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The Munich Procedure – Standardising Linear Regression Documentation in p-XRF Research

Michaela Schauer [1 2], Frank Siegmund [3], Markus Helfert [4], Brandon Lee Drake [5]

[1] Vienna Institute for Archaeological Science (VIAS), Universität Wien, Franz-Klein-Gasse 1, 1190 Wien, Austria, michaela.schauer@univie.ac.at, https://orcid.org/0000-0002-0555-3451 [corresponding author]

[2] Research Network Human Evolution and Archaeological Sciences (HEAS), Universität Wien, Djerassiplatz 1, 1030 Wien, Austria

[3] Abt. Ur- und Frühgeschichtliche Archäologie, Universität Münster, Domplatz 20-22, 48143 Münster Germany, mail@frank-siegmund.de, https://orcid.org/0000-0002-0555-3451

[4] Ceramic Research Center, Institute for Archaeological Science, Goethe-Universität Frankfurt, Norbert-Wollheimer-Platz 1, 60629 Frankfurt am Main, Germany, m.helfert@em.uni-frankfurt.de, https://orcid.org/0009-0004-4942-2615

[5] Department of Anthropology, University of New Mexico. 1 University of New Mexico, Albuquerque, NM 80634, b.lee.drake@gmail.com

Abstract

The Munich Procedure, a protocol presented as R code and initially developed on the basis of archaeometric portable X-ray fluorescence (p-XRF) data, offers adaptability and standardisation to evaluate coefficient corrections. These corrections are derived from linear regressions calculated by comparing p-XRF values with laboratory chemical analyses of the same sample set. The versatility of this procedure allows collaboration and ensures consistent data structure. Not tied to specific instrumentation, this approach helps to universally improve the accuracy of p-XRF data, benefiting specialists in a variety of industries. By providing a common baseline for performance evaluation, it enables discussion across different applications.

Keywords

coefficient correction, linear regression, reproducibility, standardisation, R-code, archaeometry

Code metadata

Nr	Code metadata description	Please fill in this column
C 1	Current code version	v1.0
C 2	Permanent link to code/repository used for this code version	https://github.com/MichaelaSchauer/MunichProcedure
C 3	Permanent link to reproducible capsule	none

C 4	Legal code license	The code was released under GPL-3.0 licence
C 5	Code versioning system used	GIT
C 6	Software code languages, tools and services used	R (version 4.3.1), RStudio (version 2023.06.1 – Build 524), Quarto plugin (version 1.3.433)
C 7	Compilation requirements, operating environments and dependencies	All necessary requirements are listed in https://github.com/MichaelaSchauer/MunichProcedure/blob/v1.0/README.md and https://github.com/MichaelaSchauer/MunichProcedure/blob/v1.0/MunichProcedure/scripts/MunichProcedure.qmd
C 8	If available, link to developer documentation/manual	https://github.com/MichaelaSchauer/MunichProcedure/blob/main/README.md
C 9	Support email for questions	michaela.schauer@univie.ac.at

Introduction

The use of linear regressions for instrument calibration and/or the development of coefficient corrections (coefcor) – also known as is type standardisation, user factors, secondary calibration, calibration correction or post-processed slope correction [1–7] – is a standard procedure used in many disciplines and for a variety of analytical methods [8,9]. This is also true for portable X-ray fluorescence (p-XRF) devices for which linear regressions [10]are performed foremost to compensate for element interferences and matrix effects, but also to assess the accuracy of the instrument by determining the agreement of its output with that of other analytical methods [8,11–21]. Yet, unlike calibrations that do consider interferences like peak overlaps, background scatter and matrix effects [8,16,21–23], empirically developed coefcors offer a straightforward comparisons of measurements taken on the same set of samples which can be performed using simple software such as Excel but also, more continently, R [24,25]. Coefcors are applied to compare data from different settings, instruments, or methods to adjust the data given by the p-XRF instrument to the samples surface and matrix properties: For example data collected on archaeological pottery, due to its composition, does need a different coefcor then environmental hazard samples even if the same measurement mode was used. However, even if regularly used, the descriptive potential of linear regression for calibrations as well as coefcors in p-XRF studies has yet not been fully exploited. Particularly important information to precisely define and assess the accuracy of the given instrument and measurement procedure is lacking [1,13,26–28]. Additionally, there is no standard procedure with benchmarks to define a sufficiently accurate linear regression. Therefore, this paper describes an algorithm, the Munich Procedure, which fills this gap with respect to coefcors of p-XRF data and is made available as R code for further use and improvement [28,29]. This protocol offers a standardised, robust, transparent, and consistent approach to data processing that can be applied to various datasets and instruments, ensuring that the resulting data is comparable across studies.

