

线性回归法复原化石标本中的残缺数据¹⁾

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摘要: 基于多元统计分析中对样本完整性的要求, 为了在分析中不抛弃大量不完整的化石标本或者不大大减少变量, 创建了一种恢复标本残缺数据的方法。本方法基于线性回归理论, 假设同类标本个体之间的区别仅仅是大小的区别, 形状的区别可以忽略不计, 因此, 在同类标本中, 可以用一件标本的已知测量数据预测另一件标本的残缺测量数据。在多件标本的情况下, 对某件标本的某个残缺数据的预测结果是用其他标本分别进行预测所得值的加权平均, 加权系数的选取与每件标本的保存完好程度相关。用现生马属头骨及肢骨标本做的数据试验证明, 该方法具有良好的稳定性, 对标本的种类、数量及残缺值的多少均不敏感, 对于尺寸较大的标本或数值较大的数据的预测效果要比对尺寸较小的标本或数值较小的数据的预测效果要好。与传统的线性回归方法的不同之处在于, 本方法利用的是样本(即标本)间的线性相关性, 传统方法利用的是变量(即测量项)间的线性相关性。在通常情况下, 样本间的线性相关程度要优于变量间的线性相关程度。本方法简单实用, 在对化石标本进行统计分析, 特别是多元统计分析中具有良好的应用前景。

关键词: 线性回归, 最小二乘法, 化石标本, 马属

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RECOVERING THE MISSING DATA OF DEFECTIVE FOSSIL SPECIMENS USING LINEAR REGRESSION METHOD

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Abstract In multivariate statistical analyses, intact specimens are essentially required. In order to help researchers avoid having to discard many defective fossil specimens or greatly reduce the number of variables in their analyses, we developed a method based on the theory of linear regression for recovering missing data for defective fossil specimens. Using this method, missing value of measurements can be predicted based on other intact or defective equivalent specimens. Numerical tests have been carried out on the head and limb bones of extant *Equus*. The results show that our method, which is relatively insensitive to the quantity, preservational quality and type of available specimens, has satisfactory stability. The predictive accuracy is best for large specimens or measurements of large magnitude. Furthermore, our method is distinct from traditional linear regression methods in utilizing linear correlations between specimens rather than between variables, since the correlations are usually stronger in the case of the former procedure. Our method is simple in theory and practice, and should be broadly applicable to statistical analyses of fossil specimens, particularly in multivariate.

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1 Introduction

Paleontologists always hope to obtain, as far as possible, intact fossil specimens which could provide integrated and abundant information. However, intact fossil specimens are very rare. Collected specimens are always defective in many ways, or significantly deformed by the pressure exerted by overlying strata. These defects or deformations of specimens cause the loss of useful information. Nowadays, multivariate statistical analyses have been widely used in paleontological research, and in such analyses plenty of intact specimens were essentially required (Bignon et al., 2005; Eisenmann and Baylac, 2000; Eisenmann and Turbot, 1978). Therefore many defective and deformed fossil specimens had to be eliminated from multivariate statistical analyses (Eisenmann, 1986), or alternatively the number of variables used had to be reduced, causing the loss of useful information.

Previously, many approaches to estimating missing characteristics have been developed based on the theory of linear regression, such as methods for estimating stature from (even fragmented) long bones (Badkur and Nath, 1990; Formicola and Franceschi, 1996; Hasegawa et al., 2009) or estimating age from the pubic symphysis (Liu et al., 1988). Regression equations or ratios were often proposed to predict single objective missing data points in these works (Liu et al., 1988; Badkur and Nath, 1990; Feldesman et al., 1990; Formicola and Franceschi, 1996; Hasegawa et al., 2009). Although mature in theory and practice, these traditional methods are not very suitable for our circumstances. In our statistical analyses, fossil specimens are always available in small quantities and defective in multiple respects. These complex missing data are hard to estimate using one or even several regression equations. Therefore, a new approach is needed to solve this problem.

