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Full Length Article

Estimating rock strength parameters across varied failure criteria: Application of spreadsheet and R-based orthogonal regression to triaxial test data

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A B S T R A C T

Triaxial tests, a staple in rock engineering, are labor-intensive, sample-demanding, and costly, making their optimization highly advantageous. These tests are essential for characterizing rock strength, and by adopting a failure criterion, they allow for the derivation of criterion parameters through regression, facilitating their integration into modeling programs. In this study, we introduce the application of an underutilized statistical technique—orthogonal regression— well-suited for analyzing triaxial test data. Additionally, we present an innovation in this technique by minimizing the Euclidean distance while incorporating orthogonality between vectors as a constraint, for the case of orthogonal linear regression. Also, we consider the Modified Least Squares method. We exemplify this approach by developing the necessary equations to apply the Mohr-Coulomb, Murrell, Hoek-Brown, and Úcar criteria, and implement these equations in both spreadsheet calculations and R scripts. Finally, we demonstrate the technique's application using five datasets of varied lithologies from specialized literature, showcasing its versatility and effectiveness.

1. Introduction

In civil, mining, and petroleum engineering, it is common to apply a rock failure criterion whose parameters must be determined when modeling the ground behavior in response to the considered construction. There are numerous failure criteria: Edelbro (2003) conducted an analysis of twelve criteria available at that time, ranging from the Mohr-Coulomb criterion, which dates back to the 18th-20th-century contributions such as the Fairhurst (1964), Murrell (1965), and Hoek and Brown (1980) criteria, among others, although it did not include the well-known Mogi criterion (Mogi, 1971) in its review. However, the number of criteria, revisions, and comparisons among them have continued to grow in the 21st century, with additions including (without intending to be exhaustive in the enumeration) Yu (2004), the review by Lakirouhani and Hasanzadehshooiili (2011), Shen et al. (2014), Moshrefi et al. (2019), Úcar (2021), Mahetaji et al. (2023) and the reviews by He et al. (2022) and Mahetaji and Brahma (2024).

Triaxial tests, crucial for deriving the parameters of the different criteria (Elliott, 1993; Mishra and Janecek, 2017), represent a budget-intensive portion of laboratory experiments in rock mechanics, and they involve intensive laboratory work where the rock's strength is assessed under controlled conditions. Therefore, it is imperative to extract the maximum and most accurate information possible from these tests to ensure a return on the investment made.

These tests feed into regression analyses, typically using methods such as Ordinary Least Squares (OLS), to correlate the stress variables σ_3 and σ_1, wherein the sum of the squares of the vertical deviations from the data points to the regression line is minimized—assuming the independent variable is constant and attributing all potential error to the dependent variable (see Fig. 1). It is worth highlighting a very interesting approach that addresses

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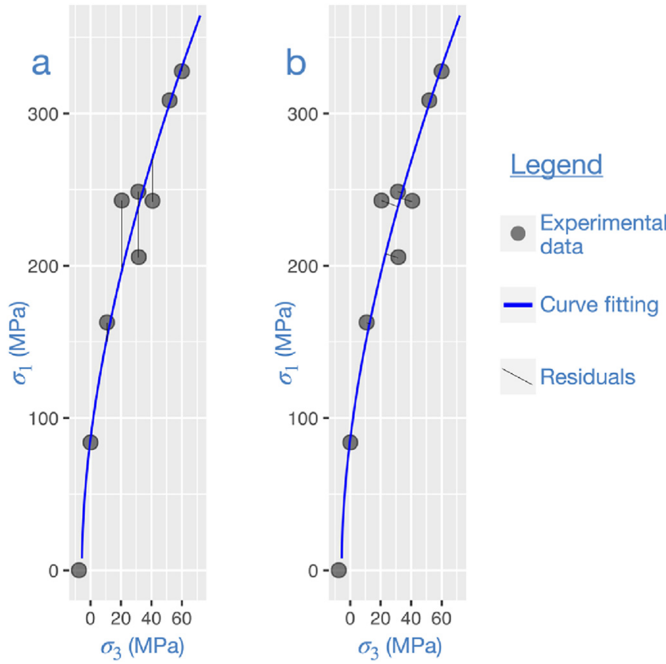

Fig. 1. (a) Conventional regression, where all potential error is attributed to the independent variable, σ_1 in our case, versus (b) orthogonal regression, which accounts for error also in the dependent variable. Data of Pniowek sandstone, sourced from Kwasniewski (1983) as cited by Sheorey (1997). Both axes are at the same scale, for clarity, the next figures will be at different scales.

this situation. This approach involves the modification proposed by Mostyn and Douglas (2000), which also addresses three other key points.

Firstly, the Hoek and Brown criterion, in its usual expression, is not defined for confining pressure values, $\sigma_3 \leq -\sigma_c/m_i$. Secondly, conventional OLS adjustments do not account for the fact that, in tensile strength tests ($\sigma_3 < 0$), the roles of the control variable and the dependent variable are reversed between σ_3 and σ_1 compared to triaxial compression tests. Thirdly, conventional OLS adjustments assign much greater influence to tests with high confining pressure because, as also observed by Pariseau (2007), logically, the residuals to be minimized will be proportionally larger for high confining pressures than for low ones.

These ideas have been incorporated into the modifications proposed by Mostyn and Douglas (2000), Douglas and Mostyn (2004) and tested by Douglas (2002) and Bertuzzi et al. (2016), which can be referred to as Modified Least Squares (MLS), providing excellent fits that surpass those obtained through conventional OLS. This justifies the special attention given to this approach. As we will see in this work, the seldom-used orthogonal regression accounts for errors in both the response variable and the predictor, leading to a more statistically robust model. This is particularly relevant in our context, given that both variables are of the same nature and are measured similarly.

Keleş and Altun (2016) acknowledge that orthogonal regression, initially developed by Adcock (1878), has been rediscovered numerous times and has been well-understood for over a century. A chronological non-exhaustive review of significant contributions to this method includes early works such as Deming (1943) with their seminal "Statistical Adjustment of Data", followed by Nievergelt (1994), Van Huffel (1997), Caizada and Scariano (2003), Carr (2012), Ding et al. (2013), Mujica (2017), Villota-Viveros (2018), Keleş (2018), and Pallavi et al. (2022) demonstrating the widespread utilization of this statistical technique among researchers.

The ultimate goal is to determine the parameters that best fit the acquired data so that the applied failure criterion faithfully replicates the rock's actual strength. When determining the regression model, one may choose between a linear or a nonlinear model. This choice, in our case, is essentially dictated by the nature of the selected failure criterion and its specific mathematical formulation. This study aims to apply orthogonal regression to four different rock failure criteria, three of which are well-known and widely used, namely Mohr-Coulomb, Murrell (1965), and Hoek and Brown (1980, 2019), and a fourth, the innovative yet still lesser-known Úcar (2021) criterion. One of them, Mohr-Coulomb (M-C), is a linear criterion, and the other three are nonlinear in nature. By comparing these methods, we aim to demonstrate the enhanced reliability and accuracy of orthogonal regression in determining rock failure parameters.

2. Orthogonal regression

2.1. Linear and nonlinear model

In this section, the statistical method utilized for regression is known as orthogonal regression (OR), also commonly referred to as total least squares (TLS) or errors-in-variables (EIV) regression. This method minimizes the sum of the squares of the orthogonal distances between the experimental data points and the regression line, accounting for errors in both variables. Through this research, the parameters or regressor coefficients are determined alongside the statistical measures of goodness of fit, such as R-squared (R^2) and the standard error of the estimate. These statistical procedures enable the comparison of observed experimental values with those predicted by the regression models applied to the four empirical failure criteria selected for analysis.

A significant challenge arises because the proposed equations generally do not conform to a linear criterion.

In certain cases, and for specific applications, the well-known Mohr-Coulomb equation can be applied. This equation is commonly expressed in the form of a straight line, thus we assert that Mohr-Coulomb is a linear criterion. Consequently, one may employ a linear regression procedure to ascertain the

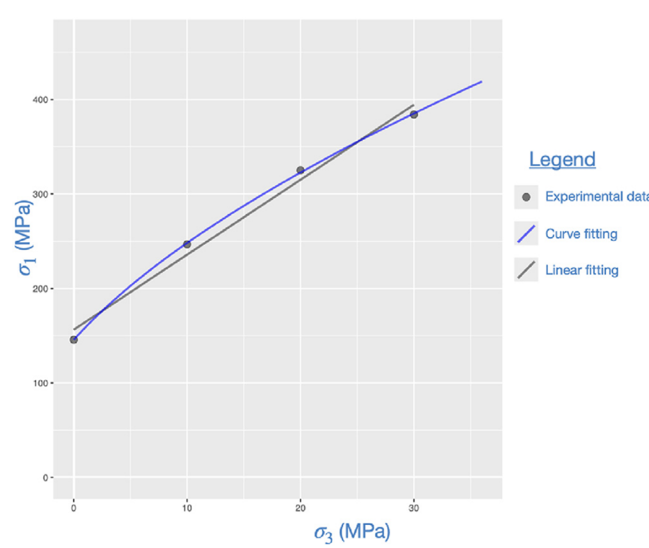

Fig. 2. Experimental data points often exhibit a better fit with a curve than a straight line, indicating the need for a nonlinear criterion. In the figure, the data is sourced from Betournay et al. (1991) as cited in Sheorey (1997). The blue curve represents the proposed criterion adjusted to the data points, while the grey line depicts the linear best fit.

corresponding parameters.

At other times (refer to Fig. 2), experimental data points are not aligned along a straight line, making it more suitable to fit a curve to the data. This necessitates the use of a nonlinear criterion, such as the Murrell (Murrell, 1965; Bieniawski, 1974), Hoek-Brown (Hoek and Brown, 1980, 2019), or Úcar criteria (Úcar, 2011, 2021), see Fig. 3 for a general view of the criteria and their main parameters applied to the same set of triaxial tests and resulting pairs (σ_3, σ_1).