The status quo - linear regressions in p-XRF studies

Linear regressions [10] are commonly used to enhance and define the accuracy of measurement data by adjusting p-XRF measurements using samples with known compositions and a matrix matching those of the samples to be analysed. For example, archaeological samples like the Frankfurt Pottery Sample Set [15,30] are often employed to develop linear regressions for archaeological pottery while powdered samples are employed for the analysis of soils. The calculations themselves then compare values or in some cases intensities measured by p-XRF (x-values or independent variable) with values obtained from the same samples by laboratory methods (such as ED-XRF, WD-XRF, NAA or ICP-MS; y-values or dependent variable) which are traditionally taken as 'true' values [8,13–18,26,27]. The slope (a) and, if applicable, intercept (b) derived from these comparisons are then used to calculate corrections for data sets generated by the specific device on similar matrices. This results in the creation of coefcors tailored to specific sample types, such as pottery or obsidian. To define the quality of a linear regression that best corrects p-XRF, the coefficient of determination (r^2) and the coefficients (a, b if applicable) are usually reported [5,6,13–19,21–23,27,31–33]. The exclusion of samples from the calculation to obtain the best possible equation is normally based on the operator's judgment, with the emphasis on introducing as little change as possible to the original p-XRF values and keeping r^2 as close to 1 as possible. This process helps not only to obtain the best correction factors but also to decide whether to use Regression Through Origin (RTO) or Ordinary Linear Regression (OLR) [33–35].

An improved approach – the Munich Procedure

Building on the previously described approach (in the archaeometric Niton-user community also know as the Frankfurt Procedure) the Munich Procedure not only includes additional quality criteria such as the standard error of the estimate (SEE) which indicates the average distance of the observed values from the regression line [33,35] but also uses a Bonferroni outlier test to identify outliers and a bootstrap algorithm to test for reproducibility [28,33]. Yet, as the SEE is given in the unit of the measurement, to ensure comparability within a data set containing very different concentrations of major (e.g. compositional, % level or ppm) and trace elements (e.g. ppm level), the relative SEE (rSEE) is introduced. This criterion is calculated as a percentage of the mean value: rSEE= (SEE/mean)*100. To accept a linear regression, the rSEE must be less than 10% and the r^2 greater than 90%. These threshold values are based on many years of experience working with archaeological pottery and are specific for the application of the Munich Procedure to this type of material. Other benchmarks may be defined for other materials or disciplines as no universally applicable threshold can exist [28,36]. In order to establish reproducibility, such as ensuring that the exclusion of samples does not significantly alter the linear regression, the bootstrap confidence intervals for the slope are calculated using the BCa approach (bias-corrected and accelerated, confidence level 0.9). Hereby random samples are drawn 2500 times from the provided sample set allowing to re-draw samples [35,37,38]. The values obtained by the bootstrap method and those calculated on the basis of the linear regression should be as close as possible (± 0.05) to the 5 % and 95 % confidence levels. To ensure that the best possible linear regression is selected for the data in question, both a RTO and an OLR are calculated and compared [28]. Additionally, factors such as the range of variation of residuals, percentage of excluded samples, and the root mean squared error (RMS or RMSE) should be taken into consideration: The RMS quantifies the deviation of values in their unit of measurement from their true position (e.g., the value obtained from a

