R, \hat{a}'_Y, \hat{a}_X) \right] ; \end{aligned} \quad (91)$$

$$[(\hat{\sigma}_{\hat{b}_R})_N]^2 = \left[ \frac{1}{\hat{a}_R} \frac{(\tilde{w}_x)_{11}}{(\tilde{w}_x)_{00}} + (\tilde{X})^2 \right] [(\hat{\sigma}_{\hat{a}_R})_N]^2 - \frac{\hat{a}_R}{n-2} \frac{(\tilde{w}_x)_{11}}{(\tilde{w}_x)_{00}} \Theta(\hat{a}_R, \hat{a}'_Y, \hat{a}_X) ; \quad (92)$$

$$(\hat{\sigma}_{\hat{a}_R})^2 = (\hat{a}_R)^2 \frac{\hat{a}_Y}{\hat{a}'_Y} \left[ \frac{1}{4} \frac{(\hat{\sigma}_{\hat{a}_Y})^2}{(\hat{a}_Y)^2} + \frac{1}{4} \frac{(\hat{\sigma}_{\hat{a}_X})^2}{(\hat{a}_X)^2} + \frac{1}{2} \frac{\hat{\sigma}_{\hat{a}_Y \hat{a}_X}}{\hat{a}_Y \hat{a}_X} \right] ; \quad (93)$$

$$\begin{aligned} (\hat{\sigma}_{\hat{b}_R})^2 &= \frac{\hat{a}_R}{n} \left[ \frac{\hat{a}_X - \hat{a}_R}{\hat{a}_R} + \frac{\hat{a}_R - \hat{a}'_Y}{\hat{a}'_Y} \right] \frac{(\tilde{w}_x)_{11}}{(\tilde{w}_x)_{00}} + (\tilde{X})^2 (\hat{\sigma}_{\hat{a}'_R})^2 \\ &\quad - \frac{2}{n} \tilde{X} (\hat{\sigma}_{\hat{b}_Y \hat{a}_R} + \hat{\sigma}_{\hat{b}_X \hat{a}_R}) ; \end{aligned} \quad (94)$$

$$\hat{\sigma}_{\hat{b}_Y \hat{a}_R} = \frac{1}{2} \left( \frac{\hat{a}_X}{\hat{a}_Y} \right)^{1/2} \frac{(\tilde{w}_x)_{12} + \hat{a}_Y \hat{a}_R (\tilde{w}_x)_{30} - (\hat{a}_Y + \hat{a}_R) (\tilde{w}_x)_{21}}{(\tilde{w}_x)_{20}} ; \quad (95)$$

$$\hat{\sigma}_{\hat{b}_X \hat{a}_R} = \frac{1}{2} \left( \frac{\hat{a}_Y}{\hat{a}_X} \right)^{1/2} \frac{(\tilde{w}_x)_{03} + \hat{a}_X \hat{a}_R (\tilde{w}_x)_{21} - (\hat{a}_X + \hat{a}_R) (\tilde{w}_x)_{12}}{(\tilde{w}_x)_{11}} ; \quad (96)$$

and, in addition:

$$(\hat{\sigma}_{\hat{a}'_R})^2 = \frac{1}{4} \left[ \frac{\hat{a}_X}{\hat{a}_Y} (\hat{\sigma}_{\hat{a}'_Y})^2 + \frac{\hat{a}_Y}{\hat{a}_X} (\hat{\sigma}_{\hat{a}_X})^2 + 2\hat{\sigma}_{\hat{a}_Y \hat{a}_X} \right] ; \quad (97)$$

where  $\hat{a}_Y = (\tilde{w}_y)_{11}/(\tilde{w}_y)_{20}$ ;  $\hat{a}'_Y = (\tilde{w}_x)_{11}/(\tilde{w}_x)_{20}$ ;  $\hat{a}_X = (\tilde{w}_x)_{02}/(\tilde{w}_x)_{11}$ ;  $R$  is defined in A,  $\hat{\sigma}_{\hat{a}_Y \hat{a}_X}$ ,  $(\hat{\sigma}_{\hat{a}'_Y})^2$ , are expressed by Eqs. (73), (80), respectively, and  $\Theta$  is formulated in terms of  $n(\tilde{w}_x)_{pq}/(\tilde{w}_x)_{00}$  instead of  $S_{pq}$ .

In absence of a rigorous proof, Eqs. (91)-(96) must be considered as approximate results.

## 2.7 Bisector regression

The bisector regression implies use of both Y and X models for determining the angle formed by related regression lines. The bisecting line is assumed to be the estimated regression line of the model.

Let  $\alpha_Y$ ,  $\alpha_X$ ,  $\alpha_B$ , be the angles formed between Y, X, B, regression line, respectively, and  $x$  axis, and  $\gamma$  the angle formed between Y and X regression lines, as outlined in Fig. 1. Accordingly,  $\gamma/2$  is the angle formed between Y or X and B regression lines.

The following relations can easily be deduced from Fig. 1:  $\alpha_X = \alpha_Y + \gamma$ ;  $\alpha_B = \alpha_Y + \gamma/2 = (\alpha_Y + \alpha_X)/2$ , and the dimensionless slope of the regression line is  $\tan \alpha_B$ . Using the trigonometric formulae:

$$\tan(u + v) = \frac{\tan u + \tan v}{1 - \tan u \tan v} \quad ; \quad \tan \frac{u}{2} = \frac{\sin u}{1 + \cos u} \quad ;$$

and the identity:

$$\frac{X(1 + S_Y) + Y(1 + S_X)}{(1 + S_X)(1 + S_Y) - XY} = \frac{XY - 1 + S_X S_Y}{X + Y} \quad ;$$

$$X = \frac{a_X}{a_u} \quad ; \quad Y = \frac{a_Y}{a_u} \quad ; \quad S_X = \sqrt{1 + X^2} \quad ; \quad S_Y = \sqrt{1 + Y^2} \quad ;$$

the regression line slope estimator, after some algebra, is expressed as [14]:

$$\hat{a}_B = \frac{\hat{a}_Y \hat{a}_X - a_u^2 + \sqrt{a_u^2 + (\hat{a}_Y)^2} \sqrt{a_u^2 + (\hat{a}_X)^2}}{\hat{a}_Y + \hat{a}_X} \quad ; \quad (98)$$

where  $a_u$  is the unit slope,  $\hat{a}_Y = S_{11}/S_{20}$ ,  $\hat{a}_X = S_{02}/S_{11}$ , and the regression line intercept estimator reads [14]:

$$\hat{b}_B = \bar{Y} - \hat{a}_B \bar{X} \quad ; \quad (99)$$

where the index, B, denotes bisector regression.

The bisector regression may be considered as a special case of oblique regression where the variance ratio,  $c^2$ , is deduced from the combination of Eqs. (54) and (98), requiring  $a_C = a_B$ . After a lot of algebra involving the roots of a second-degree equation, the result is:

$$c^2 = (a_B)^2 \frac{a_X \mp a_B}{a_B} \left( \frac{a_B \mp a_Y}{a_Y} \right)^{-1} \quad ; \quad (100)$$

where the parasite solution must be disregarded. Accordingly, Eqs. (51) and (52) also hold.

For normal residuals and homoscedastic data, the regression line slope and intercept variance estimators may be directly inferred from Eqs. (56) and (57) in the limit,  $\hat{a}_C \rightarrow \hat{a}_B$ . The result is:

$$\begin{aligned} [(\hat{\sigma}_{\hat{a}_B})_N]^2 &= \frac{(\hat{a}_B)^2}{n-2} \left[ \frac{(n-2)R_B}{\hat{a}_B S_{11}} + \Theta(\hat{a}_B, \hat{a}_Y, \hat{a}_X) \right] \\ &= \frac{(\hat{a}_B)^2}{n-2} \left[ \frac{\hat{a}_X - \hat{a}_B}{\hat{a}_B} + \frac{\hat{a}_B - \hat{a}_Y}{\hat{a}_Y} + \Theta(\hat{a}_B, \hat{a}_Y, \hat{a}_X) \right] ; \end{aligned} \quad (101)$$

$$[(\hat{\sigma}_{\hat{b}_B})_N]^2 = \left[ \frac{1}{\hat{a}_B} \frac{S_{11}}{S_{00}} + (\bar{X})^2 \right] [(\hat{\sigma}_{\hat{a}_B})_N]^2 - \frac{\hat{a}_B}{n-2} \frac{S_{11}}{S_{00}} \Theta(\hat{a}_B, \hat{a}_Y, \hat{a}_X) ; \quad (102)$$

and for non normal residuals the application of the  $\delta$ -method yields [14]:

$$(\hat{\sigma}_{\hat{a}_B})^2 = \frac{(\hat{a}_B)^2}{(\hat{a}_Y + \hat{a}_X)^2} \left[ \frac{a_u^2 + (\hat{a}_X)^2}{a_u^2 + (\hat{a}_Y)^2} (\hat{\sigma}_{\hat{a}_Y})^2 + \frac{a_u^2 + (\hat{a}_Y)^2}{a_u^2 + (\hat{a}_X)^2} (\hat{\sigma}_{\hat{a}_X})^2 + 2\hat{\sigma}_{\hat{a}_Y \hat{a}_X} \right] ; \quad (103)$$

$$\begin{aligned} (\hat{\sigma}_{\hat{b}_B})^2 &= \frac{\hat{a}_B}{n} \left[ \frac{\hat{a}_X - \hat{a}_B}{\hat{a}_B} + \frac{\hat{a}_B - \hat{a}_Y}{\hat{a}_Y} \right] \frac{S_{11}}{S_{00}} + (\bar{X})^2 (\hat{\sigma}_{\hat{a}_B})^2 \\ &\quad - \frac{2}{n} \bar{X} (\hat{\sigma}_{\hat{b}_Y \hat{a}_B} + \hat{\sigma}_{\hat{b}_X \hat{a}_B}) ; \end{aligned} \quad (104)$$

$$\hat{\sigma}_{\hat{b}_Y \hat{a}_B} = \frac{\hat{a}_B \sqrt{a_u^2 + (\hat{a}_X)^2}}{(\hat{a}_Y + \hat{a}_X) \sqrt{a_u^2 + (\hat{a}_Y)^2}} \frac{S_{12} + \hat{a}_Y \hat{a}_B S_{30} - (\hat{a}_Y + \hat{a}_B) S_{21}}{S_{20}} ; \quad (105)$$

$$\hat{\sigma}_{\hat{b}_X \hat{a}_B} = \frac{\hat{a}_B \sqrt{a_u^2 + (\hat{a}_Y)^2}}{(\hat{a}_Y + \hat{a}_X) \sqrt{a_u^2 + (\hat{a}_X)^2}} \frac{S_{03} + \hat{a}_X \hat{a}_B S_{21} - (\hat{a}_X + \hat{a}_B) S_{12}}{S_{11}} ; \quad (106)$$

where  $\hat{\sigma}_{\hat{a}_Y \hat{a}_X}$  is defined by Eq. (60) and Eqs. (103), (104), are equivalent to their counterparts expressed in the parent paper [14]. For further details refer to D.

For heteroscedastic data, the combination of Eqs. (67) and (98), requiring  $a_C = a_B$ , after a lot of algebra involving the roots of a second-degree equation, yields:

$$c^2 = (a_B)^2 \frac{a_X \mp a_B}{a_B} \left( \frac{a_B \mp a'_Y}{a'_Y} \right)^{-1} ; \quad (107)$$

where  $\hat{a}_X = (\tilde{w}_x)_{02}/(\tilde{w}_x)_{11}$ ;  $\hat{a}'_Y = (\tilde{w}_x)_{11}/(\tilde{w}_x)_{20}$ ; and the parasite solution must be disregarded. Accordingly, Eqs. (51) and (52) also hold.