According to Chatterjee and Price (1977), regression models can be categorized into two types, termed linear and nonlinear. The natural inclination, therefore, might be to fit the parameters of the Mohr-Coulomb to the experimental data using linear regression, and those of the other mentioned criteria using a nonlinear regression; however, this is not automatically valid. In statistical regression, the need to fit data to a curve does not automatically necessitate nonlinear regression. This is because the 'linear' aspect of regression refers to the coefficients and not to the form of the relationship between variables. Consider a standard linear regression model:

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 \ldots + \beta_k x_k + e \tag{1}$$

where β_i is the coefficient, x_i is the predictor, and e is the error term. The model is 'linear' in the sense that each term involving the parameters β_i is in a linear form. This linearity pertains to the parameters irrespective of whether the relationship between y and each x_i appears curved or not.

For the nonlinear models:

$$y = \beta_0 + \beta_1 x + \beta_2 x^2 + e \tag{2}$$

$$y = \beta_0 + \beta_1 \ln x + e \tag{3}$$

The parameters remain linear, despite the nonlinear relationships between the dependent variable y and the independent variable x. Additionally, both equations can be linearized through variable transformations that convert the models' formulations to a linear form.

Rivas et al. (1993) provide a straightforward method to discern the linearity of a model by examining the derivative of the function with respect to each parameter β_i. If the derivative is independent of any β_i and is linear for all model parameters, then the model is expressed as linear in parameters.

Frost (2020) posits that nonlinear models offer the same predictive power as linear models but with added flexibility due to the diversity of functional forms they can adopt.

2.2. Analytical method of orthogonal regression

Utilizing the principles of analytical geometry, we calculate the

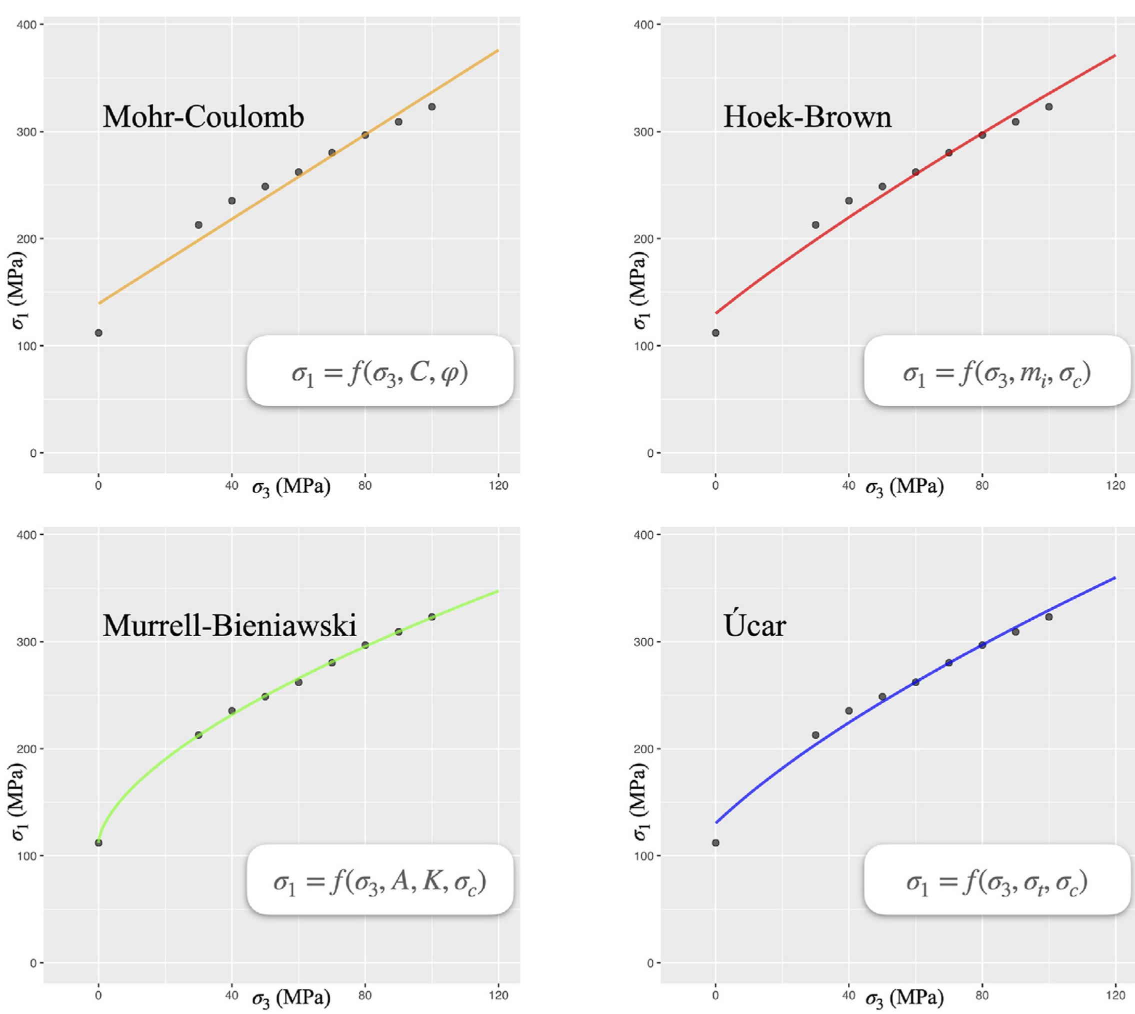

Fig. 3. The four methods that we will employ in this work, adjusted in R to the same set of triaxial data and their corresponding pairs (σ_3, σ_1). For each criterion, the parameters involved in the criterion for the determination of σ_1 are indicated. The rock tested is rhyolite from Kidd Creek Mine, as sourced from Betournay et al. (1991), cited in Sheorey (1997).

shortest distance from a point to a line, a concept central to the statistical method of orthogonal regression. Fig. 4 illustrates this with the implicit form of the line's equation. At $x = 0$, this line intersects the ordinate axis at $\beta_0 = -(C/B)$. On the other hand, the vector $\overrightarrow{PP}_i$ is defined by

$$\overrightarrow{PP}_i = x_i\,\vec{i} + \left(y_i + \frac{C}{B}\right)\vec{j} \tag{4}$$

Additionally, the normal vector to the line is obtained through the gradient vector:

$$\vec{N} = \nabla f = \frac{\partial f}{\partial x}\vec{i} + \frac{\partial f}{\partial y}\vec{j} = A\,\vec{i} + B\,\vec{j} \tag{5}$$

Being also the unit vector:

$$\vec{n} = \frac{\vec{N}}{|\vec{N}|} = \frac{A\,\vec{i} + B\,\vec{j}}{\sqrt{A^2 + B^2}} \tag{6}$$

Knowing both vectors, the distance d_i normal to the line from the point P_i (x_i, y_i) is

$$d_i = |\overrightarrow{PP}_i| \cdot |\vec{n}| \cos\theta = |\overrightarrow{PP}_i| \cos\theta \tag{7}$$

$$d_i = \left[x_i\,\vec{i} + \left(y_i + \frac{C}{B}\right)\vec{j}\right] \cdot \frac{A\,\vec{i} + B\,\vec{j}}{\pm\sqrt{A^2 + B^2}} \tag{8}$$

Resulting finally, through the scalar product:

$$d_i = \frac{Ax_i + By_i + C}{\pm\sqrt{A^2 + B^2}} \tag{9}$$

On the other hand, the equation of the line can be expressed in the form:

$$y = -\frac{A}{B}x - \frac{C}{B} \tag{10}$$

$$\left.\begin{aligned} \beta_0 &= -\frac{C}{B} \\ \beta_1 &= -\frac{A}{B} = \tan\psi \end{aligned}\right\} \tag{11}$$

Therefore, replacing Eq. (11) into Eq. (10) results in

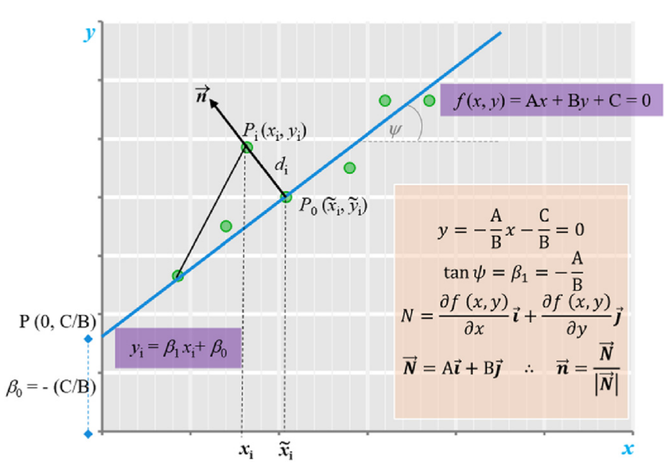

Fig. 4. Orthogonal distance (d_i) from a point P_i (x_i, y_i) to the regression line.

$$y = \beta_0 + \beta_1 x \tag{12}$$

In this context, the distance d_i from a point P_i with coordinates (x_i, y_i) to the regression line can be expressed as

$$d_i = \frac{|\beta_1 x_i - y_i + \beta_0|}{\sqrt{\beta_1^2 + 1}} \tag{13}$$

Logically, the distance d_i is the residual error e_i of the considered point P_i (x_i, y_i). Conversely, the objective is to ascertain the regression line's parameters or coefficients by minimizing the total sum of squares of the residuals for the entire triaxial test data set:

$$f(\beta_1, \beta_0) = \sum_{i=1}^{n} e_i^2 = \sum_{i=1}^{n}\left(\frac{\beta_1 x_i - y_i + \beta_0}{\sqrt{\beta_1^2 + 1}}\right)^2 \tag{14}$$