In this paper we presented a new method of linear regression to recover the complex missing value of measurements of specimens that are defective in multiple respects. In our method, linear correlations of specimens rather than variables were utilized to predict the missing data using as many additional intact or defective homogeneous specimens as possible. Numerical tests indicate that this method is simple and practical with adequate stability. Although the method could not actually replace missing information, it should prove widely applicable to statistical analyses of fossil specimens, particularly multivariate ones.

2 Specimens and measurements

All the raw data are measurements of head and limb bones of *Equus* belonging to the collections in the Muséum National d'Histoire Naturelle (MNHN), Paris, France. The bones include 21 skulls and 21 mandibles of *Equus burchelli*, as well as 12 metacarpal III and 12 anterior phalanges I of *Equus hemionus*. Sexes were not distinguished in this work because modern equids are considered to have weak sexual dimorphism. All the specimens represent adults, with M3/m3 erupted in skulls/mandibles and epiphyses completely fused in long bones. 31 measurements of skulls, 14 of mandibles, 15 of metacarpal III, and 13 of anterior phalanges I were taken (Eisenmann et al., 1988).

3 The theoretical model

The main assumption of the work is that the main difference among the homogeneous spec-

mens is merely size. Differences in shape are considered to be so small that we can neglect them. Thus, identical measurements of individual specimens in one sort are proportional. Suppose there are two intact homogeneous specimens S_1 and S_2 , with the same k measurements having been taken for each specimen. The values of the measurements are designated m_{ij} . Here the first subscript ($i = 1, 2$) identifies a particular specimen, and the second subscript ($j = 1 \dots k$) identifies a particular measurement. If the measurements of S_1 (m_{1j}) are treated collectively as an independent variable and the measurements of S_2 (m_{2j}) as a dependent variable, the resulting points $P_j(m_{1j}, m_{2j})$, $j = 1 \dots k$ should fall close to a regression line (cf Fig 1).

If a certain measurement of S_2 is missing, say m_{2q} , $q \in (1 \dots k)$, we will use other measurements (m_{1j}, m_{2j} , $j = 1 \dots k$, $j \neq q$) to fit the regression line using the least squares method and predict m_{2q} by m_{1q} . Suppose the regression line satisfies following equation

$$y = ax + b \quad (1)$$

According to the least squares method, the fitted parameters are as follows

$$a = \frac{\left(\binom{k-1}{j=1, j \neq q} \sum_{j=1, j \neq q}^k m_{1j} m_{2j} - \sum_{j=1, j \neq q}^k m_{1j} \sum_{j=1, j \neq q}^k m_{2j} \right)}{\left(\binom{k-1}{j=1, j \neq q} \sum_{j=1, j \neq q}^k m_{1j}^2 - \left(\sum_{j=1, j \neq q}^k m_{1j} \right)^2 \right)} \quad (2)$$

$$b = \left(\frac{1}{\binom{k-1}{j=1, j \neq q}} \right) \sum_{j=1, j \neq q}^k m_{2j} - \left(\frac{a}{\binom{k-1}{j=1, j \neq q}} \right) \sum_{j=1, j \neq q}^k m_{1j} \quad (3)$$

Accordingly, we can predict the value of m_{2q} according to Eqs 1-3, i.e. $m_{2q} = a \times m_{1q} + b$

In the steps above, it is not necessary that all m_{1j}, m_{2j} , $j = 1, \dots, k$, $j \neq q$ are known, but m_{1q} is needed in order to calculate m_{2q} . Furthermore, theoretically, at least two measurements $j = 1, \dots, k$, $j \neq q$, m_{1j}, m_{2j} for two different values of j must be available for both specimens. Otherwise the parameter a in Eq 2 will be equal to 0, and it will not be possible to compute a regression line. Assuming a regression line can be calculated (we always made this assumption in present work), an arbitrary set of missing measurements $m_{2q_1}, m_{2q_2}, \dots, m_{2q_s}$ can be predicted as outlined above provided $m_{1q_1}, m_{1q_2}, \dots, m_{1q_s}$, $1 \leq s \leq k-2$ are known. Simultaneously, for S_1 , the arbitrary missing measurements $m_{1q_1}, m_{1q_2}, \dots, m_{1q_t}$, $1 \leq t \leq k-2$ can be predicted from $m_{2q_1}, m_{2q_2}, \dots, m_{2q_t}$, if the latter are known.