The extension of the above results to heteroscedastic data via Eqs. (98)-(99) and (101)-(106) reads:

$$\hat{b}_B = \tilde{Y} - \hat{a}_B \tilde{X} ; \quad (108)$$

$$\begin{aligned} [(\hat{\sigma}_{\hat{a}_B})_N]^2 &= \frac{(\hat{a}_B)^2}{n-2} \left[ \frac{n-2}{n} \frac{R_B (\tilde{w}_x)_{00}}{\hat{a}_B (\tilde{w}_x)_{11}} + \Theta(\hat{a}_B, \hat{a}'_Y, \hat{a}_X) \right] \\ &= \frac{(\hat{a}_B)^2}{n-2} \left[ \frac{\hat{a}_X - \hat{a}_B}{\hat{a}_B} + \frac{\hat{a}_B - \hat{a}'_Y}{\hat{a}'_Y} + \Theta(\hat{a}_B, \hat{a}'_Y, \hat{a}_X) \right] ; \end{aligned} \quad (109)$$

$$[(\hat{\sigma}_{\hat{b}_B})_N]^2 = \left[ \frac{1}{\hat{a}_B} \frac{(\tilde{w}_x)_{11}}{(\tilde{w}_x)_{00}} + (\tilde{X})^2 \right] [(\hat{\sigma}_{\hat{a}_B})_N]^2 - \frac{\hat{a}_B}{n-2} \frac{(\tilde{w}_x)_{11}}{(\tilde{w}_x)_{00}} \Theta(\hat{a}_B, \hat{a}'_Y, \hat{a}_X); \quad (110)$$

$$(\hat{\sigma}_{\hat{a}_B})^2 = \frac{(\hat{a}_B)^2}{(\hat{a}_Y + \hat{a}_X)^2} \left[ \frac{a_u^2 + (\hat{a}_X)^2}{a_u^2 + (\hat{a}_Y)^2} (\hat{\sigma}_{\hat{a}_Y})^2 + \frac{a_u^2 + (\hat{a}_Y)^2}{a_u^2 + (\hat{a}_X)^2} (\hat{\sigma}_{\hat{a}_X})^2 + 2\hat{\sigma}_{\hat{a}_Y \hat{a}_X} \right]; \quad (111)$$

$$\begin{aligned} (\hat{\sigma}_{\hat{b}_B})^2 &= \frac{\hat{a}_B}{n} \left[ \frac{\hat{a}_X - \hat{a}_B}{\hat{a}_B} + \frac{\hat{a}_B - \hat{a}'_Y}{\hat{a}'_Y} \right] \frac{(\tilde{w}_x)_{11}}{(\tilde{w}_x)_{00}} + (\tilde{X})^2 (\hat{\sigma}_{\hat{a}'_B})^2 \\ &\quad - \frac{2}{n} \tilde{X} (\hat{\sigma}_{\hat{b}_Y \hat{a}_B} + \hat{\sigma}_{\hat{b}_X \hat{a}_B}) ; \end{aligned} \quad (112)$$

$$\hat{\sigma}_{\hat{b}_Y \hat{a}_B} = \frac{\hat{a}_B \sqrt{a_u^2 + (\hat{a}_X)^2}}{(\hat{a}_Y + \hat{a}_X) \sqrt{a_u^2 + (\hat{a}_Y)^2}} \frac{(\tilde{w}_x)_{12} + \hat{a}_Y \hat{a}_B (\tilde{w}_x)_{30} - (\hat{a}_Y + \hat{a}_B) (\tilde{w}_x)_{21}}{(\tilde{w}_x)_{20}}; \quad (113)$$

$$\hat{\sigma}_{\hat{b}_X \hat{a}_B} = \frac{\hat{a}_B \sqrt{a_u^2 + (\hat{a}_Y)^2}}{(\hat{a}_Y + \hat{a}_X) \sqrt{a_u^2 + (\hat{a}_X)^2}} \frac{(\tilde{w}_x)_{03} + \hat{a}_X \hat{a}_B (\tilde{w}_x)_{21} - (\hat{a}_X + \hat{a}_B) (\tilde{w}_x)_{12}}{(\tilde{w}_x)_{11}}; \quad (114)$$

and, in addition:

$$(\hat{\sigma}_{\hat{a}'_B})^2 = \frac{(\hat{a}_B)^2}{(\hat{a}_Y + \hat{a}_X)^2} \left[ \frac{a_u^2 + (\hat{a}_X)^2}{a_u^2 + (\hat{a}_Y)^2} (\hat{\sigma}_{\hat{a}'_Y})^2 + \frac{a_u^2 + (\hat{a}_Y)^2}{a_u^2 + (\hat{a}_X)^2} (\hat{\sigma}_{\hat{a}_X})^2 + 2\hat{\sigma}_{\hat{a}_Y \hat{a}_X} \right]; \quad (115)$$

where  $\hat{a}_Y = (\tilde{w}_y)_{11}/(\tilde{w}_y)_{20}$ ,  $\hat{a}'_Y = (\tilde{w}_x)_{11}/(\tilde{w}_x)_{20}$ ,  $\hat{a}_X = (\tilde{w}_x)_{02}/(\tilde{w}_x)_{11}$ ,  $R$  is defined in A,  $\hat{\sigma}_{\hat{a}_Y \hat{a}_X}$ ,  $(\hat{\sigma}_{\hat{a}'_Y})^2$ , are expressed by Eqs. (73), (80), respectively, and  $\Theta$  is formulated in terms of  $n(\tilde{w}_x)_{pq}/(\tilde{w}_x)_{00}$  instead of  $S_{pq}$ .

In absence of a rigorous proof, Eqs. (109)-(114) must be considered as approximate results.

## 2.8 Extension to structural models

A nontrivial question is to what extent the above results, valid for extreme structural models, can be extended to generic structural models. In

general, assumptions related to generic structural models are different from their counterparts related to extreme structural models e.g., [3], [4] Chap. 6, §6.4.5, but, on the other hand, they could coincide for a special subclass.

In any case, whatever different assumptions and models can be made with regard to generic and extreme structural models, results from the former are expected to tend to their counterparts from the latter when the instrumental scatter is negligible with respect to the intrinsic scatter. It is worth noticing that most work on linear regression by astronomers involves the situation where both intrinsic scatter and heteroscedastic data are present e.g., [1, 22, 15, 16].

A special subclass of structural models with normal residuals can be defined where, for a selected regression estimator, the regression line slope and intercept variance estimators are independent of the amount of instrumental and intrinsic scatter, including the limit of null intrinsic scatter (functional models) and null instrumental scatter (extreme structural models). More specifically, the dependence occurs only via the total (instrumental + intrinsic) scatter. In this view, the whole subclass of structural models under consideration could be related to functional modelling [8] Chap. 2, §2.1. For further details refer to the parent paper [7].

## 3 An example of astronomical application

### 3.1 Astronomical introduction

Heavy elements are synthesised within stars and (partially or totally) returned to the interstellar medium via supernovae. In an ideal situation where the initial stellar mass function (including binary and multiple systems) is universal and the gas returned after star death is instantaneously and uniformly mixed with the interstellar medium, the abundance ratio of primary elements produced mainly by large-mass ( $m \gtrsim 8m_{\odot}$ , where  $m_{\odot}$  is the solar mass) stars maintains unchanged, which implies a linear relation. This is why large-mass stars have a short lifetime with respect to the age of the universe, and related ejecta (due to type II supernovae) may be considered as instantaneously returned to the interstellar medium.

A linear relation also holds if low-mass ( $m \lesssim 8m_{\odot}$ ) stars are considered, where the stellar lifetime can no longer be neglected with respect to the age

of the universe. Close binary systems including a white dwarf with masses,  $m_{\text{WD}} + m_{\text{C}} > m_{\text{Ch}}$ , are (type Ia) supernovae progenitors, where  $m_{\text{WD}}$  is the white dwarf mass,  $m_{\text{C}}$  is the companion mass, and  $m_{\text{Ch}} \approx 1.44m_{\odot}$  is the Chandrasekhar upper mass limit for stable white dwarfs. An additional restriction, for a linear relation between two generic primary elements in the interstellar medium, is a constant number ratio of type II to type Ia supernovae at any epoch. For further details refer to F.

Restricting to iron and oxygen, the generic linear relation, Eq. (227), reads:

$$[\text{O}/\text{H}]^* = a[\text{Fe}/\text{H}]^* + b \quad ; \quad (116)$$

where  $[\text{O}/\text{H}]$ ,  $[\text{Fe}/\text{H}]$ , are logarithmic number abundances normalized to the solar value e.g., [5] and the asterisks denote the ideal situation. More specifically, oxygen and iron abundance determinations performed on ideal stars by use of ideal instruments yield coordinates of points lying on the straight line defined by Eq. (116).

The intrinsic dispersion outside or along the ideal regression line may be owing to several processes, such as fluctuations in the stellar initial mass function (including binary and multiple systems) and inhomogeneous mixing of stellar ejecta with the interstellar medium, at different rates for different elements. Accordingly, ideal points,  $\text{P}_i^* \equiv ([\text{Fe}/\text{H}]_i^*, [\text{O}/\text{H}]_i^*)$ , are shifted towards actual points,  $\text{P}_{\text{Si}} \equiv ([\text{Fe}/\text{H}]_{\text{Si}}, [\text{O}/\text{H}]_{\text{Si}})$ .

More specifically, coeval ideal stars are represented by a single point on the ideal regression line, while related actual stars correspond to points which, in general, are shifted to a different extent outside or along the ideal regression line. Conversely, stars with different age could be represented by a same actual point,  $\text{P}_{\text{Si}}$ . The occurrence of instrumental scatter, related to iron and oxygen abundance determination on a star sample, makes actual points,  $\text{P}_{\text{Si}}$ , be shifted towards observed points,  $\text{P}_i \equiv ([\text{Fe}/\text{H}]_i, [\text{O}/\text{H}]_i)$ .

With regard to the ideal regression line, there is a one-to-one correspondence between the coordinates,  $[\text{Fe}/\text{H}]$  and  $[\text{O}/\text{H}]$ , while the contrary holds for actual points and observed points. In the limit of extreme structural models, where instrumental scatter is negligible with respect to intrinsic scatter, observed points are very close to actual points (if otherwise, any linear dependence would be hidden). The latter, to a first extent, may be determined along the following steps.

**(1)** Estimate a plausible regression line.

- (2) Calculate the mean distance of observed points from the estimated regression line, parallel to each coordinate axis.
- (3) Subdivide each coordinate axis into bins of width equal to the related mean distance calculated in (2).
- (4) Evaluate the intrinsic scatter within each bin, using the method described in an earlier attempt [1].
- (5) Minimize the loss function and determine the regression line slope and intercept estimators.
- (6) Verify the absolute difference between previous and current regression line slope and intercept estimators is less than a previously assigned tolerance value. If otherwise, return to (2) taking into consideration the current estimated regression line.

In general, the total scatter,  $\sigma_{[\text{W}/\text{H}]_i}^2 = \sigma_{[\text{W}/\text{H}]_{\text{Fi}}}^2 + \sigma_{[\text{W}/\text{H}]_{\text{Si}}}^2$ , should be used for evaluating the weights,  $w_{x_i}, w_{y_i}$ ,  $1 \leq i \leq n$ , appearing in the sum of the squared residuals, expressed by Eq. (8a), which implies the knowledge of the instrumental covariance matrix e.g., [1, 16].

## 3.2 Statistical results

An astronomical application performed in an earlier attempt [7] with regard to functional models, shall be repeated here for extreme structural models. Accordingly, related samples will be left unchanged but with the additional assumptions: (i) the intrinsic scatter is dominant with respect to the instrumental scatter, and (ii) uncertainties mentioned in the parent papers and reported below are related to the intrinsic scatter.

More specifically, the following samples related to the [O/H]-[Fe/H] relation shall be considered: RB09,  $n = 49$ , heteroscedastic data [20]; Fa09,  $n = 44$ , homoscedastic data with three different [O/H] determinations, namely LTE (standard local thermodynamical equilibrium for one-dimensional hydrostatic model atmospheres), SH0 (three-dimensional hydrostatic model atmospheres in absence of LTE with no account taken of the inelastic collisions via neutral H atoms,  $S_{\text{H}} = 0$ ), SH1 (three-dimensional hydrostatic model atmospheres in absence of LTE with due account taken of the inelastic collisions via neutral H atoms,  $S_{\text{H}} = 1$ ) [9]; Sa09,  $n = 63$ , heteroscedastic data

[21]. For further details refer to the parent paper [6]. In any case,  $[\text{Fe}/\text{H}]$  and  $[\text{O}/\text{H}]$  are determined independently for each sample star.

The  $[\text{O}/\text{H}]-[\text{Fe}/\text{H}]$  empirical relations are interpolated using the regression models, G, Y, X, O, R, B, for heteroscedastic data (FB09 and Sa09 samples) and Y, X, O, R, B, for homoscedastic data (Fa09 sample, cases LTE, SH0, SH1) and heteroscedastic data where intrinsic scatters are taken equal to the typical uncertainties mentioned in the parent papers (FB09, Sa09),  $\sigma_{[\text{Fe}/\text{H}]} = 0.15$ ,  $\sigma_{[\text{O}/\text{H}]} = 0.15$ , for both FB09 and Sa09 samples. Model G relates to a general case where the slope and intercept estimators are determined via Eqs. (22) and (21), respectively. For further details refer to the parent papers [23, 25, 7]. Slope and intercept estimators together with related dispersion estimators are listed in Tables 2, 3, and 4, 5, for heteroscedastic and homoscedastic data, respectively.

Owing to high difficulties intrinsic to the determination of slope and intercept dispersion estimators for G models, related calculations were not performed, leaving only approximate expressions [23] and asymptotic formulae [B, Eq. (160) related to G models]. For the remaining models, the regression line slope and intercept estimators and related dispersion estimators are calculated using Eqs. (23)-(29) and (30)-(36), case Y, homoscedastic and heteroscedastic data, respectively; Eqs. (37)-(43) and (44)-(50), case X, homoscedastic and heteroscedastic data, respectively; Eqs. (54)-(62) and (67)-(75),  $c^2 = 1$ , case O, homoscedastic and heteroscedastic data, respectively; Eqs. (81)-(88) and (89)-(96), case R, homoscedastic and heteroscedastic data, respectively; Eqs. (98)-(106) and (108)-(114), case B, homoscedastic and heteroscedastic data, respectively.

The regression lines determined by use of the above mentioned methods are plotted in Figs. 2 and 3 for heteroscedastic and homoscedastic data, respectively, where sample denomination and population are indicated on each panel together with model captions. Homoscedastic data are conceived as a special case of heteroscedastic data in Fig. 2 to test the computer code, which is different for heteroscedastic and homoscedastic data. It can be seen that lower panels of Figs. 2 and 3 coincide, and the regression lines related to models G and O in lower panels of Figs. 2 also coincide, as expected. The whole set of regression lines for all methods and all samples is shown in the upper right panel of Figs. 2 and 3.

Regression line slope and intercept estimators have the same expression for both structural and functional models. Accordingly, Figs. 2 and 3 maintain unchanged with respect to their counterparts shown in an earlier attempt [7]

Table 2: Regression line slope estimators,  $\hat{a}$ , and related dispersion estimators,  $\hat{\sigma}_{\hat{a}}$ , for heteroscedastic models, G, Y, X, O, R, B, applied to the [O/H]-[Fe/H] empirical relation deduced from the following samples (from up to down): RB09, Sa09. Dispersion column captions: ENNR - extreme structural models with non normal residuals [14]; ENRR - extreme structural models with normal residuals [10]; FNRR - functional models with normal residuals [23, 25, 7]; YANR - approximate formula for normal residuals [23, 25, 7]; AFNR - asymptotic formula for normal residuals [B, Eq. (160) related to the appropriate model]. For G models, exact expressions of slope estimators were not evaluated in the present attempt. For Y models and normal residuals, different slope dispersion estimators yield coinciding values, as expected.