Next, we compute the partial derivatives with respect to β_0 and β_1 and set them equal to zero. This process yields this system of equations (Recio-López, 2021):

$$\left.\begin{aligned} &\sum_{i=1}^{n}(\beta_1 x_i - y_i + \beta_0)(x_i + \beta_1 y_i - \beta_1\beta_0) = 0 \\ &\sum_{i=1}^{n}(\beta_1 x_i - y_i + \beta_0) = 0 \end{aligned}\right\} \tag{15}$$

Additionally, the mean values of the set of data points are

$$\bar{x} = \frac{1}{n}\sum_{i=1}^{n} x_i;\ \bar{y} = \frac{1}{n}\sum_{i=1}^{n} y_i \tag{16}$$

Taking into account Eq. (16), the second equation indicated in (15) is transformed:

$$\beta_0 = \bar{y} - \beta_1\bar{x} \tag{17}$$

Developing the first equation in (15), and taking into account the mean values, together with the concepts of covariance s_{xy} and variances s_x^2 and s_y^2, the slope of the line that minimizes the function $f(\beta_0, \beta_1)$ is

$$\beta_1 = \frac{-\left(s_x^2 - s_y^2\right) + \sqrt{\left(s_x^2 - s_y^2\right)^2 + 4\,s_{xy}^2}}{2\,s_{xy}} \tag{18}$$

$$\left.\begin{aligned} s_x^2 &= \frac{1}{n}\sum_{i=1}^{n}\left(x_i^2 - \bar{x}^2\right) = \frac{1}{n}\sum_{i=1}^{n}(x_i - \bar{x})^2 \\ s_y^2 &= \frac{1}{n}\sum_{i=1}^{n}\left(y_i^2 - \bar{y}^2\right) = \frac{1}{n}\sum_{i=1}^{n}(y_i - \bar{y})^2 \\ s_{xy} &= \frac{1}{n}\sum_{i=1}^{n}(x_i - \bar{x})\cdot(y_i - \bar{y}) \end{aligned}\right\} \tag{19}$$

Hence, using the values of β_0 and β_1 as specified in Eqs. (17) and (18), we can derive the equation of the straight line by applying the orthogonal regression technique.

Once the function $f(\beta_0, \beta_1)$ is minimized, the regression coefficients obtained are denoted as $\widehat{\beta}_0$ and $\widehat{\beta}_1$, following the usual notation (Chatterjee and Price, 1977). So, the equation for the regression line becomes

$$\widehat{y}_i = \widehat{\beta}_0 + \widehat{\beta}_1 x_i \tag{20}$$

It should be noted that Recio-López (2021) defines the coefficient of determination R^2, specifically for the case of orthogonal regression as follows:

$$R^2 = 1 - \frac{\sum_{i=1}^{n} e_i^2}{\sum_{i=1}^{n} d(\overline{P}, P_i)^2} = \frac{s_y^2\,\widehat{\beta}_1^2 + 2\,s_{xy}\,\widehat{\beta}_1 + s_x^2}{\left(s_x^2 + s_y^2\right)\left(1 + \widehat{\beta}_1^2\right)} \tag{21}$$

As previously stated, in this study we deal with obtaining the parameters for intact rock failure criteria using triaxial tests. The coordinates of an intersection point between the normal line P_0P and the tangent line P_0P_1, at point P_0 of the curve $f(x)$, as shown in Fig. 5, serve as the basis for determining the regression coefficient parameters for both linear and nonlinear models, and are represented by the following expression:

$$y_n = -\frac{1}{f'(\tilde{x}_0)}(x - \tilde{x}_0) + f(\tilde{x}_0) \tag{22}$$

Hence, for orthogonal regression, we replace the coordinates (x, y) with (σ_3, σ_1), where σ_3, the minor principal stress at failure, is the independent variable, and σ_1, the major principal stress at the moment of failure, is the dependent variable. The experimental data points are denoted by $(\sigma_{3i}, \sigma_{1i})$ for i = 1, 2, 3, …, n.

From Fig. 6, the equation of the straight line P_0P normal to the regression line, at point P_0, when considering Eq. (22), results:

$$\sigma_1 = -\frac{1}{\tan\psi}\left(\sigma_3 - \tilde{\sigma}_{3i}\right) + \tilde{\sigma}_{1i} \tag{23}$$

For simplicity, we initially assume that the regression line's precise equation, including its slope and intercept, is unknown—these do not represent the optimal parameters. Thus, as described earlier in Eq. (12), the line is represented by

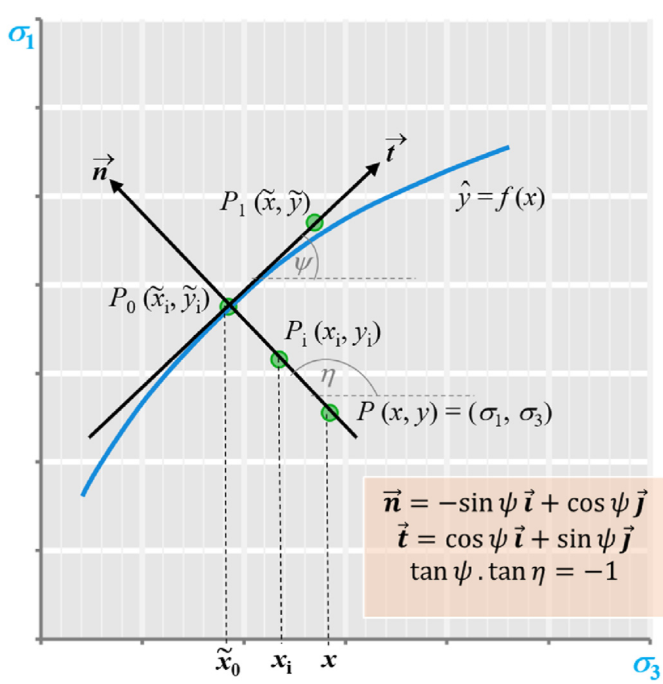

Fig. 5. Tangent line to the regression curve at point P_0 $(\tilde{x}_0, \tilde{y}_0)$. Once the fitted values are obtained, the regression equation becomes $\hat{y} = f(x_i)$, considering the estimated regression parameters $\widehat{\beta}_0, \widehat{\beta}_1, ..., \widehat{\beta}_k$.

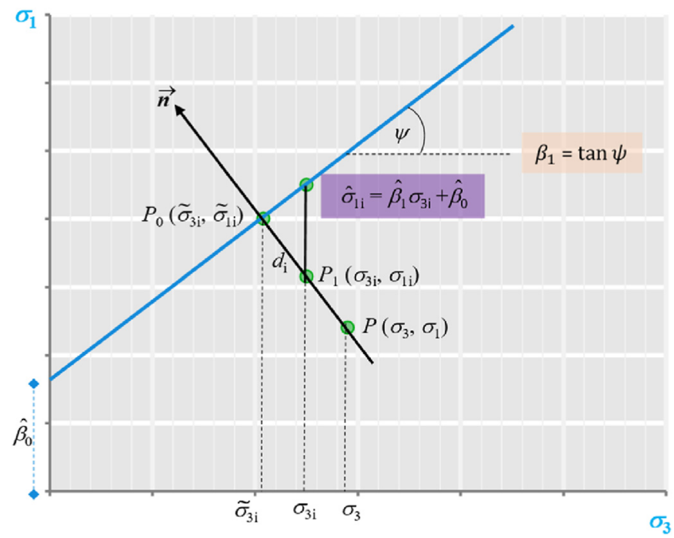

Fig. 6. Determination of the coordinates $(\tilde{\sigma}_{3i}, \tilde{\sigma}_{1i})$ belonging to the point of intersection between the fitted regression line and the normal line passing through point $P_1(\sigma_{3i}, \sigma_{1i})$. Once the residual is minimized and the regressor parameters are obtained, the fitted curve takes the form $\widehat{\sigma}_{1i} = \beta_1\widehat{\sigma}_{3i} + \widehat{\beta}_0$.

$$\sigma_1 = \beta_1\sigma_3 + \beta_0 \tag{24}$$

where $\beta_1 = \tan\psi$ is the dip, and β_0 is the intercept. Under these conditions, taking into account the point P_i $(\sigma_{3i}, \sigma_{1i})$, Eqs. (23) and (24) are transformed into:

$$\sigma_{1i} = -\frac{1}{\beta_1}(\sigma_{3i} - \tilde{\sigma}_{3i}) + \tilde{\sigma}_{1i} \tag{25}$$

On the other hand, according to Eq. (24):

$$\tilde{\sigma}_{1i} = \beta_1\tilde{\sigma}_{3i} + \beta_0 \tag{26}$$

Replacing $\tilde{\sigma}_{1i}$ in Eq. (25) and clearing $\tilde{\sigma}_{3i}$ we obtain

$$\tilde{\sigma}_{3i} = \left[\frac{\beta_1\sigma_{1i} + \sigma_{3i} - \beta_0\,\beta_1}{1 + \beta_1^2}\right] \tag{27}$$

Similarly:

$$\tilde{\sigma}_{1i} = \left[\frac{\beta_1^2\,\sigma_{1i} + \beta_1\,\sigma_{3i} + \beta_0}{1 + \beta_1^2}\right] \tag{28}$$

From Fig. 6, the distance d_i squared is

$$e_i^2 = d_i^2 = \left[(\sigma_{1i} - \tilde{\sigma}_{1i})^2 + (\sigma_{3i} - \tilde{\sigma}_{3i})^2\right] \tag{29}$$