In the case mentioned above, only two samples are considered. In fact, more than two specimens are commonly available. For example, suppose we have S_b, \dots, S_n , a total of n specimens. In order to predict any missing measurement $m_{p,q}$, $p \in (1, \dots, n)$, $q \in (1, \dots, k)$, the other r specimens S_1, \dots, S_r , $1 \leq r \leq n-1$ among the n specimens for which measurements $m_{i,q}$, $i = 1, \dots, r$, $i \neq p$ are known can each be used as the basis for a separate linear regression. Thus, r pairs of parameters $(a, b)_i$ can be obtained using r specimens. The optimum prediction of (a, b) is the weighted mean of all $(a, b)_i$ as follows

$$(a, b) = \sum_{i=1}^r c_i (a, b)_i \quad (4)$$

$$\text{where } c_i = \frac{L_i D_i}{\sum_{i=1}^r L_i D_i} \quad (5)$$

Here $L_i = \max(m_{ij}) - \min(m_{ij})$, $i = 1, \dots, r$, $j = 1, \dots, k$, $i \neq p$, $j \neq q$. Note that $m_{i,j}$

can be any measurement of specimen S_i , while D_i is the number of measurements available for specimen S_i , except $m_{i,q}$. These weights c_i are designed mathematically to reflect the fact that a larger regression region (the difference between the smallest and largest values) and a larger number of regression points can give more reliable results

4 Results and discussion

4.1 Validation of the theoretical model

In order to verify the theoretical model, we first selected two random intact skulls of *Equus burchelli* (S_1 and S_2), taking 31 measurements in each case. The measurements of S_1 were treated as an independent variable and those of S_2 as a dependent variable, and the fitted parameters and regression line could be resulted according to Eqs 1–3 (Fig 1), which yielded $a = 1.09$, $b = -3.81$. The linearity is excellent, with a coefficient of determination (r^2) of 0.9920.

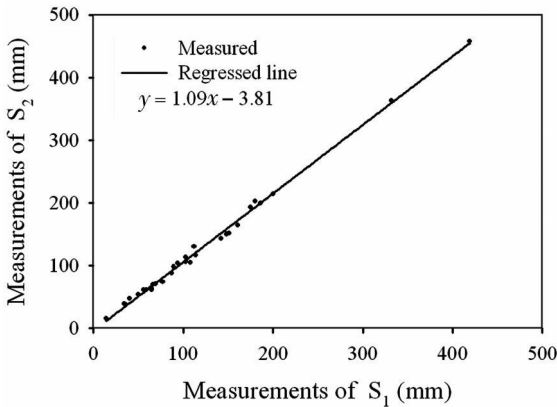


Fig 1 Linear correlation between measurements of two skulls of *Equus burchelli*

The horizontal and vertical axes are measurements $m_{1,j}$ and $m_{2,j}$, $j = 1, \dots, 31$ of specimens S_1 and S_2 respectively

lected for removal by a custom-designed Matlab 7.0 program, although the program was rerun in the very rare cases when the measurements it designated for removal were concentrated in too few specimens or the remaining measurements were insufficient to produce all of the regression lines. The distribution of the relative errors for a typical set of 65 predictions is shown in Fig 3. The result shows that the relative errors conform to a bell-shaped distribution with the peak value near to 0. This observed distribution can be fitted to a Gaussian distribution with the following parameters: mean value $\mu = 0.0071$ and standard deviation $\sigma = 0.045$. This result indicates that our method is practicable. The fact that μ is close to 0 indicates that the errors are small. The low