$m$	$\hat{a}$	$\hat{\sigma}_{\hat{a}}$					sample
		ENNR	ENRR	FNRR	YANR	AFNR	
G	0.7279				0.0294	0.0288	RB09
Y	0.6714	0.0302	0.0314	0.0314	0.0314	0.0314	
X	0.7305	0.0271	0.0290	0.0290	0.0279	0.0290	
O	0.6964	0.0277	0.0276	0.0278	0.0271	0.0274	
R	0.7050	0.0254	0.0280	0.0282	0.0272	0.0277	
B	0.7005	0.0254	0.0278	0.0280	0.0271	0.0275	
G	0.6383				0.0435	0.0582	Sa09
Y	0.6167	0.0810	0.0398	0.0398	0.0398	0.0398	
X	0.8652	0.0772	0.0833	0.0829	0.0664	0.0829	
O	0.6355	0.0753	0.0609	0.0637	0.0541	0.0580	
R	0.6927	0.0677	0.0664	0.0700	0.0560	0.0626	
B	0.7336	0.0662	0.0704	0.0738	0.0579	0.0666	

Table 3: Regression line intercept estimators,  $\hat{b}$ , and related dispersion estimators,  $\hat{\sigma}_{\hat{b}}$ , for heteroscedastic models, G, Y, X, O, R, B, applied to the [O/H]-[Fe/H] empirical relation deduced from the following samples (from up to down): RB09, Sa09. Dispersion column captions: ENNR - extreme structural models with non normal residuals [14]; ENRR - extreme structural models with normal residuals [10]; FNRR - functional models with normal residuals [23, 25, 7]; YANR - approximate formula for normal residuals [23, 25, 7]; AFNR - asymptotic formula for normal residuals [via B, Eq. (160) related to the appropriate model]. For G models, exact expressions of intercept estimators were not evaluated in the present attempt. For Y models and normal residuals, different intercept dispersion estimators yield coinciding values, as expected.

$m$	$\hat{b}$	$\hat{\sigma}_{\hat{b}}$					sample
		ENNR	ENRR	FNRR	YANR	AFNR	
G	+0.0043				0.0672	0.0660	RB09
Y	-0.1121	0.0608	0.0675	0.0675	0.0675	0.0675	
X	+0.0316	0.0636	0.0736	0.0735	0.0712	0.0735	
O	-0.0512	0.0523	0.0702	0.0707	0.0689	0.0697	
R	-0.0305	0.0521	0.0710	0.0725	0.0693	0.0704	
B	-0.0413	0.0522	0.0706	0.0711	0.0691	0.0700	
G	+0.0619				0.0251	0.0336	Sa09
Y	+0.0439	0.0105	0.0198	0.0198	0.0198	0.0198	
X	+0.3080	0.0712	0.0676	0.0673	0.0575	0.0673	
O	+0.1461	0.0396	0.0509	0.0525	0.0469	0.0491	
R	+0.1864	0.0436	0.0547	0.0549	0.0485	0.0524	
B	+0.2153	0.0455	0.0575	0.0603	0.0501	0.0552	

Table 4: Regression line slope estimators,  $\hat{a}$ , and related dispersion estimators,  $\hat{\sigma}_{\hat{a}}$ , for homoscedastic models, Y, X, O, R, B, applied to the [O/H]-[Fe/H] empirical relation deduced from the following samples (from up to down): RB09, Sa09, Fa09, cases LTE, SH0, SH1. Dispersion column captions: ENNR - extreme structural models with non normal residuals [14]; ENRR - extreme structural models with normal residuals [10]; FNRR - functional models with normal residuals [23, 25, 7]; YANR - approximate formula for normal residuals [23, 25, 7]; AFNR - asymptotic formula for normal residuals [B, Eq. (160) related to the appropriate model]. For Y models and normal residuals, different slope dispersion estimators yield coinciding values, as expected.

$m$	$\hat{a}$	$\hat{\sigma}_{\hat{a}}$					sample
		ENNR	ENRR	FNRR	YANR	AFNR	
Y	0.6917	0.0268	0.0317	0.0317	0.0317	0.0317	RB09
X	0.7600	0.0326	0.0349	0.0348	0.0332	0.0348	
O	0.7143	0.0282	0.0327	0.0331	0.0319	0.0324	
R	0.7251	0.0278	0.0332	0.0336	0.0321	0.0328	
B	0.7253	0.0278	0.0333	0.0336	0.0321	0.0329	
Y	0.5868	0.0596	0.0461	0.0461	0.0461	0.0461	Sa09
X	0.8077	0.0563	0.0637	0.0635	0.0541	0.0635	
O	0.6476	0.0620	0.0509	0.0526	0.0468	0.0491	
R	0.6885	0.0523	0.0541	0.0562	0.0479	0.0519	
B	0.6916	0.0513	0.0544	0.0565	0.0480	0.0521	
Y	0.8961	0.0333	0.0303	0.0303	0.0303	0.0303	Fa09 (LTE)
X	0.9381	0.0294	0.0318	0.0317	0.0310	0.0317	
O	0.9150	0.0319	0.0310	0.0311	0.0305	0.0308	
R	0.9168	0.0310	0.0310	0.0312	0.0305	0.0308	
B	0.9169	0.0310	0.0310	0.0312	0.0305	0.0308	
Y	1.2261	0.0459	0.0432	0.0432	0.0432	0.0432	Fa09 (SH0)
X	1.2884	0.0434	0.0454	0.0454	0.0443	0.0454	
O	1.2640	0.0449	0.0445	0.0448	0.0436	0.0443	
R	1.2569	0.0441	0.0443	0.0445	0.0435	0.0440	
B	1.2568	0.0441	0.0443	0.0445	0.0435	0.0440	
Y	1.0492	0.0358	0.0341	0.0341	0.0341	0.0341	Fa09 (SH1)
X	1.0946	0.0315	0.0356	0.0356	0.0348	0.0356	
O	1.0732	0.0337	0.0349	0.0350	0.0343	0.0347	
R	1.0716	0.0332	0.0348	0.0350	0.0343	0.0346	
B	1.0716	0.0332	0.0348	0.0350	0.0343	0.0346	



Table 5: Regression line intercept estimators,  $\hat{b}$ , and related dispersion estimators,  $\hat{\sigma}_{\hat{b}}$ , for homoscedastic models, Y, X, O, R, B, applied to the [O/H]-[Fe/H] empirical relation deduced from the following samples (from up to down): RB09, Sa09, Fa09, cases LTE, SH0, SH1. Dispersion column captions: ENNR - extreme structural models with non normal residuals [14]; ENRR - extreme structural models with normal residuals [10]; FNRR - functional models with normal residuals [23, 25, 7]; YANR - approximate formula for normal residuals [23, 25, 7]; AFNR - asymptotic formula for normal residuals [via B, Eq. (160) related to the appropriate model]. For Y models and normal residuals, different intercept dispersion estimators yield coinciding values, as expected.

$m$	$\hat{b}$	$\hat{\sigma}_{\hat{b}}$					sample
		ENNR	ENRR	FNRR	YANR	AFNR	
Y	-0.0766	0.0598	0.0737	0.0737	0.0737	0.0737	RB09
X	+0.0742	0.0811	0.0807	0.0806	0.0773	0.0806	
O	-0.0268	0.0658	0.0759	0.0766	0.0741	0.0752	
R	-0.0030	0.0664	0.0770	0.0778	0.0746	0.0762	
B	-0.0025	0.0665	0.0770	0.0778	0.0746	0.0762	
Y	+0.0908	0.0211	0.0338	0.0338	0.0338	0.0338	Sa09
X	+0.2011	0.0423	0.0431	0.0430	0.0397	0.0430	
O	+0.1212	0.0268	0.0357	0.0363	0.0343	0.0351	
R	+0.1416	0.0279	0.0373	0.0381	0.0352	0.0365	
B	+0.1431	0.0282	0.0375	0.0382	0.0352	0.0367	
Y	+0.5476	0.0761	0.0663	0.0663	0.0663	0.0663	Fa09 (LTE)
X	+0.6366	0.0665	0.0693	0.0693	0.0678	0.0693	
O	+0.5877	0.0725	0.0676	0.0680	0.0666	0.0673	
R	+0.5916	0.0706	0.0678	0.0681	0.0667	0.0674	
B	+0.5916	0.0706	0.0678	0.0681	0.0667	0.0674	
Y	+0.8717	0.1017	0.0945	0.0945	0.0945	0.0945	Fa09 (SH0)
X	+1.0037	0.1003	0.0992	0.0991	0.0968	0.0991	
O	+0.9519	0.1019	0.0973	0.0978	0.0953	0.0967	
R	+0.9369	0.0998	0.0967	0.0973	0.0950	0.0961	
B	+0.9367	0.0998	0.0967	0.0973	0.0950	0.0961	
Y	+0.6518	0.0808	0.0745	0.0745	0.0745	0.0745	Fa09 (SH1)
X	+0.7479	0.0730	0.0777	0.0777	0.0761	0.0777	
O	+0.7027	0.0772	0.0762	0.0765	0.0750	0.0758	
R	+0.6993	0.0760	0.0761	0.0764	0.0750	0.0757	
B	+0.6993	0.0760	0.0761	0.0764	0.0749	0.0757	

where, on the other hand, B models were not included.

An inspection of Tables 2-5 and Figs. 2-3 discloses the following.

(1) Either of the inequalities [14]:

$$\hat{a}_Y < \hat{a}_O < \hat{a}_R < \hat{a}_B < \hat{a}_X ; \quad \hat{a}_B < a_u ; \quad S_{11} > 0 ; \quad (117a)$$

$$\hat{a}_Y < \hat{a}_B < \hat{a}_R < \hat{a}_O < \hat{a}_X ; \quad \hat{a}_B > a_u ; \quad S_{11} > 0 ; \quad (117b)$$

where  $a_u$  is the unit slope, is satisfied for homoscedastic data but the contrary holds for heteroscedastic data. In particular,  $\hat{a}_B < \hat{a}_R < a_u$  for RB09 sample, see Table 2. In addition,  $\hat{a}_Y < \hat{a}_G < \hat{a}_X$  for heteroscedastic data, but a counterexample is provided in an earlier attempt [23].

- (2) Slope and intercept estimators from O, R and B models are in agreement within  $\mp\sigma$ . The extension of the above result to slope and intercept estimators from Y and X models holds for samples with lower dispersion (Fa09). An increasing dispersion yields marginal (RB09) or no (Sa09) agreement within  $\mp\sigma$ , for both heteroscedastic and homoscedastic data.
- (3) For normal residuals, slope and intercept dispersion estimators related to functional and structural models yield slightly different results, as expected from the fact that related asymptotic formulae coincide [B, Eq. (160) related to the appropriate model]. Asymptotic formulae used in the current attempt make a better fit with respect to earlier approximations [23, 25, 7].
- (4) Systematic variations due to different sample data are dominant with respect to the intrinsic scatter.

In conclusion, regression lines deduced from different sample data represent correct (from the standpoint of regression models considered in the current attempt) [O/H]-[Fe/H] relations, but no definitive choice can be made until systematic errors due to different methods and/or spectral lines in determining oxygen abundance, are alleviated.

## 4 Discussion

For an assigned sample, structural models belonging to a special subclass are indistinguishable from extreme structural models, as outlined in an earlier

attempt [7]. Accordingly, the results of the current paper also apply to structural models of the kind considered. The expression of regression line slope and intercept estimators and related variance estimators in terms of weighted deviation traces, for heteroscedastic and homoscedastic data, makes a second step towards a unified formalism of bivariate least squares linear regression.

Exact expressions of regression line slope and intercept estimators and related variance estimators have been rewritten in a more compact form with respect to an earlier attempt [10] in the limit of oblique regression i.e.  $(\sigma_{yy})_i/(\sigma_{xx})_i = c^2$ ,  $1 \leq i \leq n$ . It is noteworthy that a constant variance ratio,  $c^2$ , for all data points, does not necessarily imply equal variances,  $(\sigma_{xx})_i = \sigma_{xx} = \text{const}$ ,  $(\sigma_{yy})_i = \sigma_{yy} = \text{const}$ ,  $1 \leq i \leq n$ . While regression line slope and intercept estimators attain a coinciding expression in different attempts [23, 25, 14, 10], the results of the current paper show that the contrary holds for related variance estimators. The same holds for both reduced major-axis and bisector regression.

Approximate expressions provided in earlier attempts for normal residuals [23, 25] make (at least in computed cases) a lower limit to their exact counterparts, as shown in Tables 2-5, YANR vs. ENRR, FNRR. The same holds, to a better extent, for the asymptotic expressions determined in the current paper, as shown in Tables 2-5, AFNR vs. ENRR, FNRR. Related fractional discrepancies for low-dispersion data (RB09, Fa09) do not exceed a few percent, which grows up to about 10% in presence of large-dispersion data (Sa09).

It is well known that the regression line slope and intercept estimators are biased towards zero for Y models e.g., [12] Chap. 1, §1.1.1, [8] Chap. 3, §3.2 [15, 16], [4] Chap. 4, §4.4. Biases can be explicitly expressed in the special case of homoscedastic models with normal residuals. More specifically, the condition  $1 - \rho_{20} \ll 1$  ensures bias effects are negligible, where  $\rho_{20}$  is the reliability ratio:

$$\rho_{20} = \frac{S_{20}}{S_{20} + (n - 1)\sigma_{xx}} ; \quad (118)$$

which implies  $0 \leq \rho_{20} \leq 1$ . For further details refer to specific monographies e.g., [12] Chap. 1, §1.1.1, [8] Chap. 3, §3.2.1, [4] Chap. 4, §4.4.