Minimizing the sum of squares of the residuals, taking into account Eqs. (27) and (28), for the n experimental points $P(\sigma_{3i}, \sigma_{1i})$ it results

$$\text{Min}\sum_{i=1}^{n} e_i^2 = \text{Min}\sum_{i=1}^{n}\left[(\sigma_{1i} - \tilde{\sigma}_{1i})^2 + (\sigma_{3i} - \tilde{\sigma}_{3i})^2\right] \tag{30}$$

The approach suggested in this study involves minimizing the sum of the Euclidean distances from the data points to points belonging to the regression line, which equates to minimizing the following expression:

$$\text{Min}\sum_{i=1}^{n} e_{\mathrm{i}} = \text{Min}\sqrt{\sum_{i=1}^{n}\left[(\sigma_{1\mathrm{i}}-\tilde{\sigma}_{1\mathrm{i}})^2+(\sigma_{3\mathrm{i}}-\tilde{\sigma}_{3\mathrm{i}})^2\right]} \tag{31}$$

Furthermore, this is subject to a constraint that incorporates the concept of orthogonality (see Fig. 7), which necessitates that the dot product between the vector connecting the experimental points to those on the regression line, and the vector linking the points on the regression line to their mean values, must be zero:

$$\overrightarrow{\boldsymbol{P}_{\mathbf{0}}\boldsymbol{P}_{\mathbf{i}}}\cdot\overrightarrow{\overline{\boldsymbol{P}}\boldsymbol{P}_{\mathbf{0}}}=0 \tag{32}$$

After minimizing the function using either of the specified methods, the coefficients are converted to $\widehat{\beta}_1, \widehat{\beta}_0$, which define the regression adjustment equation. Additionally, this yields the benefit of determining, through Eqs. (27) and (28), the coordinates of the intersection between the fitted regression line and the normal line passing through the experimental point. Finally, it's notable that in Fig. 7, as point P_{i} approaches P_0, the distance d nears to zero, thus the ratio of the two distances converges to one. Additionally, incorporating the concept of variance, the value of R^2, based on the left side of Eq. (20), can be succinctly formulated in a more concise expression:

$$R^2=\frac{\sum_{i=1}^{n}\left[\frac{(\tilde{x}_{\mathrm{i}}-\overline{x})^2+(\tilde{y}_{\mathrm{i}}-\overline{y})^2}{(n-1)}\right]}{\sum_{i=1}^{n}\left[\frac{(x_{\mathrm{i}}-\overline{x})^2+(y_{\mathrm{i}}-\overline{y})^2}{(n-1)}\right]} \tag{33}$$

In terms of variances, takes the form:

$$R^2=\frac{\text{Var}(\tilde{x})+\text{Var}(\tilde{y})}{\text{Var}(x)+\text{Var}(y)}=\left(\frac{{s_{\tilde{x}}}^2+{s_{\tilde{y}}}^2}{s_{x}^2+s_{y}^2}\right) \tag{34}$$

2.3. Modified least squares

As anticipated in the introduction of this work, Mostyn and Douglas (2000) presented a procedure that was further developed and discussed by Douglas (2002), Douglas and Mostyn (2004), Sari (2012), Bertuzzi (2013), and Bertuzzi et al. (2016), addressing several issues that arise when fitting regression models to strength test data under varying confining pressures. Initially proposed for application to the Hoek and Brown (HB) criterion, some of its aspects—those not specific to any particular criterion—are sufficiently valuable to have been adapted and tested in this study.

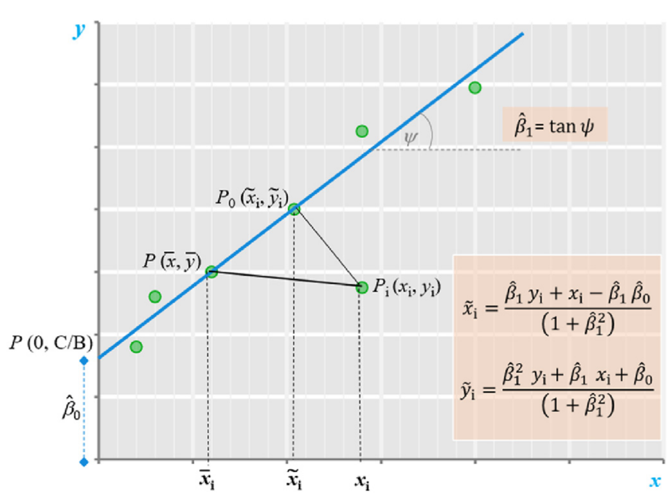

Fig. 7. Graphical representation of the orthogonal regression line and the mean values ($\overline{x}$, $\overline{y}$) of the experimental data set P_{i} (x_{i}, y_{i}). Note that the vector from P_0 to P_{i} is orthogonal to the vector from the mean point $\overline{P}$ to P_0, i.e., $\overrightarrow{\boldsymbol{P}\boldsymbol{P}_{\mathbf{i}}}\cdot\overrightarrow{\overline{\boldsymbol{P}}\boldsymbol{P}_{\mathbf{0}}}=0$.

These authors focused on the HB criterion, as mentioned, and pointed out that its usual expression is not defined for values of $\sigma_3 \leq -\sigma_{\mathrm{c}}/m_{\mathrm{i}}$, leading to an indeterminate condition. Additionally, in tensile strength tests, where $\sigma_3 < 0$, the roles of the control variable and the dependent variable are reversed between σ_3 and σ_1, meaning that regression should be performed accordingly, without assuming error solely in the control variable (note that this issue is not relevant in the context of orthogonal regression). Finally, since the OLS fitting process involves minimizing the sum of residuals that arise from the comparison between the criterion's prediction and the observed data, the larger the predicted and observed values, the larger the residuals will be, and consequently, their proportional weight in the overall fit will be greater (Pariseau, 2007). In other words, triaxial tests conducted under high confining pressures disproportionately influence the determination of the optimal fit compared to tests conducted under low confining pressures. Since the minimizing parameter involves the residual sum of squares (RSS), the squaring of residuals further penalizes larger residuals (Uriel, 2019). This effect is common to most regression techniques, not just OLS.

The first concern is addressed by redefining the HB criterion (Mostyn and Douglas, 2000) to cover the full range of confining stresses:

$$\left.\begin{array}{ll}\sigma_1=\sigma_3+\sigma_{\mathrm{c}}\left[m_{\mathrm{i}}\dfrac{\sigma_3}{\sigma_{\mathrm{c}}}+s\right]^{0.5} & \text{for } \sigma_3>\dfrac{\sigma_{\mathrm{c}}}{m_{\mathrm{i}}}\\ \sigma_1=\sigma_3 & \text{for } \sigma_3\leq-\dfrac{\sigma_{\mathrm{c}}}{m_{\mathrm{i}}}\end{array}\right\} \tag{35}$$

Furthermore, Douglas (2002) and Douglas and Mostyn (2004) found that the HB criterion provided better results when, instead of using the exponent 0.5 as in Eq. (35), an exponent a_i was used, with a_{i} ranging between 0.4 and 0.9. The second issue is resolved—for the HB criterion—by modifying the way residuals are computed, (measured σ_1 − predicted σ_1), for $\sigma_1 > 3\sigma_3$, and (measured σ_3 − predicted σ_3)m_i, for $\sigma_1 \leq$ - $3\sigma_3$. For different criteria, this modification must, logically, be adapted. The third problem is addressed by redefining the residuals again, incorporating a normalization using the value of σ_1 considered in each pair.

Following their procedure, two fitting loops are performed. In the first loop, the value of a_{i} is determined through least squares regression of the triaxial test data for the studied samples (with a_{i} constrained within the range specified by the authors). This value of a_{i} then allows for the estimation, in a second regression loop, of the adjusted values of the rest of parameters for the studied dataset.

The findings of Douglas (2002) and Bertuzzi et al. (2016) demonstrate a significantly improved fit compared to conventional OLS fitting of the original HB criterion (Eq. (45)). Consequently, this study will explore the comparison between the Mostyn and Douglas (2000) equation—henceforth referred to as HB-MD, following the nomenclature of Bertuzzi et al. (2016)—and the HB criterion, using both OLS and orthogonal regressions.

2.4. Orthogonal regression in R

The aforementioned procedures have been implemented in specially designed spreadsheets, yet similar results can be achieved using R (R Core Team, 2023). R natively provides linear regression functionalities, including capabilities such as fitting a model and deriving its parameters, computing correlation coefficients like Pearson's or Spearman's, and graphically depicting data alongside the resulting regression curve. Likewise, tools for performing nonlinear regression are also integrated into the main program via the "nls" function, which calculates nonlinear (weighted) least-squares estimates of a nonlinear model's parameters. Additionally, the "nlstools" package (Baty et al., 2015) is required for a more nuanced analysis. For orthogonal regression, R offers the "onls" package (Spiess, 2022), providing orthogonal nonlinear least-squares regression capabilities. The package starts by fitting to the data a conventional (non-orthogonal) nonlinear model by nls.lm. This is because the parameters of the orthogonal model are usually within a small window of those of a standard nls model. Then, through two loops, it performs first a Levenberg-Marquardt minimization of the orthogonal distance sum-of-squares and then minimizes and returns the vector of orthogonal distances.

The scripts, one tailored for each criterion and accessible to readers, begin by initializing a vector with the data. Given that the dataset typically comprises just a handful of (σ_3 – σ_1) pairs, importing data from.csv or spreadsheet files was deemed superfluous. Therefore, data is directly inputted into the script's body.

Depending on the chosen failure criterion, the script, after data loading, includes the relevant criterion's equations (model_function) to be fitted to the data. In all cases, seed values, starting values, or initial estimates are required to commence the iterative search for the best fit. Fully commented scripts are available to the reader.

3. Failure criteria. Change of notation

3.1. Ucar's nolinear failure criterion

The quadratic criterion recently introduced by Úcar (2011, 2021) correlates the principal stresses σ_1 and σ_3 at failure, alongside the analytical formulation for shear strength in rocks and other brittle materials like concrete.