Then we eliminated each measurement $m_{2,j}$, $j = 1, \dots, 31$ of S_2 in turn, and attempted to predict its value. The distribution of the absolute values of the relative errors associated with all 31 measurements was plotted in Fig 2. The result shows that most relative errors have absolute values of less than 10%, with only 4 errors (12.9% of 31 measurements) exceeding this level. The result indicates that even a single intact specimen can give relatively good predictions for another defective specimen.

Next we considered 21 intact skulls of *Equus burchelli*, eliminated 10% of the measurements, that is, 65 $m_{i,j}$, $i = 1, \dots, 21$, $j = 1, \dots, 31$, and predict them simultaneously. Measurements were randomly se-

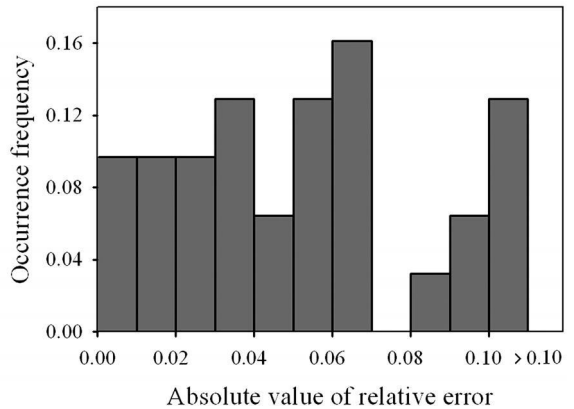


Fig 2 The distribution (bars) of absolute values of relative errors, which comes from the predictions of measurements $m_{2,j}$ of specimens S_2 one by one using present method

value of σ , which implies that 68.27% of all calculated error values are situated in the interval $[-\sigma, \sigma]$, shows that the method's predictions are stable. In the following section, we used the two parameters μ and σ to test the accuracy of the predictions.

4.2 Stability of the method

In the results above, we verified that our method is practicable. We would then test whether the method could give relatively stable predictions in each of 10 different cases (Table 1). In each case we carried out 10 tests independently (except case 7, see Table 1) and use their individual means and standard deviations to create an average mean $\langle \mu \rangle$, and average standard deviation $\langle \sigma \rangle$. Firstly, the percentage of measurements m_{ij} of 21 skulls of *Equus burchelli* removed from the analysis varies from 1% to 20%, resulting in $\langle \mu \rangle$ values varying from 0.0007 to 0.0053 and $\langle \sigma \rangle$ values varying from 0.060 to 0.068 (Table 1, cases 1–4). $\langle \mu \rangle$ is very close to 0 when only 1% of the measurements m_{ij} are removed (case 1). Even when the percentage of removed data is higher (cases 2–4), $\langle \mu \rangle$ is also close to 0 and its magnitude is relatively stable. Furthermore, the $\langle \sigma \rangle$ values are very close one another in all 4 cases. These results indicate that our method is stable when varying proportions of measured data were missing.

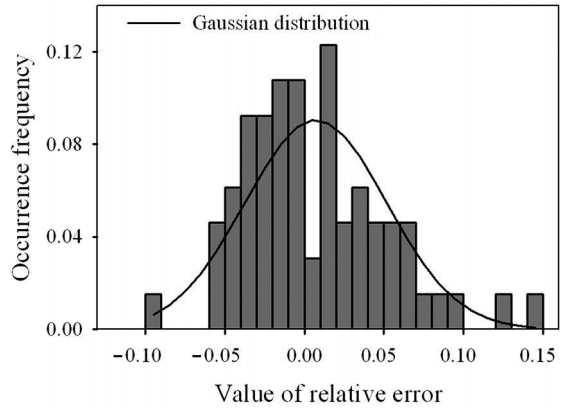


Fig. 3 The distribution (bars) of relative errors of predictions when simultaneously removing 65 measurements m_{ij} , $i = 1 \dots, 21$, $j = 1 \dots, 31$, of 21 skulls of *Equus burchelli* at one time.