Similarly, it can be seen that regression line slope and intercept variance estimators are biased towards infinity for X models. In the special case of homoscedastic models with normal residuals, the condition  $1 - \rho_{02} \ll 1$

ensures bias effects are negligible, where  $\rho_{02}$  is the reliability ratio:

$$\rho_{02} = \frac{S_{02}}{S_{02} + (n - 1)\sigma_{yy}} ; \quad (119)$$

which implies  $0 \leq \rho_{02} \leq 1$  e.g., [7].

Accordingly, slopes are underestimated in Y models and overestimated in X models by a factor,  $\rho_{20}$  and  $1/\rho_{02}$ , respectively. For C models (oblique regression), O models (orthogonal regression), R models (reduced major-axis regression), B models (bisector regression), the regression line slope estimators lie between their counterparts related to Y and X models, according to Eqs. (118) and (119), which implies bias corrections e.g., [8] Chap. 3, §3.4.2. Though there is skepticism about an indiscriminate use of oblique regression estimators, still it is accepted the method is viable provided both instrumental and intrinsic covariance matrix are known e.g., [8] Chap. 3, §3.4.2, [4] Chap. 4, §4.5.

With regard to heteroscedastic data, an inspection of Tables 2-5 shows that for lower data dispersion (RB09 sample) the values of regression line slope and intercept estimators, deduced for weighted (Tables 2-3) and unweighted (Tables 4-5) data, are systematically smaller in the former case with respect to the latter, but are still in agreement within  $\mp\sigma$ . For larger dispersion data (Sa09 sample) no systematic trend of the kind considered appears, but the values of regression line slope and intercept estimators are still in agreement within  $\mp\sigma$  for O, R, and B models. It may be a general property of the regression models considered in the current attempt or, more realistically, intrinsic to the samples selected for the application performed in subsection 3.2.

The reliability ratios, Eqs. (118) and (119), have been calculated for all sample data and the inequalities,  $\rho_{20} > 0.92$ ,  $\rho_{02} > 0.91$ , hold in any case except  $\rho_{02} > 0.86$  for the Sa09 sample, which implies poorly biased regression line slope and intercept estimators for the samples considered using Y and X models and, a fortiori, using C, O, R, and B models.

Numerical simulations can determine the performance of the regression coefficients in presence of small samples and large scatter, and evaluate whether the approximations made in deriving variances are accurate. According to the results of a classical paper [14], the uncertainties to the slope predicted by O models are, on average, larger than those predicted by Y, R, or B models. For this reason, skepticism is expressed towards O models and,

in any case, caution is urged in interpreting slopes when small samples and large scatter are involved [14].

On the other hand, O models are special cases of C models, which could also include R and B models, and the predicted slopes lie between their counterparts related to the limiting cases of Y and X models. Extended numerical simulations should be used for searching a relation between the family of C models,  $c^2 = c_{\min}^2$ , with the lowest uncertainty to the slope, and values of population variances and covariance, namely  $c_{\min}^2 = f(\sigma_{XX}, \sigma_{YY}, \sigma_{XY})$ . In this view, it should be recommended use of C models where  $c^2 = c_{\min}^2$  for assigned sample variances and covariance, which estimate their counterparts related to the parent population.

Concerning samples listed in Tables 2-5 and represented in Figs. 2-3, the slope uncertainty predicted by O models is slightly larger than the slope predicted by R and B models for non normal residuals (ENNR), while the reverse occurs for normal residuals (ENNR). In addition, the slope uncertainty predicted by G models (the general case), when estimated, is close to the slope uncertainty predicted by O, R, and B models.

## 5 Conclusion

From the standpoint of a unified analytic formalism of bivariate least squares linear regression, extreme structural models have been conceived as a limiting case where the instrumental scatter is negligible (ideally null) with respect to the intrinsic scatter.

Within the framework of a variant of the classical additive error model e.g., [8] Chap.1, §1.2, Chap.3, §3.2.1, [4] Chap.4, §4.3, [16], the classical results presented in earlier papers [14, 10] have been rewritten in a more compact form using a new formalism in terms of weighted deviation traces which, for homoscedastic data, reduce to usual quantities, leaving aside an unessential (but dimensional) multiplicative factor.

Regression line slope and intercept estimators, and related variance estimators, have been expressed in the special case of uncorrelated errors in  $X$  and in  $Y$  for the following models: (Y) errors in  $X$  negligible (ideally null) with respect to errors in  $Y$ ; (X) errors in  $Y$  negligible (ideally null) with respect to errors in  $X$ ; (C) oblique regression; (O) orthogonal regression; (R) reduced major-axis regression; (B) bisector regression. Related variance estimators have been expressed for both non normal and normal residuals and

compared to their counterparts determined for functional models [7].

Under the assumption that regression line slope and intercept variance estimators for homoscedastic and heteroscedastic data are connected to a similar extent in functional and structural models, the above mentioned results have been extended from homoscedastic to heteroscedastic data. In absence of a rigorous proof, related expressions have been considered as approximate results.

An example of astronomical application has been considered, concerning the [O/H]-[Fe/H] empirical relations deduced from five samples related to different populations and/or different methods of oxygen abundance determination. For low-dispersion samples and assigned methods, different regression models have been found to yield results which are in agreement within the errors ( $\mp\sigma$ ) for both heteroscedastic and homoscedastic data, while the contrary has been shown to hold for large-dispersion samples. In any case, samples related to different methods have been found to produce discrepant results, due to the presence of (still undetected) systematic errors, which implies no definitive statement can be made at present.

Asymptotic expressions have been found to approximate regression line slope and intercept variance estimators, for normal residuals, to a better extent with respect to earlier attempts [23, 25]. Related fractional discrepancies have been shown to be not exceeding a few percent for low-dispersion data, which has grown up to about 10% in presence of large-dispersion data.

An extension of the formalism to generic structural models has been left to further investigation.

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## A Euclidean and statistical squared residual sum

For homoscedastic data, the sum of squared (dimensional) Euclidean distances between observed points,  $P_i(X_i, Y_i)$ , and adjusted points on the estimated regression line,  $\hat{P}_i(x_i, y_i)$ ,  $y_i = \hat{a}x_i + \hat{b}$ , is expressed as e.g., [12] Chap. 1, §1.3.3, [10, 7]:

$$(n - 2)R = \sum_{i=1}^n [(Y_i - \bar{Y}) - \hat{a}(X_i - \bar{X})]^2 = S_{02} + (\hat{a})^2 S_{20} - 2\hat{a}S_{11} \quad ; \quad (120)$$

where  $R$  is denoted as  $s_{vv}$  in the earlier quotation [12].

The sum of squared (dimensionless) statistical distances e.g., [12] Chap. 1, §1.3.3, between the above mentioned points,  $P_i(X_i, Y_i)$  and  $\hat{P}_i(x_i, y_i)$ , reads [7]:

$$T_{\bar{R}} = W [S_{02} + (\hat{a})^2 S_{20} - 2\hat{a}S_{11}] \quad ; \quad (121)$$

which, for heteroscedastic data, takes the general expression [7]:

$$T_{\tilde{R}} = \tilde{W}_{02} + (\hat{a})^2 \tilde{W}_{20} - 2\hat{a}\tilde{W}_{11} \quad ; \quad (122)$$

accordingly, the extension of Eq. (120) to heteroscedastic data reads:

$$(n - 2)R = \frac{n[\tilde{W}_{02} + (\hat{a})^2 \tilde{W}_{20} - 2\hat{a}\tilde{W}_{11}]}{\tilde{W}_{00}} \quad ; \quad (123)$$

which, in the limit of homoscedastic data,  $W_i = W = \bar{W}$ ,  $1 \leq i \leq n$ ,  $\tilde{W}_{00} = n\bar{W} = nW$ ,  $\tilde{W}_{pq} = W S_{pq}$ , via Eqs. (9), (10), reduces to Eq. (120), as expected.

## B Equivalence between earlier and current formulation

Let oblique regression models be taken into consideration under the following restrictive assumptions: (1) homoscedastic data; (2) uncorrelated

errors in  $Y$  and in  $X$ ; (3) normal residuals. Accordingly, the regression line slope variance estimator is expressed by Eq. (56) where the function,  $\Theta(\hat{a}_C, \hat{a}_Y, \hat{a}_X)$ , may be different for different methods and/or models, as shown in Table 1. Aiming to a formal demonstration, some preliminary relations are needed.

In terms of dimensionless ratios, using Eqs. (23) and (37), Eq. (120) translates into:

$$\frac{(n-2)R}{\hat{a}S_{11}} = \frac{\hat{a}_X}{\hat{a}} + \frac{\hat{a}}{\hat{a}_Y} - 2 = \frac{\hat{a}_X - \hat{a}}{\hat{a}} + \frac{\hat{a} - \hat{a}_Y}{\hat{a}_Y} ; \quad (124)$$

where the following identities:

$$\frac{\hat{a}_X - \hat{a}}{\hat{a}} + \frac{\hat{a} - \hat{a}_Y}{\hat{a}_Y} = \frac{\hat{a}_X - \hat{a}_Y}{\hat{a}_Y} - \frac{\hat{a}_X - \hat{a}}{\hat{a}} \frac{\hat{a} - \hat{a}_Y}{\hat{a}_Y} ; \quad (125)$$

$$\frac{\hat{a}_X - \hat{a}}{\hat{a}} \frac{\hat{a} - \hat{a}_Y}{\hat{a}_Y} = \frac{\hat{a}_X - \hat{a}_Y}{\hat{a}_Y} - \frac{\hat{a}_X - \hat{a}}{\hat{a}} - \frac{\hat{a} - \hat{a}_Y}{\hat{a}_Y} = \frac{\hat{a}_X - \hat{a}}{\hat{a}_Y} - \frac{\hat{a}_X - \hat{a}}{\hat{a}} ; \quad (126)$$

may easily be verified.

In the case under discussion of oblique regression models,  $\hat{a} = \hat{a}_C$ , the following inequalities hold [14]:

$$\hat{a}_X \geq \hat{a}_C \geq \hat{a}_Y ; \quad S_{11} > 0 ; \quad (127)$$

$$\hat{a}_X \leq \hat{a}_C \leq \hat{a}_Y ; \quad S_{11} < 0 ; \quad (128)$$

which makes the left-hand side of Eq. (124) always positive provided  $S_{11} \neq 0$ .

Using the method of partial differentiation, the regression line slope variance estimator in the case under discussion is [7]:

$$(\hat{\sigma}_{\hat{a}_C})^2 = \frac{(\hat{a}_C)^2}{n-2} \left[ 2 \frac{S_{02}S_{20} - (S_{11})^2}{(S_{11})^2} + 2 - \frac{S_{02} + (\hat{a}_C)^2 S_{20}}{\hat{a}_C S_{11}} \right] ; \quad (129)$$

and the substitution of Eqs. (23) and (37) into (129), using (125) and (126) yields after some algebra:

$$(\hat{\sigma}_{\hat{a}_C})^2 = \frac{(\hat{a}_C)^2}{n-2} \left[ \frac{\hat{a}_X - \hat{a}_C}{\hat{a}_C} + \frac{\hat{a}_C - \hat{a}_Y}{\hat{a}_Y} + 2 \frac{\hat{a}_X - \hat{a}_C}{\hat{a}_C} \frac{\hat{a}_C - \hat{a}_Y}{\hat{a}_Y} \right] ; \quad (130)$$

from which the following is inferred by comparison with Eq. (56):

$$\Theta(\hat{a}_C, \hat{a}_Y, \hat{a}_X) = 2 \frac{\hat{a}_X - \hat{a}_C}{\hat{a}_C} \frac{\hat{a}_C - \hat{a}_Y}{\hat{a}_Y} ; \quad (131)$$

as listed in Table 1.

Using the method of moments estimators, the elements sample covariance matrix are:

$$m_{XX} = \frac{S_{20}}{n-1} ; \quad m_{YY} = \frac{S_{02}}{n-1} ; \quad m_{XY} = m_{YX} = \frac{S_{11}}{n-1} ; \quad (132)$$

which, in terms of the variance estimators,  $(\hat{\sigma}_{xx})_S$  (intrinsic  $x$  error distribution),  $(\hat{\sigma}_{xx})_F$  (instrumental  $x$  error distribution),  $(\hat{\sigma}_{yy})_F$  (instrumental  $y$  error distribution) via  $c_F^2 = (\sigma_{yy})_F/(\sigma_{xx})_F$ , and regression line slope estimator,  $\hat{a}_C$ , are expressed as:

$$m_{XX} = (\hat{\sigma}_{xx})_S + (\hat{\sigma}_{xx})_F ; \quad (133a)$$

$$m_{YY} = (\hat{a}_C)^2(\hat{\sigma}_{xx})_S + (c_F)^2(\hat{\sigma}_{xx})_F ; \quad (133b)$$

$$m_{XY} = m_{YX} = \hat{a}_C(\hat{\sigma}_{xx})_S ; \quad (133c)$$

for further details and specification of the model refer to the parent paper [12] Chap. 1, §1.3.2.

The substitution of Eqs. (132) and (133) into (120) yields:

$$(n-2)R_C = (n-1)[(\hat{a}_C)^2 + (c_F)^2](\hat{\sigma}_{xx})_F ; \quad (134)$$

where the variance ratio,  $(c_F)^2$ , may explicitly be expressed using Eqs. (132) and (133). The result is:

$$(c_F)^2 = \frac{\hat{a}_C(S_{02} - \hat{a}_C S_{11})}{\hat{a}_C S_{20} - S_{11}} ; \quad (135)$$

which, using Eq. (120) and performing some algebra, takes the equivalent form:

$$(\hat{a}_C)^2 + (c_F)^2 = \frac{\hat{a}_C(n-2)R_C}{\hat{a}_C S_{20} - S_{11}} ; \quad (136)$$

finally, the substitution of Eq. (136) into (134) yields:

$$(\hat{\sigma}_{xx})_F = \frac{\hat{a}_C S_{20} - S_{11}}{(n-1)\hat{a}_C} ; \quad (137)$$

where the dependence on the variance ratio,  $(c_F)^2$ , has been eliminated.