This novel two-dimensional rupture criterion enables the parametric determination of normal and tangential stresses based on the angle made by the tangent to the failure envelope or the intrinsic resistance curve. This angle, referred to as the instantaneous internal friction angle, changes in response to varying levels of normal stresses.

For computational convenience, the correlation between the principal stresses σ_1 and σ_3 at failure is expressed in a non-dimensional form by the following plane curve equation:

$$\frac{\sigma_1}{\sigma_c} = k_1\left(\frac{\sigma_3}{\sigma_c} - \xi\right) + k_2\left(\frac{\sigma_3}{\sigma_c} - \xi\right)^{1/2} \tag{36}$$

where σ_c represents the unconfined compressive strength of the intact rock (rock matrix), σ_t is the uniaxial tensile strength, and $\xi = \sigma_t/\sigma_c$, a parameter that controls the position and curvature of the failure parabola.

A characteristic of the criterion is that the quadratic equation linking the principal stresses σ_1 and σ_3 defines a conic section, specifically a parabola, which accurately reflects the overall trend of experimental strength data for various rocks studied.

The values of k_1 and k_2, which depend directly on ξ were obtained (Úcar, 2021) through the properties of the parabola in its canonical form, and taking into account the latus rectum (chord) passing through the focus and perpendicular to the axis of the parabola:

$$\left.\begin{aligned} k_1 &= \frac{-(1+|\xi|)+\sqrt{1+6|\xi|-7\xi^2}}{2|\xi|} \\ k_2 &= \frac{1+k_1\xi}{\sqrt{-\xi}} \end{aligned}\right\} \tag{37}$$

Now, we can apply the analysis presented in previous sections to this criterion. In dimensionless form with respect to σ_c, the quadratic curve to be fitted is as follows for the intact rock condition:

$$\tilde{\sigma}_{1i} = k_1(\tilde{\sigma}_{3i} - \xi) + k_2(\tilde{\sigma}_{3i} - \xi)^{1/2} \tag{38}$$

And its derivative:

$$\tan\psi_i = \left(\frac{d\tilde{\sigma}_{1i}}{d\tilde{\sigma}_{3i}}\right) = k_1 + 0.5k_2\left(\tilde{\sigma}_{3i} - \xi\right)^{-1/2} \tag{39}$$

Considering Eq. (23), we obtain

$$\sigma_{1i}\tan\psi_i = (\tilde{\sigma}_{3i} - \sigma_{3i}) + \tilde{\sigma}_{1i}\tan\psi_i \tag{40}$$

By replacing Eqs. (38) and (39) in the previous expression:

$$\sigma_{1i}\left(k_1 + \frac{0.5\,k_2}{(\tilde{\sigma}_{3i} - \xi)^{1/2}}\right) = \tilde{\sigma}_{3i}\left(1 + k_1^2\right) + \frac{3}{2}k_1k_2(\tilde{\sigma}_{3i} - \xi)^{1/2} + \left(\frac{k_2^2}{2} - \sigma_{3i} - \xi\,k_1^2\right) \tag{41}$$

Eq. (41) takes the forms of a cubic equation. Analysis of the solutions based on its coefficients reveals one real root and two imaginary ones. This is demonstrated in the accompanying spreadsheet, where the regression parameters are derived using optimization procedures implemented through mathematical algorithms. Given these circumstances, we minimize the sum of orthogonal distances from each experimental point P_i (σ_{3i}, σ_{1i}) to the tangent line of the curve for $i = 1, 2, 3, \ldots, n$. Consequently, we ascertain the regression parameter ξ, and accordingly, the values of k_1 and k_2, along with the standard error to assess the regression fit. Concurrently, the optimization process also calculates the values of $\tilde{\sigma}_{3i} = f(\xi, k_1, k_2, \sigma_{3i}, \sigma_{1i})$ for each experimental point. The equation to minimize:

$$\mathrm{Min}\,d_i^2 = \mathrm{Min}\sum_{i=1}^{n}(\sigma_{3i} - \tilde{\sigma}_{3i})^2 + \left[\sigma_{1i} - \underbrace{\left(k_1(\tilde{\sigma}_{3i} - \xi) + k_2\sqrt{(\tilde{\sigma}_{3i} - \xi)}\right)}_{\tilde{\sigma}_{1i}}\right]^2 \tag{42}$$

3.2. Mohr-Coulomb's linear failure criterion

This well-known and widely used criterion of failure in rocks and soils is represented by the linear equation:

$$\sigma_1 = \sigma_3\tan^2(45 + \varphi/2) + 2C\tan(45 + \varphi/2) \tag{43}$$

where C is the shear strength when the normal stress, σ_n, equals to zero, and φ is the angle of internal friction. Expressing this equation in terms of the regressor parameters we have

$$\hat{\sigma}_1 = \sigma_3 \hat{\beta}_1 + \hat{\beta}_0 \tag{44}$$

Applying the orthogonal regression technique through Eqs. (17) and (18), and with the help of iterative optimization, the coefficients $\hat{\beta}_0$ and $\hat{\beta}_1$, and the shear parameters C and φ are determined. It should be noted that this procedure compares the results with the one proposed in this research using Eqs. (31) and (32).

3.3. Hoek and Brown's nonlinear failure criterion

Given that the Hoek-Brown criterion (Hoek and Brown, 1980, 2019) is indeed prevalent in the field of rock engineering, this section is expected to be of utmost interest. As it is well known, the generalized Hoek-Brown (HB) criterion is expressed as follows:

$$\sigma_1 = \sigma_3 + \sqrt{m\sigma_3\sigma_c + s\sigma_c^2} \tag{45}$$

where m, s and a are constants depending on rock properties. For intact rock, the material constants are denoted by m_i, $s = 1$ and $a = 0.5$ (Hoek and Brown, 1980, 2019). It may be beneficial at this juncture to consult Hoek and Brown (2019) for an analysis of the distinctions between σ_c (the experimental uniaxial compressive strength, UCS) and σ_{ci} (the value of σ_1 when $\sigma_3 = 0$ on the fitted regression curve). Following their clue, we will call σ_{ci} the value obtained by regression, and σ_c the experimental value. Of course, when considering σ_{ci} in the aforementioned equation, the model ceases to be linear in its parameters, as we can confirm by deriving:

$$\left.\begin{aligned} \frac{\partial\sigma_1}{\partial\sigma_{ci}} &= \frac{(m\sigma_3 + 2\sigma_{ci})}{2\sqrt{m\sigma_3\sigma_{ci} + \sigma_{ci}^2}} \\ \frac{\partial\sigma_1}{\partial m} &= \frac{\sigma_{ci}\,\sigma_3}{2\sqrt{m\sigma_{ci} + \sigma_{ci}^2}} \end{aligned}\right\} \tag{46}$$

A practical and straightforward solution, though, involves utilizing the original equation to determine m_i and σ_{ci} as regression parameters. To address the nonlinearity of the parameters, the function can be converted into a linear model. With this approach, σ_c is assumed to be known, and the parameters m_i and s to be determined. The necessary transformation for linearity involves the following variable change:

$$y = \left(\frac{\sigma_1}{\sigma_c} - \frac{\sigma_3}{\sigma_c}\right)^2;\ x = \frac{\sigma_3}{\sigma_c} \tag{47}$$

Resulting in the linear equation:

$$y = mx + s \tag{48}$$

The next step is to determine the coefficients of the orthogonal regression. In the case that s is different from one, the new value of σ_c must be calculated. That is, σ_c is obtained by multiplying the previous value by $\sqrt{s}$. The iterative process continues until $s = 1$ is achieved, and therefore the desired resistance σ_{ci} is obtained. It should be emphasized that this streamlined approach aligns with outcomes derived via orthogonal nonlinear regression in R (see sections 2.4 and 4.2). This confirms the efficacy of the simplified method.

3.4. Murrell's nonlinear failure criterion

Another classical failure criterion was proposed by Murrell (1965), and although several authors have modified its formulation, (Sheorey et al., 1986, for instance), probably the best-known version is the one by Bieniawski (1974), that simplified Murrell's equation by converting it into a normalized form and empirically determined the constants within the equation through testing. In its dimensionless representation, the equation is as follows:

$$\sigma_1 = \sigma_c + F\,\sigma_3^K \tag{49}$$

That Bieniawski (1974) transforms into:

$$\frac{\sigma_1}{\sigma_c} = A\left(\frac{\sigma_3}{\sigma_c}\right)^K + 1 \tag{50}$$

where $F = A\sigma_c^{1-K}$, A depends on the type of rock, and K remains constant for most rocks at 0.75. In the specific scenario where $K = 1$, the Murrell-Bieniawski expression simplifies to a straight line, rendering the shear strength linear as well. Consequently, this yields the linear Mohr-Coulomb failure equation.