Line shows the Gaussian fit of the distribution, which has the following parameters: $\mu = 0.0071$ and $\sigma = 0.045$.

Table 1 Results of independent numerical tests in different cases

C	T	S	B	M	P (%)	N	$\langle \mu \rangle (10^{-3})$	$\langle \sigma \rangle (10^{-2})$
1	10	<i>E. burchelli</i>	Skull	31	1	21	0.74	6.03
2	10	<i>E. burchelli</i>	Skull	31	5	21	4.59	6.75
3	10	<i>E. burchelli</i>	Skull	31	10	21	3.92	6.68
4	10	<i>E. burchelli</i>	Skull	31	20	21	5.32	6.81
5	10	<i>E. burchelli</i>	Skull	31	5	13	6.66	6.31
6	10	<i>E. burchelli</i>	Skull	31	5	7	6.06	5.28
7	31	<i>E. burchelli</i>	Skull	31	1	2	-13.70	—
8	10	<i>E. burchelli</i>	Mandible	14	5	21	-4.44	6.25
9	10	<i>E. henionus</i>	MCIII	15	5	12	-16.24	6.70
10	10	<i>E. henionus</i>	API	13	5	12	16.45	10.81

Abbreviations: C, case; T, number of independent tests; S, species; B, type of bone; M, measurements; P, proportion of removed data; N, number of specimens; $\langle \mu \rangle$, average of means; $\langle \sigma \rangle$, average of standard deviations; MCIII, metacarpal III; API, anterior phalange I.

Secondly, we set the specimen size of skull of *Equus burchelli* at values of 21, 13, to 7 while keeping the percentage of removed data fixed at 5%, which respectively resulted in $\langle \mu \rangle$ values of 0.0046, 0.0067 and 0.0061 and $\langle \sigma \rangle$ values of 0.067, 0.063 and 0.053 (Table 1, cases 2, 5 and 6). Both $\langle \mu \rangle$ and $\langle \sigma \rangle$ are relatively small and consistent in magnitude across all 3 cases. Furthermore, even if only 2 specimens remain, our methods could still lead to a low $\langle \mu \rangle$ value of -0.0137 provided that only 1% of the data (a single datum) was removed.

(Table 1, case 7). Therefore our method is stable across a range of specimen sizes

Thirdly we used 21 mandibles (14 measurements) of *Equus burchelli* as well as 12 metacarpal III (15 measurements) and 12 anterior phalanges I (13 measurements) of *Equus hemionus* to test whether or not our method could be applied to other specimens. We fixed the percentage of removed data at 5% (Table 1, cases 8–10). For mandibles of *Equus burchelli*, $\langle \mu \rangle = 0.0044$ and $\langle \sigma \rangle = 0.063$, values close to those obtained using skulls of *Equus burchelli*. As a result the method is clearly applicable to mandibles of *Equus*. For 12 metacarpal III of *Equus hemionus*, $\langle \sigma \rangle = 0.067$, a value close to that obtained from skulls of *Equus burchelli*. However $\langle \mu \rangle = -0.0162$, close to 0 but larger than the result for the skulls. The reason may be that all of the measurements for the metacarpal apart from m_{i1} and m_{i2} are radial and therefore of small magnitude (Eisenmann et al., 1988). For a small true value, a given absolute error will represent a larger relative error than will be obtained if the true value are larger. For 12 anterior phalanges I of *Equus hemionus*, both $\langle \mu \rangle$ (0.0165) and $\langle \sigma \rangle$ (0.108) are substantially larger than those obtained for skulls of *Equus burchelli*. Most measurements are again radial in the case of the phalanges, and furthermore the largest measurement is far less than in either the skulls or the mandibles. This results in a very small regression region, which will tend to give worse regression results. Thus, for skulls and mandibles, our method can give better predictions than are possible for metapodials and phalanges. The larger the bones, the more accurate the predictions that can be obtained, although the predictions even for small bones were likely to be acceptable in many cases.