In the limit of large samples ( $n \gg 1$ , ideally  $n \rightarrow +\infty$ ) where, in addition,  $S_{11} \neq 0$ , the regression line slope variance estimator is [12] Chap. 1, §1.3.2:

$$(\hat{\sigma}_{\hat{a}_C})^2 = \frac{1}{n-1} \frac{1}{[(\hat{\sigma}_{xx})_S]^2} \left\{ [(\hat{\sigma}_{xx})_S + (\hat{\sigma}_{xx})_F] R_C - (\hat{a}_C)^2 [(\hat{\sigma}_{xx})_F]^2 \right\} ; \quad (138)$$

and the substitution of Eqs. (124), (132), (133), (137), into (138) yields after some algebra:

$$\begin{aligned} (\hat{\sigma}_{\hat{a}_C})^2 &= \frac{(\hat{a}_C)^2}{n-2} \\ &\times \left[ \frac{\hat{a}_X - \hat{a}_C}{\hat{a}_C} + \frac{\hat{a}_C - \hat{a}_Y}{\hat{a}_Y} + \frac{\hat{a}_X - \hat{a}_C}{\hat{a}_C} \frac{\hat{a}_C - \hat{a}_Y}{\hat{a}_Y} + \frac{1}{n-1} \left( \frac{\hat{a}_C - \hat{a}_Y}{\hat{a}_Y} \right)^2 \right] ; \quad (139) \end{aligned}$$

from which the following is inferred by comparison with Eq. (56):

$$\Theta(\hat{a}_C, \hat{a}_Y, \hat{a}_X) = \frac{\hat{a}_X - \hat{a}_C}{\hat{a}_C} \frac{\hat{a}_C - \hat{a}_Y}{\hat{a}_Y} + \frac{1}{n-1} \left( \frac{\hat{a}_C - \hat{a}_Y}{\hat{a}_Y} \right)^2 ; \quad (140)$$

as listed in Table 1.

On the other hand, the regression line slope variance estimator reported in an earlier attempt [10] Eq. (4) therein, reads:

$$\begin{aligned} (\hat{\sigma}_{\hat{a}_C})^2 &= \frac{(\hat{a}_C)^2}{n-2} \left[ \frac{(n-2)R_C}{\hat{a}_C S_{11}} + \frac{\hat{a}_C(S_{02} - \hat{a}_C S_{11})}{(c_S)^2} \frac{(n-2)R_C}{\hat{a}_C (S_{11})^2} \right. \\ &\quad \left. - \frac{n-2}{n-1} \frac{(\hat{a}_C)^2}{(S_{11})^2} \left( \frac{S_{02} - \hat{a}_C S_{11}}{(c_S)^2} \right)^2 \right] ; \quad (141) \end{aligned}$$

where  $c_S = c$  and the counterpart of Eq. (135) holds [7]:

$$c^2 = c_S^2 = \frac{\hat{a}_C(S_{02} - \hat{a}_C S_{11})}{\hat{a}_C S_{20} - S_{11}} ; \quad (142)$$

and the substitution of Eqs. (124), (142), into (141), after some algebra yields Eq. (139). Then the regression line slope variance estimator, expressed by Eq. (141), coincides with its counterpart deduced by use of the method of moment estimators, expressed by Eq. (139).

Using the method of least squares estimation, under the assumption that the entire instrumental covariance matrix is known, the regression line slope variance estimator reads [12] Chap. 1, §1.3.3:

$$(\hat{\sigma}_{\hat{a}_C})^2 = \frac{1}{n-1} \frac{1}{(\hat{m}_{XX})^2} \left\{ \hat{m}_{XX} \hat{\sigma}_{vv} + (\sigma_{xx})_F \hat{\sigma}_{vv} - (\hat{\sigma}_{xv})^2 \right\} ; \quad (143)$$

$$\hat{\sigma}_{vv} = (\sigma_{yy})_F + (\hat{a}_C)^2 (\sigma_{xx})_F - 2\hat{a}_C (\sigma_{xy})_F ; \quad (144)$$

$$\hat{\sigma}_{xv} = (\sigma_{xy})_F - \hat{a}_C (\sigma_{xx})_F ; \quad (145)$$

where  $\hat{m}_{XX}$  is the maximum likelihood estimator for  $(\sigma_{xx})_S$ ,  $\hat{m}_{XX} = (\hat{\sigma}_{xx})_S$ .

In the special case under consideration,  $(\sigma_{yy})_F = (c_F)^2 (\sigma_{xx})_F$ ,  $(\sigma_{xy})_F = 0$ , Eqs. (143), (144), (145), reduce to:

$$(\hat{\sigma}_{\hat{a}_C})^2 = \frac{1}{n-1} \frac{1}{(\hat{m}_{XX})^2} \left\{ [\hat{m}_{XX} + (\sigma_{xx})_F] \hat{\sigma}_{vv} - (\hat{a}_C)^2 [(\sigma_{xx})_F]^2 \right\} ; \quad (146)$$

$$\hat{\sigma}_{vv} = [(\hat{a}_C)^2 + (c_F)^2] (\sigma_{xx})_F ; \quad (147)$$

$$\hat{\sigma}_{xv} = -\hat{a}_C (\sigma_{xx})_F ; \quad (148)$$

if, in addition, least squares estimators are proportional to corresponding moments estimators, the following relations hold:

$$[(\hat{\sigma}_{xx})_U]_{lsc} = C_{X_U} [(\hat{\sigma}_{xx})_U]_{mme} ; \quad U = F, S ; \quad (149a)$$

$$(\hat{\sigma}_{vv})_{lsc} = C_v (\hat{\sigma}_{vv})_{mme} ; \quad (149b)$$

where  $C_{X_U}$ ,  $C_v$ , are constants and the indices, lsc, mme, mean least squares estimators and methods of moments estimators, respectively.

The substitution of Eq. (149) into (146) yields:

$$\begin{aligned} (\hat{\sigma}_{\hat{a}_C})^2 = \frac{1}{n-1} \frac{1}{(C_{X_S})^2 [(\hat{\sigma}_{xx})_S]^2} & \left\{ [C_{X_S} (\hat{\sigma}_{xx})_S + C_{X_F} (\hat{\sigma}_{xx})_F] C_v [(\hat{a}_C)^2 + (c_F)^2] \right. \\ & \left. \times (\hat{\sigma}_{xx})_F - (\hat{a}_C)^2 [C_{X_F} (\hat{\sigma}_{xx})_F]^2 \right\} ; \quad (150) \end{aligned}$$

where the index, mme, has been omitted for simplifying the notation.

The substitution of Eq. (134) into (150) produces:

$$\begin{aligned} (\hat{\sigma}_{\hat{a}_C})^2 = \frac{1}{n-1} \frac{1}{[(\hat{\sigma}_{xx})_S]^2} \\ \times \left\{ \frac{C_v}{C_{X_S}} \left[ (\hat{\sigma}_{xx})_S + \frac{C_{X_F}}{C_{X_S}} (\hat{\sigma}_{xx})_F \right] \frac{n-2}{n-1} R_C - (\hat{a}_C)^2 \frac{(C_{X_F})^2}{(C_{X_S})^2} [(\hat{\sigma}_{xx})_F]^2 \right\} ; \quad (151) \end{aligned}$$

where the estimators,  $(\hat{\sigma}_{xx})_F$  and  $(\hat{\sigma}_{xx})_S$ , are expressed by Eqs. (132), (133), (135), (137). Accordingly, the explicit expression of Eq.(151) after some algebra reads:

$$(\hat{\sigma}_{\hat{a}_C})^2 = \frac{(\hat{a}_C)^2}{(S_{11})^2} \left\{ \frac{C_v}{C_{X_S}} \left[ \frac{S_{11}}{\hat{a}_C} + \frac{C_{X_F}}{C_{X_S}} \frac{S_{02} - \hat{a}_C S_{11}}{(c_F)^2} \right] \frac{n-2}{n-1} R_C - \frac{(C_{X_F})^2 (\hat{a}_C)^2}{(C_{X_S})^2 n-1} \left[ \frac{S_{02} - \hat{a}_C S_{11}}{(c_F)^2} \right]^2 \right\}; \quad (152)$$

where the restrictive assumptions:

$$\frac{C_{X_F}}{C_{X_S}} = 1 \quad ; \quad \frac{C_v}{C_{X_S}} = \frac{n-1}{n-2} \quad ; \quad (153)$$

make Eq. (152) reduce to:

$$(\hat{\sigma}_{\hat{a}_C})^2 = \frac{(\hat{a}_C)^2}{(S_{11})^2} \left\{ \left[ \frac{S_{11}}{\hat{a}_C} + \frac{S_{02} - \hat{a}_C S_{11}}{(c_F)^2} \right] R_C - \frac{(\hat{a}_C)^2}{n-1} \left[ \frac{S_{02} - \hat{a}_C S_{11}}{(c_F)^2} \right]^2 \right\}; \quad (154)$$

which formally coincides with the result of an earlier attempt where  $c_S = c$  appears instead of  $c_F$  [10] Eq. (4) therein.

Finally, the substitution of Eqs. (124) and (135) into (154) yields after some algebra:

$$(\hat{\sigma}_{\hat{a}_C})^2 = \frac{(\hat{a}_C)^2}{n-2} \times \left[ \frac{\hat{a}_X - \hat{a}_C}{\hat{a}_C} + \frac{\hat{a}_C - \hat{a}_Y}{\hat{a}_Y} + \frac{\hat{a}_X - \hat{a}_C}{\hat{a}_C} \frac{\hat{a}_C - \hat{a}_Y}{\hat{a}_Y} + \frac{1}{n-1} \left( \frac{\hat{a}_C - \hat{a}_Y}{\hat{a}_Y} \right)^2 \right]; \quad (155)$$

from which the following is inferred by comparison with Eq. (56):

$$\Theta(\hat{a}_C, \hat{a}_Y, \hat{a}_X) = \frac{\hat{a}_X - \hat{a}_C}{\hat{a}_C} \frac{\hat{a}_C - \hat{a}_Y}{\hat{a}_Y} + \frac{1}{n-1} \left( \frac{\hat{a}_C - \hat{a}_Y}{\hat{a}_Y} \right)^2 \quad ; \quad (156)$$

as listed in Table 1.

The revised version of the regression line variance estimator reported in an earlier attempt [10] Eq. (4) therein, [11] reads:

$$(\hat{\sigma}_{\hat{a}_C})^2 = \frac{(\hat{a}_C)^2}{n-2} \left\{ \frac{(n-2)R_C}{\hat{a}_C S_{11}} + \frac{1}{n-1} \frac{(\hat{a}_C)^2}{(\hat{a}_C)^2 + c^2} \left[ 1 - \frac{n-2}{n-1} \frac{(\hat{a}_C)^2}{(\hat{a}_C)^2 + c^2} \right] \left[ \frac{(n-2)R_C}{\hat{a}_C S_{11}} \right]^2 \right\}; \quad (157)$$

and the substitution of Eqs. (124), (142), into (157), after a lot of algebra yields:

$$(\hat{\sigma}_{\hat{a}_C})^2 = \frac{(\hat{a}_C)^2}{n-2} \left\{ \frac{\hat{a}_X - \hat{a}_C}{\hat{a}_C} + \frac{\hat{a}_C - \hat{a}_Y}{\hat{a}_Y} + \frac{1}{n-1} \left[ \frac{\hat{a}_X - \hat{a}_C}{\hat{a}_C} \frac{\hat{a}_C - \hat{a}_Y}{\hat{a}_Y} + \frac{1}{n-1} \left( \frac{\hat{a}_C - \hat{a}_Y}{\hat{a}_Y} \right)^2 \right] \right\} ; \quad (158)$$

from which the following is inferred by comparison with Eq. (56):

$$\Theta(\hat{a}_C, \hat{a}_Y, \hat{a}_X) = \frac{1}{n-1} \left[ \frac{\hat{a}_X - \hat{a}_C}{\hat{a}_C} \frac{\hat{a}_C - \hat{a}_Y}{\hat{a}_Y} + \frac{1}{n-1} \left( \frac{\hat{a}_C - \hat{a}_Y}{\hat{a}_Y} \right)^2 \right] ; \quad (159)$$

as listed in Table 1.

The asymptotic expression ( $n \rightarrow +\infty$ ) of Eq. (158) is obtained neglecting the terms of higher order with respect to  $1/n$ . The result is:

$$(\hat{\sigma}_{\hat{a}_C})^2 = \frac{(\hat{a}_C)^2}{n-2} \left\{ \frac{\hat{a}_X - \hat{a}_C}{\hat{a}_C} + \frac{\hat{a}_C - \hat{a}_Y}{\hat{a}_Y} \right\} ; \quad (160)$$

which implies  $\Theta(\hat{a}_C, \hat{a}_Y, \hat{a}_X) = 0$ , as listed in Table 1. The asymptotic formula, Eq. (160), coincides with an approximation reported in earlier attempts [23, 25] for Y models and makes a better approximation for X, C, O, R, and B models.

## C Data-independent residuals

Let  $u_A, u_B$ , be independent random variables,  $f_A(u_A) du_A, f_B(u_B) du_B$ , related distributions,  $u_A^*, u_B^*$ , related expectation values, and  $\hat{u}_A, \hat{u}_B$ , related estimators. The random variable,  $u = u_A u_B$ , obeys the distribution,  $f(u) du = \int_U f_A(u_A) f_B(u_B) du_A du_B$ , where U is the domain for which the product,  $u_A u_B$ , equals a fixed  $u$ . According to a theorem of statistics, the expectation value is  $u^* = (u_A u_B)^* = u_A^* u_B^*$  and the related estimator is  $\hat{u} = \widehat{u_A u_B} \approx \hat{u}_A \hat{u}_B$ .