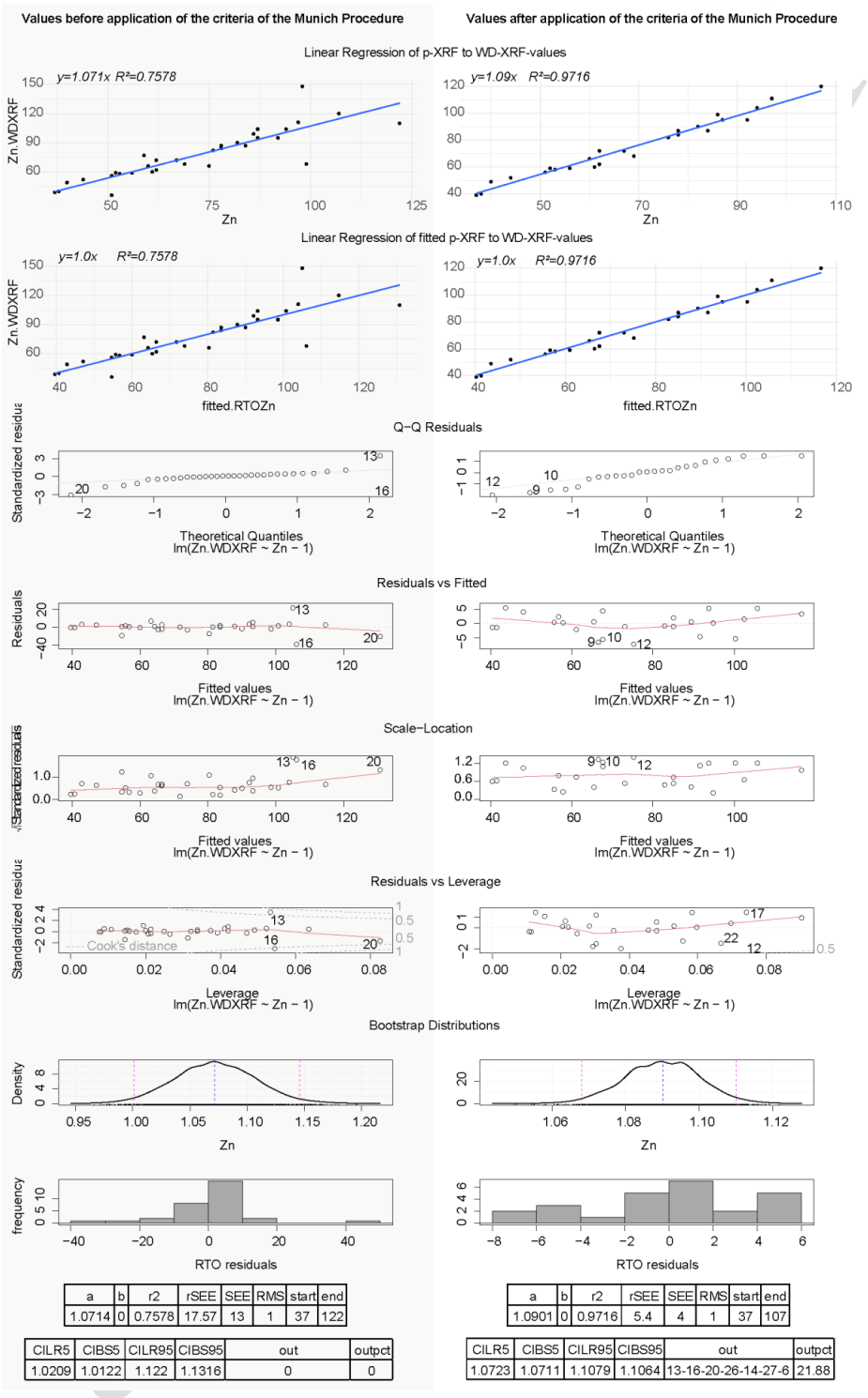
laboratory method) [33,34,36]. In this instance, the RMS is preferred over the mean absolute error (MAE) to take outliers into account [36].