4.3 Predictions for different measurements

Above we discussed the stability of our method across different cases. In addition, we wished to consider how the method performs for measurements of different magnitudes within a homogeneous collection of specimens. We used the same 21 skulls of *Equus burchelli* to carry out the necessary numerical tests. Firstly we calculated the average value of each measurement across all 21 skulls $\langle m_j \rangle$, $j = 1, \dots, 31$, and reordered these averaged measurements from small to large as follows $\langle m_{(1)} \rangle, \dots, \langle m_{(j)} \rangle, \dots, \langle m_{(31)} \rangle$. Then we removed each measured datum and predicted it in turn. Note that only 1 datum was removed at a time and all the data known for all the specimen were predicted one by one. For each measured datum $m_{i(j)}$ we

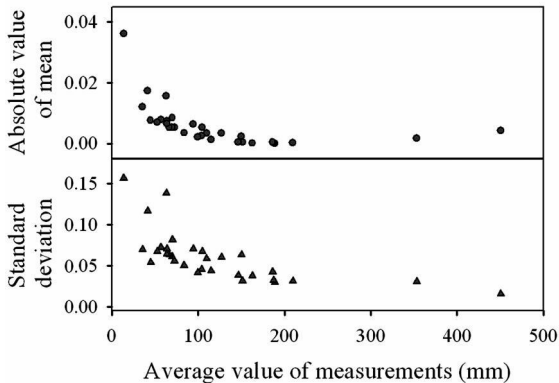


Fig. 4 $|\langle e_{(j)} \rangle|$ (upper panel) and $s_{(j)}$ (lower panel) vary according to the magnitudes of 31 ordered measurements $\langle m_{(j)} \rangle$, $j = 1, \dots, 31$ of 21 skulls of *Equus burchelli*. $|\langle e_{(j)} \rangle|$ and $s_{(j)}$ respectively represent the averaged absolute value and standard deviation of the errors associated with predicting each ordered $(j)^{\text{th}}$ measurement.

obtained a relative error $e_{i(j)}$, $i = 1, \dots, 21$, $j = 1, \dots, 31$. Then we calculated the mean $\langle e_{(j)} \rangle$ and standard deviation $s_{(j)}$ of the error associated with every ordered measurement. The results show that $|\langle e_{(j)} \rangle|$ and $s_{(j)}$ are both strongly dependent on the average value of the measurement $\langle m_{(j)} \rangle$ (Fig. 4), noting that $|\langle e_{(j)} \rangle|$ designates the absolute value of $\langle e_{(j)} \rangle$. The $s_{(j)}$ and $|\langle e_{(j)} \rangle|$ decrease rapidly with increasing $\langle m_{(j)} \rangle$, except that $|\langle e_{(j)} \rangle|$ increases slightly over the two points at the high end of the $\langle m_{(j)} \rangle$ distribution. Since larger $|\langle e_{(j)} \rangle|$ and $s_{(j)}$ values imply a worse prediction, our method performs well when predicting measurements with larger values, but may be less applicable when predicting measurements with very small values.