The special case of the arithmetic mean reads  $\bar{u} = \overline{u_A u_B} \approx \bar{u}_A \bar{u}_B$  or:

$$\frac{1}{n} \sum_{i=1}^n (u_A)_i (u_B)_i \approx \frac{1}{n} \sum_{i=1}^n (u_A)_i \frac{1}{n} \sum_{i=1}^n (u_B)_i ; \quad (161)$$

with regard to  $u_A$  and  $u_B$  samples with population equal to  $n$ .

With these general results in mind, let Eqs. (27), (41), (60), be rewritten into the explicit form [14] Eqs. (A4)-(A6) therein<sup>2</sup>:

$$(\hat{\sigma}_{\hat{a}_Y})^2 = \frac{1}{(S_{20})^2} \sum_{i=1}^n \left\{ (X_i - \bar{X})^2 [(Y_i - \bar{Y}) - \hat{a}_Y(X_i - \bar{X})]^2 \right\} ; \quad (162)$$

$$(\hat{\sigma}_{\hat{a}_X})^2 = \frac{1}{(S_{11})^2} \sum_{i=1}^n \left\{ (Y_i - \bar{Y})^2 [(Y_i - \bar{Y}) - \hat{a}_X(X_i - \bar{X})]^2 \right\} ; \quad (163)$$

$$\begin{aligned} \hat{\sigma}_{\hat{a}_Y \hat{a}_X} &= \frac{1}{S_{20} S_{11}} \sum_{i=1}^n \left\{ (X_i - \bar{X})(Y_i - \bar{Y}) [(Y_i - \bar{Y}) - \hat{a}_Y(X_i - \bar{X})] \right. \\ &\quad \left. \times [(Y_i - \bar{Y}) - \hat{a}_X(X_i - \bar{X})] \right\} ; \end{aligned} \quad (164)$$

where (dimensional) residuals related to Y and X models are enclosed in square brackets via Eqs. (24) and (38), respectively.

If residuals are independent of coordinates of observed points,  $P_i \equiv (X_i, Y_i)$ ,  $1 \leq i \leq n$ , then the particularization of Eq. (161) to  $u_A = (X_i - \bar{X})^2, (Y_i - \bar{Y})^2, (X_i - \bar{X})(Y_i - \bar{Y})$ ;  $u_B = [(Y_i - \bar{Y}) - \hat{a}_Y(X_i - \bar{X})]^2, [(Y_i - \bar{Y}) - \hat{a}_X(X_i - \bar{X})]^2, [(Y_i - \bar{Y}) - \hat{a}_Y(X_i - \bar{X})][(Y_i - \bar{Y}) - \hat{a}_X(X_i - \bar{X})]$ ; respectively, makes Eqs. (162)-(164) reduce to:

$$(\hat{\sigma}_{\hat{a}_Y})^2 = \frac{1}{n} \frac{1}{(S_{20})^2} \sum_{i=1}^n (X_i - \bar{X})^2 \sum_{i=1}^n [(Y_i - \bar{Y}) - \hat{a}_Y(X_i - \bar{X})]^2 ; \quad (165)$$

$$(\hat{\sigma}_{\hat{a}_X})^2 = \frac{1}{n} \frac{1}{(S_{11})^2} \sum_{i=1}^n (Y_i - \bar{Y})^2 \sum_{i=1}^n [(Y_i - \bar{Y}) - \hat{a}_X(X_i - \bar{X})]^2 ; \quad (166)$$

$$\begin{aligned} \hat{\sigma}_{\hat{a}_Y \hat{a}_X} &= \frac{1}{n} \frac{1}{S_{20} S_{11}} \sum_{i=1}^n (X_i - \bar{X})(Y_i - \bar{Y}) \sum_{i=1}^n [(Y_i - \bar{Y}) - \hat{a}_Y(X_i - \bar{X})] \\ &\quad \times [(Y_i - \bar{Y}) - \hat{a}_X(X_i - \bar{X})] ; \end{aligned} \quad (167)$$

as outlined in an earlier attempt [14].

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<sup>2</sup>With regard to the above quoted Eqs. (A4)-(A6), it is worth noticing  $a_Y, a_X$ , are denoted as  $\beta_1, \beta_2$ , respectively, and  $\beta_1$  has to be replaced by  $(\beta_1)^{-1}$  in Eq. (A6) to get the right dimensions and to be consistent with the expression of the covariance term [14] note to Table 1 therein.



Using Eqs. (15), (23), (37), while performing some algebra, Eqs. (165)-(167) may be cast into the form:

$$(\hat{\sigma}_{\hat{a}_Y})^2 = \frac{(\hat{a}_Y)^2 \hat{a}_X - \hat{a}_Y}{n \hat{a}_Y} ; \quad (168)$$

$$(\hat{\sigma}_{\hat{a}_X})^2 = \frac{(\hat{a}_X)^2 \hat{a}_X - \hat{a}_Y}{n \hat{a}_Y} ; \quad (169)$$

$$\hat{\sigma}_{\hat{a}_Y \hat{a}_X} = \frac{(\hat{a}_Y)^2 \hat{a}_X - \hat{a}_Y}{n \hat{a}_Y} ; \quad (170)$$

which provide correct asymptotic ( $n \rightarrow +\infty$ ) formulae but underestimate the true regression coefficient uncertainty in samples with low ( $n \lesssim 50$ ) or weakly correlated population [10].

An inspection of Table 1 shows Eq. (25) and the asymptotic ( $n \rightarrow +\infty$ ) expression of Eq. (39) match Eqs. (168) and (169), respectively, provided  $n$  therein is replaced by  $(n - 2)$ . Accordingly, Eqs. (168)-(170) translate into:

$$(\hat{\sigma}_{\hat{a}_Y})^2 = \frac{(\hat{a}_Y)^2 \hat{a}_X - \hat{a}_Y}{n - 2 \hat{a}_Y} ; \quad (171)$$

$$(\hat{\sigma}_{\hat{a}_X})^2 = \frac{(\hat{a}_X)^2 \hat{a}_X - \hat{a}_Y}{n - 2 \hat{a}_Y} ; \quad (172)$$

$$\hat{\sigma}_{\hat{a}_Y \hat{a}_X} = \frac{(\hat{a}_Y)^2 \hat{a}_X - \hat{a}_Y}{n - 2 \hat{a}_Y} ; \quad (173)$$

which are expected to yield improved values for samples with low or weakly correlated population.

With regard to oblique regression models, the substitution of Eqs. (171)-(173) into (63) yields after some algebra:

$$(\hat{\sigma}_{\hat{a}_C})^2 = \frac{(\hat{a}_C)^2}{n - 2} \times \left\{ A_{XY} + \frac{2(\hat{a}_Y)^2 (\hat{a}_C)^2 (A_{XY})^2 A_{XC} A_{CY}}{4(\hat{a}_Y)^2 (\hat{a}_C)^2 A_{XC} A_{CY} + [\hat{a}_Y \hat{a}_X A_{CY} - (\hat{a}_C)^2 A_{XC}]^2} \right\}; \quad (174)$$

where the identity:

$$A_{XY} = A_{XU} + A_{UY} + A_{XU} A_{UY} ; \quad (175)$$

may easily be verified, being  $U = C$  in the case under discussion. Accordingly, Eq. (174) may be cast under the form:

$$(\hat{\sigma}_{\hat{a}_C})^2 = \frac{(\hat{a}_C)^2}{n-2} [A_{XC} + A_{CY} + \Theta(\hat{a}_C, \hat{a}_Y, \hat{a}_X)] ; \quad (176)$$

$$\Theta(\hat{a}_C, \hat{a}_Y, \hat{a}_X) = A_{XC}A_{CY} \times \left\{ 1 + \frac{2(\hat{a}_Y)^2(\hat{a}_C)^2(A_{XY})^2}{4(\hat{a}_Y)^2(\hat{a}_C)^2A_{XC}A_{CY} + [\hat{a}_Y\hat{a}_XA_{CY} - (\hat{a}_C)^2A_{XC}]^2} \right\} \quad (177)$$

where Eqs. (176) and (56) coincide in the limit,  $\Theta \rightarrow 0$ .

With regard to reduced major axis regression models, the substitution of Eqs. (171)-(173) into (85) yields after some algebra:

$$(\hat{\sigma}_{\hat{a}_R})^2 = \frac{(\hat{a}_R)^2}{n-2} \frac{A_{XY}}{2} \left( 1 + \frac{\hat{a}_Y}{\hat{a}_X} \right) ; \quad (178)$$

where the identity:

$$\frac{\hat{a}_Y}{\hat{a}_X} = \frac{1}{A_{XY} + 1} ; \quad (179)$$

may easily be verified. Accordingly, Eq. (178) via (175) may be cast into the form:

$$(\hat{\sigma}_{\hat{a}_R})^2 = \frac{(\hat{a}_R)^2}{n-2} [A_{XR} + A_{RY} + \Theta(\hat{a}_R, \hat{a}_Y, \hat{a}_X)] ; \quad (180)$$

$$\Theta(\hat{a}_R, \hat{a}_Y, \hat{a}_X) = A_{XR}A_{RY} - \frac{1}{2} \frac{(A_{XY})^2}{A_{XY} + 1} ; \quad (181)$$

where Eqs. (180) and (83) coincide in the limit,  $\Theta \rightarrow 0$ .

With regard to bisector regression models, the substitution of Eqs. (171)-(173) into (103) yields after some algebra:

$$(\hat{\sigma}_{\hat{a}_B})^2 = \frac{(\hat{a}_B)^2}{n-2} \frac{A_{XY}(\hat{a}_Y)^2}{(\hat{a}_Y + \hat{a}_X)^2} \left[ \frac{a_u^2 + (\hat{a}_X)^2}{a_u^2 + (\hat{a}_Y)^2} + \frac{a_u^2 + (\hat{a}_Y)^2}{a_u^2 + (\hat{a}_X)^2} \frac{(\hat{a}_X)^2}{(\hat{a}_Y)^2} + 2 \right] ; \quad (182)$$

which, using Eqs. (175) and (179), may be cast under the form:

$$(\hat{\sigma}_{\hat{a}_B})^2 = \frac{(\hat{a}_B)^2}{n-2} [A_{XB} + A_{BY} + \Theta(\hat{a}_B, \hat{a}_Y, \hat{a}_X)] ; \quad (183)$$

$$\Theta(\hat{a}_B, \hat{a}_Y, \hat{a}_X) = \frac{A_{XY}}{(A_{XY} + 2)^2} \left[ \frac{a_u^2 + (\hat{a}_X)^2}{a_u^2 + (\hat{a}_Y)^2} + \frac{a_u^2 + (\hat{a}_Y)^2}{a_u^2 + (\hat{a}_X)^2} \frac{(\hat{a}_X)^2}{(\hat{a}_Y)^2} + 2 \right] - A_{XY} + A_{XB}A_{BY} ; \quad (184)$$

where Eqs. (183) and (101) coincide in the limit,  $\Theta \rightarrow 0$ .

## D Special cases of oblique regression

With regard to homoscedastic data, special cases of oblique regression may be considered starting from the expression of regression line slope and intercept estimators, Eqs. (54) and (55), and related variance estimators, Eqs. (56) and (57) for normal residuals or (58) and (59) for non normal residuals. As outlined in the parent paper [10], the special cases,  $c \rightarrow +\infty$ ,  $c \rightarrow 0$ ,  $c \rightarrow 1$ , correspond to errors in  $X$  negligible with respect to errors in  $Y$ , errors in  $Y$  negligible with respect to errors in  $X$ , and orthogonal regression, respectively. In addition, the limiting case,  $c \rightarrow c_{\text{rma}} = \sqrt{a_X a_Y}$ , corresponds to reduced major-axis regression e.g., [14, 7]. An exhaustive discussion related to regression line slope and intercept estimators, can be found in an earlier attempt [7]. Finally, the limiting case,  $c \rightarrow c_{\text{bis}}$ , where  $c_{\text{bis}}$  is expressed by Eq. (100), corresponds to bisector regression. The result is:

$$\lim_{c \rightarrow +\infty} \hat{a}_C = \hat{a}_Y ; \quad \lim_{c \rightarrow 0} \hat{a}_C = \hat{a}_X ; \quad \lim_{c \rightarrow 1} \hat{a}_C = \hat{a}_O ; \quad \lim_{c \rightarrow c_{\text{rma}}} \hat{a}_C = \hat{a}_R ; \quad (185a)$$

$$\lim_{c \rightarrow c_{\text{bis}}} \hat{a}_C = \hat{a}_B ; \quad (185b)$$

where related models are denoted by the indices, Y, X, O, R, B, respectively.