Conversely, by evaluating the slope of Eq. (50), we derive

$$\left(\frac{d\sigma_1}{d\sigma_3}\right) = KA\left(\frac{\sigma_3}{\sigma_c}\right)^{K-1} \tag{51}$$

Acknowledging that, in numerous instances, it is likely that $K < 1$, it is more suitable to express:

$$\left(\frac{d\sigma_1}{d\sigma_3}\right) = \left[\frac{K\,A}{\left(\frac{\sigma_3}{\sigma_c}\right)^{1-K}}\right] \tag{52}$$

In this expression, it is evident that for the specific case where $\sigma_3 = 0$, as occurs in a uniaxial compression test, the slope becomes perpendicular to the abscissa axis at the origin:

$$\frac{\sigma_3}{\sigma_c} \rightarrow 0 \Rightarrow \frac{d\sigma_1}{d\sigma_3} \rightarrow \infty \tag{53}$$

Simultaneously, this suggests that the minor principal stress cannot manifest in the negative or tensile stress domain (Sheorey et al., 1986), marking a clear limitation of this criterion. Conversely, it is important to recognize that while applying the Mohr-Coulomb equation allows for the substitution of σ_c with σ_{ci} as a regression parameter, this exchange cannot be made with the normalized Bieniawski equation. This is due to the nonlinearity of the model $(\partial f/\partial\sigma_c)$ and $(\partial f/\partial K)$ in the parameters. Additionally, the equation exhibits nonlinearity due to the independent variable being raised to the exponent K. Thus, modifying the variables as follows enables the linearization of the equation:

$$\left.\begin{aligned} y' &= \left(\frac{\sigma_1}{\sigma_c} - 1\right) \\ x' &= \left(\frac{\sigma_3}{\sigma_c}\right) \end{aligned}\right\} \tag{54}$$

This conversion results in $y' = A\,x'\,K$. By applying logarithms to both sides, we obtain a linear equation:

$$\ln y' = \ln A + K \ln x' \tag{55}$$

Calling $= \ln y'$; $x = \ln x' = \ln(\sigma_3/\sigma_c)$, and $b = \ln A$, it is finally obtained:

$$y = b + Kx \tag{56}$$

Indeed, with K treated as a model parameter, its evaluation will reveal whether it remains constant ($K = 0.75$), as suggested by

Bieniawski (1974), across all rock types, although the examples provided by this author include values of K such as 0.70, 0.75, 0.78, and 0.80. Consequently, this approach facilitates the determination and subsequent verification of whether K is consistent or varies.

4. Results and discussion

The data used to apply and exemplify the proposed procedures are presented in Table 1, with their sources specified in its caption. As some criteria do not account for negative values of σ_3, such data of tensile strength, although available and thus meriting inclusion in the table, were not considered in the regressions.

This study employs least squares regression along with linear and nonlinear orthogonal regression, to compare the effectiveness of the procedures when applying the outlined failure criteria across all datasets. In the least squares regression, the sum of the squared residuals of the ordinates serves as the objective function to minimize, adjusting each parameter based on an initial value specific to each failure criterion:

(1) In orthogonal regression for Úcar criterion, the objective function—minimizing the squared distance as detailed in Eq. (42) —is solved considering various initial values for σ_c and σ_t.
(2) For Mohr-Coulomb criterion, orthogonal linear regression technique applied to Eqs. (17) and (18) helps to determine the coefficients of Eq. (43) through the scalar product outlined in Eqs. (31) and (32). This represents the innovative approach introduced in this study.
(3) Regarding the Hoek and Brown criterion, the orthogonal regression coefficients for Eqs. (17) and (18) are calculated by linearizing the equation as demonstrated in Eq. (48), with the stipulation that $s = 1$, to ascertain m and σ_{ci}.
(4) Lastly, for Murrell's failure criterion, Eq. (56) is linearized, and the orthogonal regression coefficients for Eqs. (17) and (18) are determined employing, as in the rest of criteria, the spreadsheet and R script.

A common observation across the three implemented procedures (OLS, orthogonal regression in a spreadsheet, and orthogonal regression in R) is that when σ_t is one of the adjusted parameters, its variation relative to experimental observations far exceeds the variation observed in σ_c. The primary cause of this phenomenon is the intrinsic difficulty in obtaining the "correct" experimental value.

The ISRM and ASTM have published a suggested method (ISRM, 1978) and standards (ASTM D3967-16, 2016; ASTM D2936-20, 2020), respectively. Nevertheless, multiple approaches exist for obtaining tensile strength (Tarokh et al., 2022). Direct tensile strength (DTS) can be obtained by testing specimens glued using epoxy cement directly to separating end caps (Mogi, 1967; ISRM, 1978); by biaxial extension (Brace, 1964); asymmetric extension on dog-bone specimens (Brace, 1964; Hoek, 1964; Ramsey and Chester, 2004; Patel and Martin, 2018), or by using a compression-to-tension load converter (Gorski, 1993; Klanphumeesri, 2010).

Indirect methods were introduced to bypass the difficulties intrinsic to DTS specimen preparation, which can produce highly varied and erroneous results (Pérez-Rey et al., 2023). Indirect methods include unconfined (Mellor and Hawkes, 1971; ISRM, 1978) and confined (Jaeger and Hoskins, 1966; Yawei and Ghassemi, 2018) Brazilian tensile strength (BTS), and flexural/three-point bending (TPB) (ASTM C78-15, 2015).

The variety of stress configurations during testing and the difficulty of correctly interpreting the fracture relationship with the principal stress axes introduce considerable uncertainty when assessing tensile strength. Peak strength results from BTS tests are typically significantly greater than those measured in DTS tests (Perras and Diederichs, 2014; Packulak et al., 2024). Some solutions have been proposed: Perras and Diederichs (2014) established a correction factor relating BTS and DTS results according to the lithology of the specimens (DTS = f•BTS, where f ranges from 0.86 for metamorphic, 0.82 for igneous, and 0.70 for sedimentary rocks). Packulak et al. (2024) found that the average measured DTS is 0.81BTS for granitoids, 0.75•BTS for limestones, and 0.85•BTS for metamorphic rocks. Sainsbury and McDonald (2024) found that the correction factor to adjust BTS values and TPB results to DTS values depends on the UCS of the considered rock.

Given this situation, and adding natural variation and dispersion of results during testing, it is not surprising that the considered failure criteria struggle with tensile strength. When additional information from uniaxial and triaxial compression tests is considered, the criteria adjust the tensile strength to values that may significantly differ from the experimental observations.

4.1. OLS and MLS regression

A summary of the results achieved with this procedure for the five example data sets is in Table 2. Fig. 8 illustrates the case of the rhyolite. Overall, it is evident that the computed σ_{ci} values for the Úcar and HB criteria show a close resemblance, although HB-MD achieves better results compared to HB, and the optimal fit is

Table 1
Test data for the presented procedures. T1: Rhyolite from Kidd Creek Mine, sourced from Betournay et al. (1991), as cited in Sheorey (1997). T2: Georgia Marble, from Schwartz (1963). T3: Indiana limestone, from Schwartz (1963). T4: Pniowek sandstone from Borecki et al. (1982) as cited in Sheorey (1997). T5: Tyndall limestone, from Carter et al. (1991) as cited in Guo et al. (2020). All values in MPa.

T1 Rhyolite		T2 Marble		T3 Limestone		T4 Sandstone		T5 Limestone	
σ_3	σ_1	σ_3	σ_1	σ_3	σ_1	σ_3	σ_1	σ_3	σ_1
−12.5	0	−4.48	0	−2.49	0	−10.9	0	−4.0	0
0	112.0	0.0	28.9	0.0	44.0	0	125.4	0	52
30	212.8	6.89	75.8	6.89	66.0	6.3	164.4	5	88
40	235.4	13.79	104.1	13.79	85.0	12.1	193.0	10	106
50	248.7	20.68	124.8	20.68	99.0	18.1	204.5	15	118
60	262.1	27.58	142.7	27.58	109.0	24.2	229.1	20	137
70	280.2	34.47	160	34.47	119.0	30.2	241.2	25	149
80	296.8	41.37	175.2	41.37	128.2	37.2	283.0	30	164
90	309.1	48.26	189.6	48.26	135.1	41.4	292.9	35	176
100	323.0	55.16	202.7	55.16	141.9	47.9	282.8	40	190
		62.05	215.2	62.05	149.1	53.9	315.3		
		68.95	229.6	68.95	156.5	60.8	313.3		

Table 2
Results achieved by classical OLS regression. Notice that σ_{ci} is obtained in the regression process. Values of SE are obtained from vertical distances.

Failure criterion	T1 Rhyolite	T2 Marble	T3 Limestone	T4 Sandstone	T5 Limestone	T1 Rhyolite
Úcar	σci (MPa)	127.79	39.61	51.56	138.87	57.87
	σ_t (MPa)	−23.04	−3.11	−10.95	−16.41	−5.33
	ξ	−0.18	−0.08	−0.21	−0.12	−0.09
	SE vert. (MPa)	9.02	4.50	4.61	11.12	3.44
HB	σ_{ci} (MPa)	129.47	38.05	55.96	137.54	58.58
	m_i	2.99	10.13	1.56	6.49	8.33
	s	1.00	1.00	1.00	1.00	1.00
	SE vert. (MPa)	12.34	6.37	7.08	11.98	4.15
HB-MD	σ_{ci} (MPa)	124.42	30.65	54.13	134.88	57.15
	m_i	4.82	25.82	2.48	8.45	10.32
	s	1.00	1.00	1.00	1.00	1.00
	a_i	0.40	0.41	0.40	0.44	0.46
	SE vert. (MPa)	9.94	2.36	6.21	10.72	3.38
Murrell	σ_{ci} (MPa)	112.15	28.58	39.54	123.51	53.03
	A	2.00	4.08	2.33	2.62	3.10
	F	12.57	14.96	10.74	12.55	10.46
	K	0.61	0.61	0.59	0.67	0.69
	SE vert. (MPa)	2.04	0.81	4.21	9.89	2.07

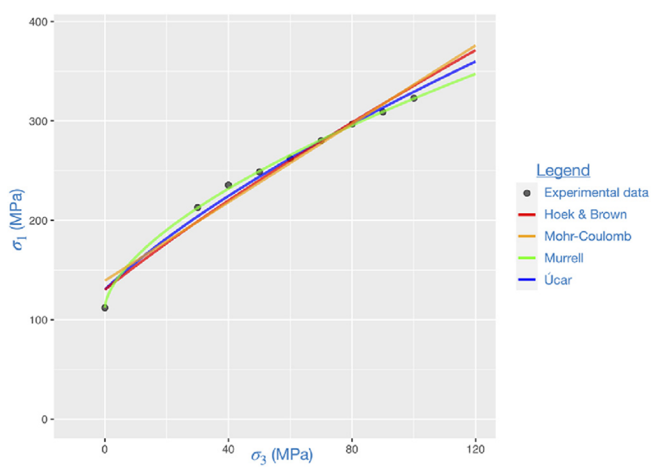

Fig. 8. Overlay of the four criteria included in this work, applied to the T1 Rhyolite data set. For each of the data sets in Table 1, both conventional and orthogonal fitting have been carried out in a spreadsheet (with and without the constraint imposed by the dot product) and with R.

attained using Murrell's criterion, where the fitting process entails adjusting both A and K parameters, rather than holding K at a constant value of 0.75 as suggested by Bieniawski's modification.