4.4 Comparisons with traditional linear regression methods

Linear regression methods have been widely used to predict missing data, for example when using long bones to predict individual stature (Fomicola and Franceschi 1996; Hasegawa et al., 2009). In a traditional analysis of this kind, the predictions are typically based on linear relations among variables (i.e. measurements) rather than individual specimens. In the works mentioned above, large numbers of specimens were used to establish simple or multiple regression equations with which we could predict missing data for defective fossil specimens. Here, traditional methods were applied to 21 skulls of *Equus burchelli* for comparison with our method. For one thing, linear relationships between paired variables were tested by calculating their correlation coefficients. A cross 465 pairs of variables (representing all the possible paired combinations of 31 measurements), the mean correlation coefficient $\langle r \rangle$ is only 0.2046, and some pairs of variables are even negatively correlation. The correlation coefficient exceeds 0.80 for only five pairs, and in no case does the value exceed 0.90. A cross 210 pairs of specimens (representing the 210 possible paired combinations of 21 specimens), the mean correlation coefficient $\langle r \rangle$ is 0.9968, and none of the individual correlation coefficients is less than 0.99. Therefore, the linear correlations between specimens are much better than those between variables, demonstrating that our method is more reliable than the traditional method.

Furthermore, five pairs of variables having correlation coefficients greater than 0.80, namely measurements 5 and 17, 6 and 24, 7 and 9, 18 and 19, and finally 19 and 24 (details seen Eisenmann et al. 1988), were selected for a further numerical test of the traditional method. For example, if we wanted to predict measurement 19 of the specimen MNHN 1909-069 based on measurement 24, we used measurement 19 (independent variable) and 24 (dependent variable) of the other twenty specimens to establish a simple regression equation, i.e. $y = 0.74x + 48.29$. We then substituted measurement 24 of the specimen (186 mm), into the equation, yielding $y = 185.42$ as a prediction of the true measurement 19 of the specimen (180 mm). The absolute value of the relative error of the prediction is 0.0031. By extension, any measurement of any specimen could be predicted on the basis of other specimens, and their absolute mean relative errors could be calculated for comparison with values arising from our method, as shown in Table 2.

Table 2 Comparisons of the two methods

P	Traditional method		Our method		
	I	$ \langle e \rangle (10^{-3})$	$s (10^{-2})$	$ \langle e \rangle (10^{-3})$	$s (10^{-2})$
M19	M24	0.45	2.72	0.16	3.22
M5	M17	0.96	2.83	0.21	3.14
M18	M19	1.37	3.12	0.49	4.25
M7	M9	0.36	3.18	3.50	5.07
M6	M24	0.63	2.14	4.27	1.57

Abbreviations: P, measurement to be predicted; I, independent variable (measurement) for simple linear regression; $|\langle e \rangle|$, absolute mean relative error; s , standard deviation; M19, measurement 19, etc.

As discussed above, smaller $|\langle e \rangle|$ and s values imply a better prediction. Thus, according to Table 2, the traditional method can yield predictions as good as those arising from our method for these particular 5 pairs of variables. For measurements 7 and 6, the predictions of the traditional method are even better than those of our method. However, these results only applied to pairs of variables with high linear dependences, and did not extend to variables with low linear dependences. A multiple regression analysis was also carried out but the result is not shown, since the multiple regression method could not produce enhanced predictions. Traditional methods can offer a formula that makes the process of calculation very explicit, but a

large number of specimens is necessary and we have to be very careful in the choice of variables. Moreover, traditional methods are not very suitable for multivariate statistical analyses in paleontology, since there are always large amounts of missing data which must be predicted from available specimens showing different levels of damage.

5 Conclusions

In this work, we developed a method which is very simple in theory and practice, for predicting missing measurements of imperfect specimens based on linear regression theory. The predictions of this method are not strongly dependent on the quantity or type of specimens available, or on their completeness. Accordingly, this method displays satisfying stability and reliability. The accuracy of the predictions decreases when using small bones or predicting measurements of particularly small magnitude, so the method should be applied only with care in such instances. In comparison to traditional methods, our method is advantageous in that the linear dependences between specimens are much better than those between variables, and also more suitable for multivariate statistical analyses of fossil specimens. Finally, the method has so far been verified merely with respect to specimens of *Equus*. Its applicability to a wider range of fossil material will need to be verified by further studies.

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