Concerning regression line slope variance estimators for normal residuals, the following relations can be inferred from Eq. (56):

$$\lim_{c \rightarrow +\infty} [(\hat{\sigma}_{\hat{a}_C})_N]^2 = \frac{(\hat{a}_Y)^2}{n-2} \left[ \frac{\hat{a}_X - \hat{a}_Y}{\hat{a}_Y} + \Theta(\hat{a}_Y, \hat{a}_Y, \hat{a}_X) \right] ; \quad (186)$$

$$\lim_{c \rightarrow 0} [(\hat{\sigma}_{\hat{a}_C})_N]^2 = \frac{(\hat{a}_X)^2}{n-2} \left[ \frac{\hat{a}_X - \hat{a}_Y}{\hat{a}_Y} + \Theta(\hat{a}_X, \hat{a}_Y, \hat{a}_X) \right] ; \quad (187)$$

$$\lim_{c \rightarrow 1} [(\hat{\sigma}_{\hat{a}_C})_N]^2 = \frac{(\hat{a}_O)^2}{n-2} \left[ \frac{\hat{a}_X - \hat{a}_O}{\hat{a}_O} + \frac{\hat{a}_O - \hat{a}_Y}{\hat{a}_Y} + \Theta(\hat{a}_O, \hat{a}_Y, \hat{a}_X) \right] ; \quad (188)$$

$$\lim_{c \rightarrow c_{\text{rma}}} [(\hat{\sigma}_{\hat{a}_C})_N]^2 = \frac{(\hat{a}_R)^2}{n-2} \left[ \frac{\hat{a}_X - \hat{a}_R}{\hat{a}_R} + \frac{\hat{a}_R - \hat{a}_Y}{\hat{a}_Y} + \Theta(\hat{a}_R, \hat{a}_Y, \hat{a}_X) \right] ; \quad (189)$$

$$\lim_{c \rightarrow c_{\text{bis}}} [(\hat{\sigma}_{\hat{a}_C})_N]^2 = \frac{(\hat{a}_B)^2}{n-2} \left[ \frac{\hat{a}_X - \hat{a}_B}{\hat{a}_B} + \frac{\hat{a}_B - \hat{a}_Y}{\hat{a}_Y} + \Theta(\hat{a}_B, \hat{a}_Y, \hat{a}_X) \right] ; \quad (190)$$

where the function,  $\Theta$ , is listed in Table 1 for different methods and/or models.

A comparison between Eqs. (25), (39), and (186), (187), respectively, yields:

$$\lim_{c \rightarrow +\infty} [(\hat{\sigma}_{\hat{a}_C})_N]^2 = [(\hat{\sigma}_{\hat{a}_Y})_N]^2 ; \quad (191)$$

$$\lim_{c \rightarrow 0} [(\hat{\sigma}_{\hat{a}_C})_N]^2 = [(\hat{\sigma}_{\hat{a}_X})_N]^2 ; \quad (192)$$

and, on the other hand:

$$\lim_{c \rightarrow 1} [(\hat{\sigma}_{\hat{a}_C})_N]^2 = [(\hat{\sigma}_{\hat{a}_O})_N]^2 ; \quad (193)$$

$$\lim_{c \rightarrow c_{rma}} [(\hat{\sigma}_{\hat{a}_C})_N]^2 = [(\hat{\sigma}_{\hat{a}_R})_N]^2 ; \quad (194)$$

$$\lim_{c \rightarrow c_{bis}} [(\hat{\sigma}_{\hat{a}_C})_N]^2 = [(\hat{\sigma}_{\hat{a}_B})_N]^2 ; \quad (195)$$

by definition of orthogonal regression e.g., [8] Chap. 3, §4.4.2, reduced major-axis regression e.g., [14, 7], and bisector regression e.g., [14].

Concerning regression line intercept variance estimators for normal residuals, the following relations can be inferred from Eq. (57):

$$\lim_{c \rightarrow +\infty} [(\hat{\sigma}_{\hat{b}_C})_N]^2 = \frac{\hat{a}_Y}{n-2} \frac{\hat{a}_X - \hat{a}_Y}{\hat{a}_Y} \frac{S_{11}}{S_{00}} + (\bar{X})^2 [(\hat{\sigma}_{\hat{a}_Y})_N]^2 ; \quad (196)$$

$$\lim_{c \rightarrow 0} [(\hat{\sigma}_{\hat{b}_C})_N]^2 = \frac{\hat{a}_X}{n-2} \frac{\hat{a}_X - \hat{a}_Y}{\hat{a}_Y} \frac{S_{11}}{S_{00}} + (\bar{X})^2 [(\hat{\sigma}_{\hat{a}_X})_N]^2 ; \quad (197)$$

$$\lim_{c \rightarrow 1} [(\hat{\sigma}_{\hat{b}_C})_N]^2 = \frac{\hat{a}_O}{n-2} \left[ \frac{\hat{a}_X - \hat{a}_O}{\hat{a}_O} + \frac{\hat{a}_O - \hat{a}_Y}{\hat{a}_Y} \right] \frac{S_{11}}{S_{00}} + (\bar{X})^2 [(\hat{\sigma}_{\hat{a}_O})_N]^2 ; \quad (198)$$

$$\lim_{c \rightarrow c_{rma}} [(\hat{\sigma}_{\hat{b}_C})_N]^2 = \frac{\hat{a}_R}{n-2} \left[ \frac{\hat{a}_X - \hat{a}_R}{\hat{a}_R} + \frac{\hat{a}_R - \hat{a}_Y}{\hat{a}_Y} \right] \frac{S_{11}}{S_{00}} + (\bar{X})^2 [(\hat{\sigma}_{\hat{a}_R})_N]^2 ; \quad (199)$$

$$\lim_{c \rightarrow c_{bis}} [(\hat{\sigma}_{\hat{b}_C})_N]^2 = \frac{\hat{a}_B}{n-2} \left[ \frac{\hat{a}_X - \hat{a}_B}{\hat{a}_B} + \frac{\hat{a}_B - \hat{a}_Y}{\hat{a}_Y} \right] \frac{S_{11}}{S_{00}} + (\bar{X})^2 [(\hat{\sigma}_{\hat{a}_B})_N]^2 ; \quad (200)$$

due to Eqs. (185) and (191)-(195).

A comparison between Eqs. (26), (40), and (196), (197), respectively, yields:

$$\lim_{c \rightarrow +\infty} [(\hat{\sigma}_{\hat{b}_C})_N]^2 = [(\hat{\sigma}_{\hat{b}_Y})_N]^2 ; \quad (201)$$

$$\lim_{c \rightarrow 0} [(\hat{\sigma}_{\hat{b}_C})_N]^2 = [(\hat{\sigma}_{\hat{b}_X})_N]^2 ; \quad (202)$$

and, on the other hand:

$$\lim_{c \rightarrow 1} [(\hat{\sigma}_{\hat{b}_C})_N]^2 = [(\hat{\sigma}_{\hat{b}_O})_N]^2 ; \quad (203)$$

$$\lim_{c \rightarrow c_{rma}} [(\hat{\sigma}_{\hat{b}_C})_N]^2 = [(\hat{\sigma}_{\hat{b}_R})_N]^2 ; \quad (204)$$

$$\lim_{c \rightarrow c_{bis}} [(\hat{\sigma}_{\hat{b}_C})_N]^2 = [(\hat{\sigma}_{\hat{b}_B})_N]^2 ; \quad (205)$$

by definition of orthogonal regression e.g., [8] Chap. 3, §4.4.2, reduced major-axis regression e.g., [14, 7], and bisector regression e.g., [14].

Concerning regression line slope variance estimators for non normal residuals, the following relations can be inferred from Eq. (58):

$$\lim_{c \rightarrow +\infty} (\hat{\sigma}_{\hat{a}_C})^2 = (\hat{\sigma}_{\hat{a}_Y})^2 ; \quad (206)$$

$$\lim_{c \rightarrow 0} (\hat{\sigma}_{\hat{a}_C})^2 = (\hat{\sigma}_{\hat{a}_X})^2 ; \quad (207)$$

$$\lim_{c \rightarrow 1} (\hat{\sigma}_{\hat{a}_C})^2 = (\hat{a}_O)^2 \frac{a_u^4 (\hat{\sigma}_{\hat{a}_Y})^2 + (\hat{a}_Y)^4 (\hat{\sigma}_{\hat{a}_X})^2 + 2(\hat{a}_Y)^2 a_u^2 \hat{\sigma}_{\hat{a}_Y \hat{a}_X}}{(\hat{a}_Y)^2 [4(\hat{a}_Y)^2 a_u^2 + (\hat{a}_Y \hat{a}_X - a_u^2)^2]} ; \quad (208)$$

where  $a_u = 1$  is the (dimensional) unit slope, according to their counterparts expressed in the parent paper [14] provided  $|\hat{a}_Y|$  is replaced by  $\hat{a}_Y$  therein.

On the other hand, the following relation holds:

$$\lim_{c \rightarrow 1} (\hat{\sigma}_{\hat{a}_C})^2 = (\hat{\sigma}_{\hat{a}_O})^2 ; \quad (209)$$

by definition of orthogonal regression e.g., [8] Chap. 3, §4.4.2.

The intercept variance estimators for special cases of oblique regression, are expressed by a single formula characterized by different dimensionless coefficients,  $\gamma_{1k}$ ,  $\gamma_{2k}$ , where  $k = 1, 2, 4$ , for Y, X, O, models, respectively [14]. The extended expressions for oblique regression, where  $k = 6$  for C models, read:

$$\gamma_{16} = \frac{\hat{a}_C c^2}{\hat{a}_Y [4(\hat{a}_Y)^2 c^2 + (\hat{a}_Y \hat{a}_X - c^2)^2]^{1/2}} ; \quad (210)$$

$$\gamma_{26} = \frac{\hat{a}_C \hat{a}_Y}{[4(\hat{a}_Y)^2 c^2 + (\hat{a}_Y \hat{a}_X - c^2)^2]^{1/2}} ; \quad (211)$$

which, for the above mentioned special cases, reduce to:

$$\gamma_{11} = \lim_{c \rightarrow +\infty} \gamma_{16} = 1 ; \quad (212)$$

$$\gamma_{21} = \lim_{c \rightarrow +\infty} \gamma_{26} = 0 ; \quad (213)$$

$$\gamma_{12} = \lim_{c \rightarrow 0} \gamma_{16} = 0 ; \quad (214)$$

$$\gamma_{22} = \lim_{c \rightarrow 0} \gamma_{26} = 1 ; \quad (215)$$

according to their counterparts expressed in the parent paper [14] and, in addition:

$$\gamma_{14} = \lim_{c \rightarrow 1} \gamma_{16} = \frac{\hat{a}_O a_u^2}{\hat{a}_Y [4(\hat{a}_Y)^2 a_u^2 + (\hat{a}_Y \hat{a}_X - a_u^2)^2]^{1/2}} ; \quad (216)$$

$$\gamma_{24} = \lim_{c \rightarrow 1} \gamma_{26} = \frac{\hat{a}_O \hat{a}_Y}{[4(\hat{a}_Y)^2 a_u^2 + (\hat{a}_Y \hat{a}_X - a_u^2)^2]^{1/2}} ; \quad (217)$$

where  $a_u = 1$  is the (dimensional) unit slope, according to their counterparts expressed in the parent paper [14] provided  $|\hat{a}_Y|$  is replaced by  $\hat{a}_Y$  therein.

The validity of Eqs. (212)-(217) implies the validity of the following relations:

$$\lim_{c \rightarrow +\infty} (\hat{\sigma}_{\hat{b}_C})^2 = (\hat{\sigma}_{\hat{b}_Y})^2 ; \quad (218)$$

$$\lim_{c \rightarrow 0} (\hat{\sigma}_{\hat{b}_C})^2 = (\hat{\sigma}_{\hat{b}_X})^2 ; \quad (219)$$

$$\lim_{c \rightarrow 1} (\hat{\sigma}_{\hat{b}_C})^2 = (\hat{\sigma}_{\hat{b}_O})^2 ; \quad (220)$$

in the general case of non normal residuals.

The above results cannot be extended to R and B models i.e.  $k = 5, 3$ , respectively, due to use of the  $\delta$ -method for determining variance estimators [14], which implies  $\lim_{u_C \rightarrow u_U} (\hat{\sigma}_{\hat{u}_C})^2 \neq (\hat{\sigma}_{\hat{u}_U})^2$ ;  $u = a, b$ ;  $U = R, B$ .

With regard to heteroscedastic data, the above results can be extended starting from the expression of regression line slope and intercept estimators, Eqs. (69) and (70) for normal residuals, which yields counterparts of Eqs. (196)-(199) where  $n(\tilde{w}_x)_{pq}/(\tilde{w}_x)_{00}$  appears in place of  $S_{pq}$  and  $\hat{a}'_Y = (\tilde{w}_x)_{11}/(\tilde{w}_x)_{20}$  in place of  $\hat{a}_Y = (\tilde{w}_y)_{11}/(\tilde{w}_y)_{20}$ . A similar procedure can be used for non normal residuals, starting from Eqs. (71) and (72).

## E C11 erratum

Due to the occurrence of printing errors, Eqs. (147) and (152) in an earlier attempt [7] were lacking of a dimensionless factor and must be corrected as follows:

$$(\hat{\sigma}_{\hat{a}_R})^2 = \frac{2}{n-2} \frac{(\tilde{w}_x)_{02}}{(\tilde{w}_x)_{20}} \left\{ \frac{1}{(\lambda_{w_x})^2} - \text{sgn}[(\tilde{w}_x)_{11}] \frac{1}{\lambda_{w_x}} \right\} ; \quad (147)$$

$$(\hat{\sigma}_{\hat{a}_R})^2 = \frac{2}{n-2} \frac{S_{02}}{S_{20}} \left[ \frac{1}{(\lambda_S)^2} - \text{sgn}(S_{11}) \frac{1}{\lambda_S} \right] ; \quad (152)$$

which are equivalent to their alternative expressions, Eqs. (149) and (154) therein, respectively.

Sample FB09 listed in Table 2 therein has to be read as RB09.

## F A linear relation between primary elements from stellar nucleosynthesis

The composition of the interstellar medium, from which a star generation was born, remains locked in stellar atmospheres. Attention shall be restricted to primary elements i.e. those synthesized in stellar cores starting from hydrogen and helium regardless of the initial composition. Conversely, secondary elements can be synthesized only in presence of heavier (with respect to hydrogen and helium) nuclides, which are called metals in astrophysics.

The ideal situation, where a linear relation holds between primary elements in stellar atmospheres, is defined by the following assumptions.