When evaluating the performance of MLS (implemented in R, see Table 3) compared to conventional OLS (Table 2), we can corroborate the positive outcomes reported by Bertuzzi et al. (2017). Applying MLS leads to significant improvements over OLS. For the HB criterion, for which the procedure was originally developed, MLS results in an average reduction of 13% in the obtained SE (with reductions reaching up to 36% in some cases). For the Úcar criterion, the reduction is 11%, and for the Murrel criterion, it is 9.4%.

4.2. Orthogonal regression results

When the outcomes of orthogonal regression (see Table 4) are contrasted with those from least squares regression, a minor increase in the standard deviation is noted due to the fitting of the uniaxial compressive strength parameter σ_{ci}, which, though slightly larger, results in a more comprehensive fit to the dataset, enhancing the alignment with the remaining experimental data. Overall, the match of the uniaxial compressive strength with the various failure criteria examined shows a marginally superior performance in orthogonal regression.

For instance, when comparing the outcomes of the linear orthogonal regression for the Mohr-Coulomb criterion with and without the scalar product introduced in this study, the main distinction is observed in the reduction of the standard error. Incorporating the scalar product there is a variation in σ_{ci}, which is 141.75 MPa with the scalar product and 134.51 MPa without it. Fig. 9 visually illustrates the comparative analysis of both techniques for the Mohr-Coulomb criterion applied to the T1 data set: Kidd Creek Mine rhyolite from Betournay et al. (1991) cited by Sheorey (1997).

In R, we executed orthogonal linear regression for the Mohr-Coulomb (M − C) criterion, while for the other criteria, we applied both nonlinear orthogonal and non-orthogonal regression using their original, non-linearized expressions. In this regard, it should be noted that the equations and variables used in the nonlinear fittings have been as follows:

(1) Murrell: the expression by Murrell (1965) as articulated by Bieniawski (1974), although with a small change in notation for internal consistency: $\sigma_1 = \sigma_c + F\sigma_3^K$, by adjusting the values of K, F, and σ_c. It requires to introduce seed values for the three parameters.
(2) Hoek-Brown: the expression used as model-function is (Hoek and Brown, 2019): $\sigma_1 = \sigma_3 + \sigma_{ci}\sqrt{m_i\frac{\sigma_3}{\sigma_{ci}} + 1}$ adjusting the values of m_i and σ_c.
(3) HB-MD: we implement a double regression loop as explained in section 3.3, to first obtain a_i and then, using the obtained a_i as a constant, derive the values for m_i and σ_{ci}.
(4) Úcar: the expression used for model-function in the case of Úcar's criterion is: $\sigma_1 = k_1(\sigma_3 - \sigma_t) + k(\sigma_3 - \sigma_t)^{1/2}$ (that is equivalent to Eq. (36)), by adjusting the values of σ_t and σ_c.

Fig. 10 presents a case in point: the outcomes for the T1 Rhyolite employing the Úcar failure criterion, where both the nonlinear least squares regression (nls) and nonlinear orthogonal regression (onls) were performed utilizing the "onls" package (Spiess, 2022). The results are detailed in Table 5. The values obtained for σ_{ci} are slightly higher for the classical regressions and orthogonal

Table 3
Results achieved by MLS regression in R. Notice that σ_{ci} is obtained in the regression process. Values of SE are obtained from vertical distances.

Failure criterion	T1 Rhyolite	T2 Marble	T3 Limestone	T4 Sandstone	T5 Limestone	T1 Rhyolite
Úcar	σ_{ci} (MPa)	124.37	36.14	51.56	135.06	56.98
	σ_t (MPa)	−21.62	−2.60	−10.95	−15.24	−5.14
	Ξ	−0.17	−0.07	−0.21	−0.11	−0.09
	SE vert. (MPa)	9.02	4.49	4.61	11.12	3.45
HB	σ_{ci} (MPa)	129.47	38.03	56.17	137.54	58.57
	m_i	2.99	10.14	1.55	6.48	8.33
	S	1	1	1	1	1
	SE vert. (MPa)	12.34	6.37	6.35	11.98	4.15
HB-MD	σ_{ci} (MPa)	124.43	30.64	54.13	132.71	54.74
	m_i	4.82	25.84	2.48	10.46	15.35
	S	1	1	1	1	1
	a_i	0.4	0.41	0.4	0.4	0.41
	SE vert. (MPa)	10.63	2.47	6.54	10.60	2.83
Murrell	σ_{ci} (MPa)	112.16	28.58	42.66	123.51	53.03
	A	2.01	4.08	2.00	2.62	3.1
	F	12.57	14.95	8.46	12.55	10.46
	K	0.61	0.61	0.59	0.67	0.69
	SE vert. (MPa)	2.2	0.8	2.05	10.49	2.23

Table 4
Results of orthogonal regression (spreadsheet). Notice that σ_{ci} is obtained in the regression process. In the case of Mohr-Coulomb criterion, the values of R^2 in use are obtained with Eq. (34). Values of SE are obtained both from vertical distances and from orthogonal distances, as explained in the main text.

Failure criterion	T1 Rhyolite	T2 Marble	T3 Limestone	T4 Sandstone	T5 Limestone	T1 Rhyolite
Úcar	σ_{ci} (MPa)	133.82	47.28	55.89	141.38	59.54
	σ_t (MPa)	−25.77	−4.45	−13.04	−17.11	−5.69
	Ξ	−0.19	−0.09	−0.23	−0.12	−0.10
	SE vert. (MPa)	9.93	6.41	5.07	11.56	3.66
	SE ortho. (MPa)	3.69	1.13	2.28	3.79	0.78
HB	σ_{ci} (MPa)	132.54	51.27	55.97	134.94	61.36
	m_i	2.83	6.87	1.59	6.81	7.69
	S	1	1	1	1	1
	SE vert. (MPa)	12.41	8.20	9.96	12.07	4.37
	SE ortho. (MPa)	10.77	2.88	7.09	6.14	1.32
HB-MD	σ_{ci} (MPa)	133.62	43.94	55.62	132.22	61.02
	m_i	3.96	14.59	2.3	8.90	7.15
	s	1	1	1	1	1
	a_i	0.40	0.56	0.40	0.40	0.52
	SE vert. (MPa)	10.80	8.57	6.55	10.80	4.71
Murrell	A	2.01	4.04	1.96	2.71	3.05
	F	12.89	14.39	6.4	10.57	12.14
	K	0.61	0.62	0.69	0.72	0.65
	SE vert. (MPa)	2.06	1.01	3.07	10.11	2.60
	SE ortho. (MPa)	1.06	0.89	0.98	1.22	1.09
Mohr Coulomb	σ_{ci} (MPa)	134.51	54.68	57.73	147.00	65.46
	φ (°)	20.23	27.92	12.92	31.86	32.21
	C (MPa)	46.89	16.45	22.99	39.68	18.06
	SE vert. (MPa)	15.53	13.45	8.07	15.17	7.47
	SE ortho. (MPa)	6.79	4.58	4.33	4.48	2.18
	R^2	0.974	0.972	0.986	0.963	0.982

regression in the spreadsheet. In general, the orthogonal regression has a better fit for all other data. When comparing the fit obtained with OLS and orthogonal regression, an interesting problem arises due to the lack of a reliable metric for such comparison. Most, if not all, coefficients describing the goodness of fit are based on the measurement of residuals—the difference between the predicted values obtained from the fitted function and the experimental observations. In OLS adjustments, this measurement is intuitive and straightforward: for each value of the control variable, the predicted value is compared to the observed value, and coefficients are derived from this comparison.

In orthogonal regression, the control, or explanatory, variable assumes part of the error. Therefore, when obtaining the residual, it cannot be measured solely in terms of the dependent variable; it must involve both variables. Geometrically, the minimal, orthogonal, distance between the observed point and the predictor function must be used. However, this approach is not quite "fair" for comparison with OLS, as the orthogonal distance will always be smaller than the "vertical" distance, even for identical functions (see Fig. 1). Conversely, using vertical distance as the criterion of goodness does not fully recognize the power of orthogonal regression, as it ignores the possible error in the explanatory

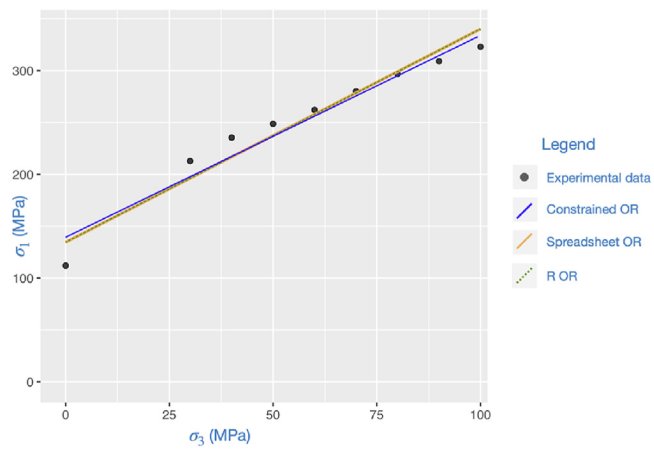

Fig. 9. Comparison of the Mohr-Coulomb failure criterion by orthogonal linear regression including the constraint of the dot product. Notice that the line resulting from orthogonal regression without constraints in the spreadsheet and R are the same and appear superimposed.