- (i) The initial stellar mass function is universal, which implies the star distribution in mass (including binary and multiple systems), normalized to unity, maintains unchanged regardless of the formation place and the formation epoch.
- (ii) Gas returned after star death is instantaneously and uniformly mixed with the interstellar medium.
- (iii) The yield of primary elements synthesized within a star depends only on the mass regardless of the initial composition.
- (iv) Supernovae may occur as either type II ( $m > 8m_{\odot}$ ) or type Ia ( $m \leq 8m_{\odot}$ ).

Accordingly, the composition of the interstellar medium is due to the accretion of newly synthesized material via supernovae. With regard to a sufficiently short time step,  $\Delta t$ , let  $n_{\text{I}}$  and  $n_{\text{II}}$  be the number of type Ia and type II supernovae, respectively; in addition, let  $\delta m_{\text{WI}}$  and  $\delta m_{\text{WII}}$  be the mean mass in the primary element, W, newly synthesized and returned to the interstellar medium via type Ia and type II supernovae, respectively.

Within a time range equal to the first  $\ell$  steps,  $t_{\ell} - t_0 = \ell \Delta t$ , the interstellar medium has been enriched by a mass in the primary element, W, as:

$$\begin{aligned}
 m_{\text{W}} &= \sum_{k=1}^{\ell} [(n_{\text{II}})_k \delta m_{\text{WII}} + (n_{\text{I}})_k \delta m_{\text{WI}}] = \\
 &= \sum_{k=1}^{\ell} (n_{\text{II}})_k \delta m_{\text{WII}} \left[ 1 + \frac{(n_{\text{I}})_k}{(n_{\text{II}})_k} \frac{\delta m_{\text{WI}}}{\delta m_{\text{WII}}} \right] ; \quad (221)
 \end{aligned}$$

where  $\delta m_{\text{WI}}$  and  $\delta m_{\text{WII}}$  may be considered, to a good extent, as time independent.

The further assumption of time independent number ratios:

$$\frac{(n_{\text{I}})_k}{(n_{\text{II}})_k} = \frac{n_{\text{I}}}{n_{\text{II}}} ; \quad (222)$$

makes Eq. (221) reduce to:

$$m_{\text{W}} = \sum_{k=1}^{\ell} (n_{\text{II}})_k \delta m_{\text{WII}} \left[ 1 + \frac{n_{\text{I}}}{n_{\text{II}}} \frac{\delta m_{\text{WI}}}{\delta m_{\text{WII}}} \right] ; \quad (223)$$

which implies an abundance ratio of two generic primary elements, A and B, in stellar atmospheres i.e. interstellar medium, as:

$$\begin{aligned} \frac{\exp_{10} [\text{A}/\text{H}]}{\exp_{10} [\text{B}/\text{H}]} &\approx \frac{\phi_{\text{A}}}{\phi_{\text{B}}} = \frac{Z_{\text{A}}/(Z_{\text{A}})_{\odot}}{Z_{\text{B}}/(Z_{\text{B}})_{\odot}} = \frac{m_{\text{A}} (Z_{\text{B}})_{\odot}}{m_{\text{B}} (Z_{\text{A}})_{\odot}} \\ &= \frac{\delta m_{\text{AII}}}{\delta m_{\text{BII}}} \frac{1 + \frac{n_{\text{I}}}{n_{\text{II}}} \frac{\delta m_{\text{AI}}}{\delta m_{\text{AII}}} \frac{(Z_{\text{B}})_{\odot}}{(Z_{\text{A}})_{\odot}}}{1 + \frac{n_{\text{I}}}{n_{\text{II}}} \frac{\delta m_{\text{BI}}}{\delta m_{\text{BII}}} \frac{(Z_{\text{A}})_{\odot}}{(Z_{\text{A}})_{\odot}}} ; \quad (224) \end{aligned}$$

where  $[\text{A}/\text{H}]$ ,  $[\text{B}/\text{H}]$ , are logarithmic number abundances normalized to the solar value;  $\phi_{\text{A}}$ ,  $\phi_{\text{B}}$ , are mass abundances normalized to the solar value;  $Z_{\text{A}}$ ,  $Z_{\text{B}}$ , are mass abundances; values are related to the interstellar medium from which the star considered was born, with the exception of  $(Z_{\text{A}})_{\odot}$ ,  $(Z_{\text{B}})_{\odot}$ , denoting solar abundances. For further details refer to the parent paper [5].

In terms of logarithmic number abundances, Eq. (224) may be cast under the form:

$$[\text{A}/\text{H}] = [\text{B}/\text{H}] + b ; \quad (225)$$

$$b = \log \left[ \frac{\delta m_{\text{AII}}}{\delta m_{\text{BII}}} \frac{1 + \frac{n_{\text{I}}}{n_{\text{II}}} \frac{\delta m_{\text{AI}}}{\delta m_{\text{AII}}} \frac{(Z_{\text{B}})_{\odot}}{(Z_{\text{A}})_{\odot}}}{1 + \frac{n_{\text{I}}}{n_{\text{II}}} \frac{\delta m_{\text{BI}}}{\delta m_{\text{BII}}} \frac{(Z_{\text{A}})_{\odot}}{(Z_{\text{A}})_{\odot}}} \right] ; \quad (226)$$

which is a linear relation with unit slope. The general case:

$$[\text{A}/\text{H}] = a[\text{B}/\text{H}] + b ; \quad (227)$$

could arise under different assumptions.



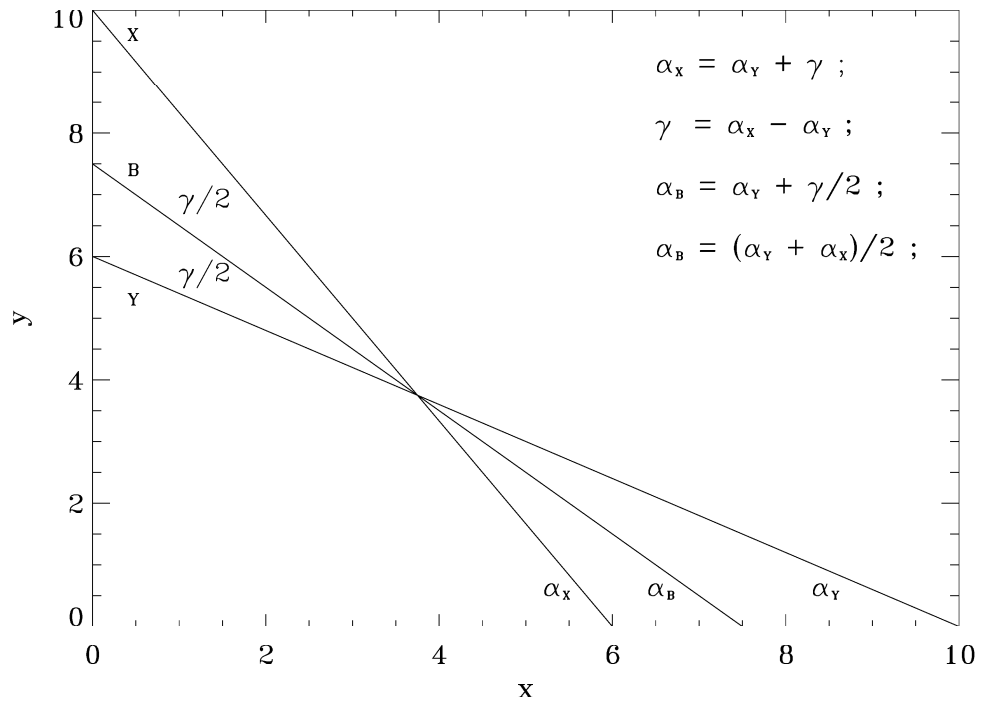


Figure 1: Regression lines related to Y, X, and B models, for an assigned sample. By definition, the B line bisects the angle,  $\gamma$ , formed between Y and X lines. The angle,  $\alpha_B$ , formed between B line and  $x$  axis, is the arithmetic mean of the angles,  $\alpha_Y$  and  $\alpha_X$ , formed between Y line and  $x$  axis and between X line and  $x$  axis, respectively.

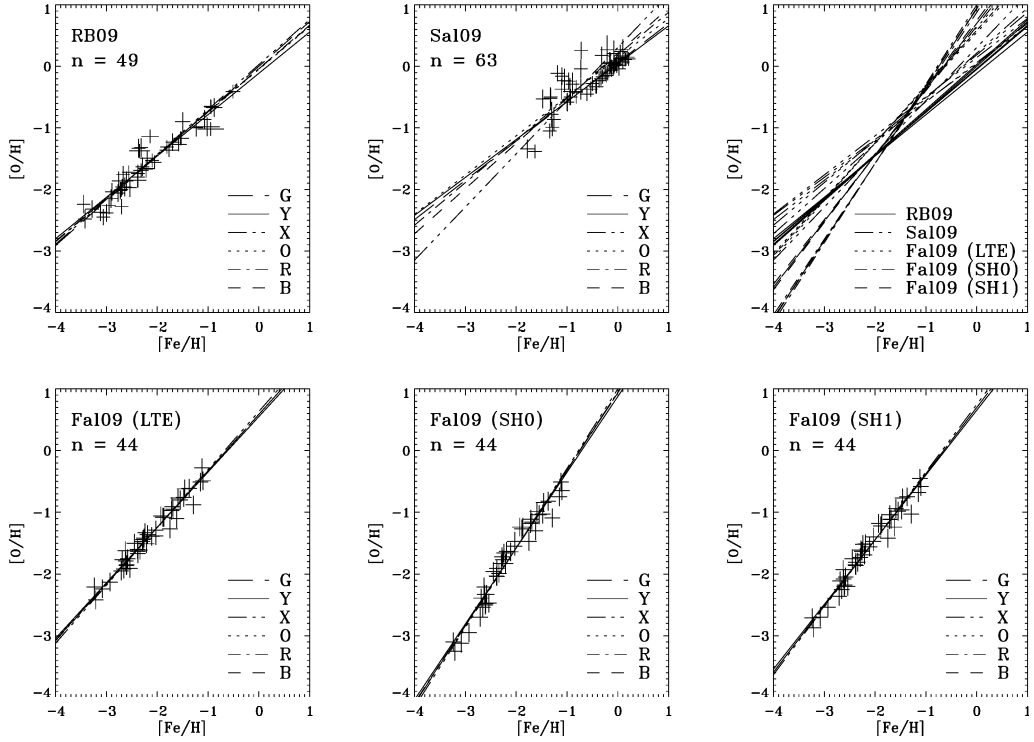


Figure 2: Regression lines related to  $[O/H]$ - $[Fe/H]$  empirical relations deduced from two samples with heteroscedastic data, RB09 and Sa09, and three samples with homoscedastic data (using the computer code for heteroscedastic data), Fa09, cases LTE, SH0, and SH1, indicated on each panel together with related population and model captions. The regression lines related to six different methods are shown for each sample on the top right panel. For further details refer to the text.

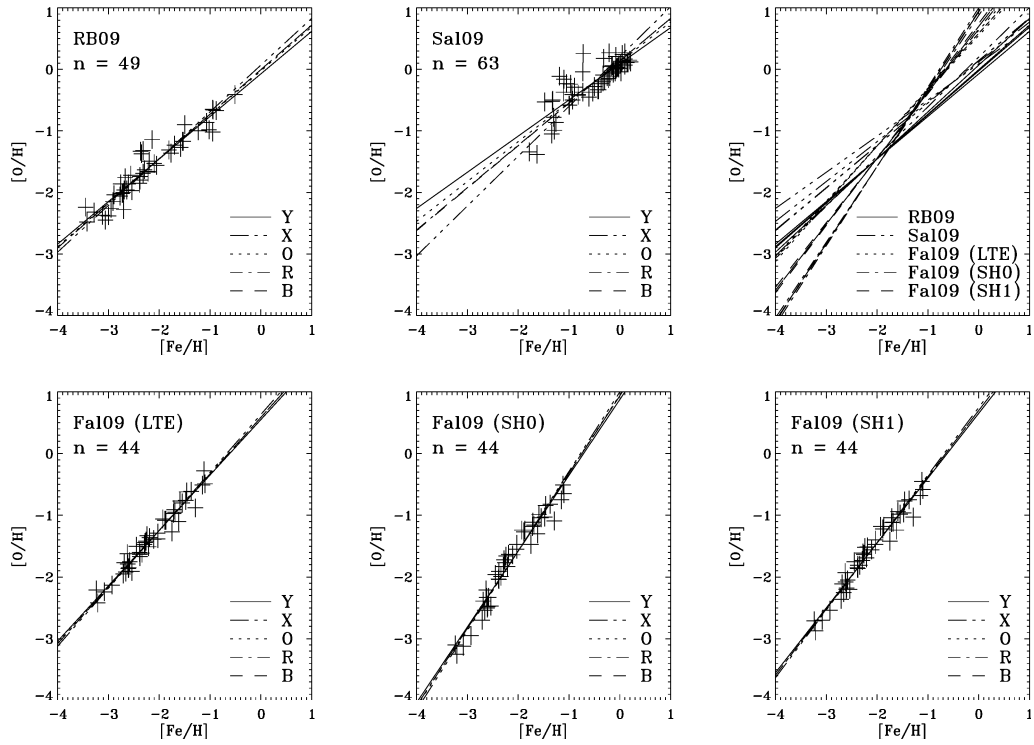


Figure 3: Regression lines related to  $[O/H]$ - $[Fe/H]$  empirical relations deduced from two samples with heteroscedastic data (with instrumental scatters taken equal to related typical values), RB09 and Sa09, and three samples with homoscedastic data, Fa09, cases LTE, SH0, and SH1, indicated on each panel together with related population and model captions. The regression lines related to five different methods are shown for each sample on the top right panel. For further details refer to the text.