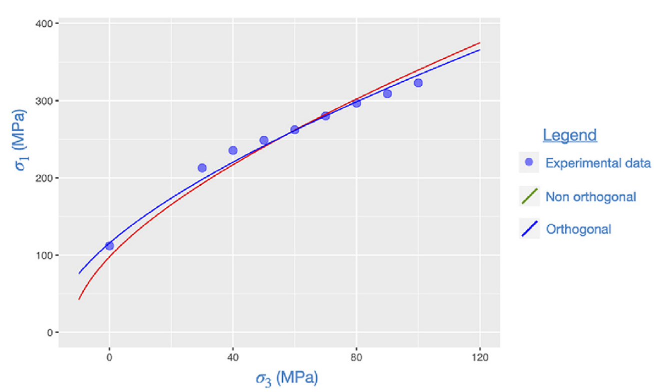

Fig. 10. Nonlinear, non-orthogonal and nonlinear orthogonal fit of the T1 data set (Kidd Creek rhyolite) for the Úcar criterion.

variable.

In Table 5, the standard error of the estimate values obtained using both vertical and orthogonal distances (provided by the "onls" package) are presented, clearly illustrating this situation.

5. Conclusions

The primary advantage of fitting experimental triaxial data using orthogonal regression is that it eliminates the asymmetry inherent in the OLS method, which arises from placing all the error weight on the dependent variable σ_1. Since σ_3, considered the controlled or independent variable, is also measured similarly during the experimental procedure, orthogonal regression provides a more refined fit for the parameters of the chosen failure criterion. This results in more accurate parameter estimation, enhancing the return on investment in testing within a project. That is, for the analyzed criteria:

(1) Úcar: Obtain the adjusted values of σ_c and σ_t (which implies having adjusted ξ and, consequently, k_1 and k_2).
(2) Hoek-Brown (HB): Obtain m_i and σ_{ci} (iteratively, ensuring the condition $s = 1$ is met).
(3) Hoek-Brown as modified by Mostyn and Douglas (2000) (HB-MD), obtain a, m_i and σ_{ci} as results of a double regression loop. The first one obtains the value of a_i that will treated as a constant in the second loop, that derives the values of m_i and σ_{ci}.
(4) Mohr-Coulomb (M − C): Obtain the slope, φ, and the intercept, C.
(5) Murrell: Obtain σ_c, A, K, and F.

It is shown that implementing orthogonal linear regression and minimizing the Euclidean distance, under the constraint that the scalar product is zero, as proposed in this study, results in an enhancement to the method efficacy. Also, in terms of methodological advancement, we have tested Recio-López (2021) new procedure to determine the R-squared value, by applying it to linear orthogonal regression on the Mohr-Coulomb criterion with good results.

With respect to the performance of the tested criteria, we can observe that the Mohr-Coulomb criterion, when applied using both least squares and orthogonal linear regression, results in a higher standard error in fitting the experimental data compared to the other criteria evaluated in this research. This outcome is expected given the nonlinear nature of the data sets.

The Murrell criterion, as a nonlinear criterion, achieves outstanding results when its parameters are linearized for the application of both least squares and orthogonal regression, allowing for the adjustment of the F, A and K parameters, considering σ_c as constant, within the spreadsheet, instead of considering a constant value for K as suggested by Bieniawski (1974). It accommodates a broad range of values for F, from 8.19 to 15.8, for A, from 2 to 4.07 and for K, from 0.5 to 0.74. This procedure yields better results than by adjusting the values of K, F, and σ_c, as tested in R.

In least squares regression, the Hoek and Brown criterion fits the parameters m_i and σ_c assuming $s = 1$ for intact rock. For orthogonal regression, the Hoek and Brown mathematical equation is linearized under the condition that $s = 1$. The process involves iteration to find values of σ_{ci} and m_i that satisfy the aforementioned condition, resulting in a curve that aligns well with the data. Applying the modifications proposed by Mostyn and Douglas (2000) and conducting a double loop regression (Douglas, 2002) significantly enhances the performance of the criterion. The standard error of the estimate values obtained are systematically lower than those using the conventional HB criterion, in both OLS and orthogonal regression modes, making this approach highly recommended. Additionally, the MLS procedure (Mostyn and Douglas, 2000; Douglas, 2002) represents a significant improvement in the quality of the fits obtained in the other criteria considered, especially when compared to conventional OLS regression, although it does require implementation in a double-loop regression process. The reduction achieved probably will be dependent on the range of confining pressure in the considered triaxial tests, as the procedure seeks to minimize the undue influence of high confining pressure tests on the overall fitting.

The Úcar criterion gives good results when compared to the nonlinear criterion applying the least squares regression fits the parameters σ_{ci} and σ_t. The curve fits very well and the standard deviations obtained are slightly smaller when compared to the criterion, though larger than Murrell's. It is noteworthy that Úcar's failure criterion has the advantage that the parameters k_1 and k_2 are

Table 5
Results of orthogonal regression implemented in R. Notice that σ_{ci} is obtained in the regression process. The standard error of the estimate is shown from vertical distances (SE vert.), and from orthogonal distances (SE ortho.), see discussion in the main text.

Failure criterion	T1 Rhyolite	T2 Marble	T3 Limestone	T4 Sandstone	T5 Limestone	T1 Rhyolite
Úcar	σ_{ci} (MPa)	124.37	36.14	50.58	135.06	57.22
	σ_t (MPa)	−21.62	−2.6	−9.24	−15.24	−5.24
	ξ	−0.17	−0.07	−0.18	−0.11	−0.09
	SE vert. (MPa)	9.02	4.50	6.79	11.12	3.76
	SE ortho. (MPa)	3.64	1.10	2.28	3.7	0.91
HB	σ_{ci} (MPa)	129.47	38.04	55.97	134.94	61.36
	m_i	2.99	10.13	1.59	6.81	7.69
	s	1	1	1	1	1
	SE vert. (MPa)	12.34	6.36	9.96	12.07	4.37
	SE ortho. (MPa)	5.25	1.86	7.09	6.14	1.32
HB - MD	σ_{ci} (MPa)	129.13	48.13	54.36	133.97	58.01
	m_i	3.69	6.11	2.44	9.52	11.47
	s	1	1	1	1	1
	a_i	0.44	0.54	0.4	0.42	0.43
	SE vert. (MPa)	11.49	8.17	6.59	11.01	3.63
	SE ortho. (MPa)	4.51	2.42	3.39	3.66	1.14
Murrell	σ_{ci} (MPa)	138.24	26.56	28.29	116.33	52.06
	F	6.1	15.8	15.11	13.82	10.4
	K	0.74	0.6	0.5	0.66	0.7
	SE vert. (MPa)	2.00	1.07	5.14	10.37	2.17
	SE ortho. (MPa)	1.14	0.29	0.59	3.81	0.82
Mohr Coulomb	σ_{ci} (MPa)	134.51	58.34	57.73	147.18	65.46
	φ (°)	20.23	15.55	12.92	31.86	32.21
	C (MPa)	46.89	22.16	22.99	39.68	18.06
	SE vert. (MPa)	15.53	10.64	8.07	15.17	7.47
	R^2	0.948	0.958	0.954	0.948	0.975

functions of $\xi = \sigma_t/\sigma_c$ and can be directly obtained, for intact rock, from Eq. (37). Additionally, these parameters can also be determined based on the quality of the rock mass, according to Úcar (2021).

CRediT authorship contribution statement

Roberto Úcar: Writing – original draft, Methodology, Conceptualization. **Luis Arlegui:** Writing – original draft, Visualization, Software, Methodology, Data curation. **Norly Belandria:** Writing – original draft, Visualization, Software, Data curation. **Francisco Torrijo:** Writing – original draft.

Code and data availability

All spreadsheets and R scripts mentioned are available, from the corresponding author [L.A.], upon request. Hardware requirements: All code in this paper is multiplatform compatible.

Software required: Spreadsheet with installed Solver complement, or R program (R Core Team, 2023) with packages (available at CRAN): dplyr (Wickham et al., 2023), ggplot2 (Wickham, 2016), nlstools (Baty et al., 2015), onls (Spiess, 2022).

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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List of symbols or Abbreviations

a	Exponent in HB-MD procedure
(β_0, β_1)	Regression coefficients of the fitted curve
$(\hat{\beta}_0, \hat{\beta}_1)$	Regression coefficients of the fitted curve
C	Mohr-Coulomb criterion: cohesion
e	Random error, representing the difference in the approximation
φ	Mohr-Coulomb criterion: angle of internal friction
K, A, F	Murrell-Bieniawski criterion: parameters
k_1, k_2	Úcar criterion: parameters dependent on ξ
m_i, s	Hoek-Brown criterion: parameters
ξ	Úcar criterion: parameter (σ_t/σ_c)
σ_c	Uniaxial Compressive strength (UCS)
σ_{ci}	Unconfined Compressive strength obtained from the dataset by curve fitting
σ_t	Uniaxial Tensile strength
σ_1	Major principal stress at failure
σ_3	Minor principal stress at failure
s_{xy}	Covariance of variable (x_i, y_i)
s_x^2	Covariance of variable x_i
s_y^2	Covariance of variable y_i
$\tilde{s}_x^2$	Variance of $\tilde{x}_i$
$\tilde{s}_y^2$	Variance of $\tilde{y}_i$
$\tilde{s}_{xy}$	Variance of variable $(\tilde{x}_i, \tilde{y}_i)$
(x_i, y_i)	Experimental values from a dataset
$(\bar{x}, \bar{y})$	Mean values of variables
$(\tilde{x}_i, \tilde{y}_i)$	Coordinates of orthogonally fitted curve
$\hat{y}_i$	Response variable of fitted curve

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