In the Munich Procedure, both linear regressions can be refined by excluding samples that are identified as significant outliers through the Bonferroni outlier test [28,33]. To accept a linear regression, no significant outliers should remain. In addition, different outliers should be reported for RTO and OLR. Yet, the later is no hard criterion – if the other criteria are met well enough or excluding the sample results in a worsening of r^2 and/or rSEE this can be disregarded. A decision on the most appropriate linear regression, and thus the coefficients for a particular element, is made when one or both of the regressions meet the benchmarks described above. All the named factors play a crucial role in comparing coefcors and documenting their quality transparently – which is up to now only rarely the case. Therefore, using the Munich Procedure does provide a broader basis to identify but also produce high quality coefcor. This is especially true as the whole procedure is provided as R-code [25,28,29].

Impact Overview: Application of the Munich Procedure, potentials and limitations

Since the Munich Procedure was only published in February 2024, it is too early to assess its reception. An extensive application of data from the Niton XL3t (No. 97390), owned by the Department of Cultural Sciences at Ludwig-Maximilians-Universität München, was used to generate a total of 9 coefficients [28,29]. These coefficients pertain to both internal instrument adjustments and the comparison of p-XRF measurements with laboratory methods, offering a comprehensive example dataset for understanding how to implement the method. Furthermore, future publications utilizing data from this instrument will have access to the coefficients presented transparently. This utilization of the Munich Procedure can thus serve as a reference and starting point for further applications.

The Munich Procedure is designed to generate coefcors using R [28,29]. The straightforward code to compare measurements can be used to align different settings, instruments, or methods but also to adjust the values of an instrument after a necessary recalibration due to an instrument defect. Thus, the produced coefcors can be used to compare the performance of the same instrument before and after certain events, but also to correlate the measured values with those obtained by other analytical methods. This process documented by the Munich Procedure enhances the accuracy of p-XRF data (Fig. 1), making it a crucial step in data processing. Incorporating factors such as rSEE and reproducibility testing with bootstrap methods not just into coefcor but also calibration procedures would be highly advantageous. However, calibrations are typically conducted by manufacturers or specialized programs provided by them, which may not allow for customization in terms of statistical values and procedures. This is particularly unfortunate as customized corrections are almost always necessary as the manufacturer's own calibrations are not tailored to the matrices or surfaces encountered in real-life settings by users [1–7]. Therefore, this limitation currently restricts the application of the Munich Procedure to analytical data provided by the instrument after method-specific calculations (black box) or analytical data pre-processed by manufacturer-specific software and customised algorithms (such as Bayesian deconvolution in the Artax software 8.0.0.46).



a	b	r2	rSEE	SEE	RMS	start	end
1.0714	0	0.7578	17.57	13	1	37	122

CILR5	CIBS5	CILR95	CIBS95	out	outpct
1.0209	1.0122	1.122	1.1316	0	0

a	b	r2	rSEE	SEE	RMS	start	end
1.0901	0	0.9716	5.4	4	1	37	107

CILR5	CIBS5	CILR95	CIBS95	out	outpct
1.0723	1.0711	1.1079	1.1064	13-16-20-26-14-27-6	21.88

Fig. 1: Comparison of data documented by the Munich Procedure before (left) and after (right) aligning it with the benchmarks and criteria. The table displays slope (a) and intercept (b) corrections, values of rSEE, SEE, RMS, as well as the lowest (start) and highest (end) concentrations covered by the coefcor. It also includes the 0.5 and 0.95 confidence intervals calculated by the linear regression (CILS) or bootstraph algorithm (CIBS). Additionally, it provides row numbers (out) and the percentage (outpct) of excluded samples (data = Zn of coefcor III [28,29])

Another key strength of the Munich Process is its versatility: Because it is available as R code, sharing and collaboration within the scientific community is strongly encouraged: Researchers can easily add to and improve the method. This could include, for example, developing a more elegant way of coding, adding criteria that improve the results when the Munich Procedure is applied to a variety of datasets, but also automating aspects of the algorithm that currently need to be individually monitored and adjusted by the user. For the latter aspect in particular, AI learning algorithms could play an important role. In addition, the code could be integrated into existing calibration routines, such as those provided by manufacturers, but also open source programs like CloudCal [39]. In addition, the use of an R code ensures a consistent data structure, as maintaining uniformity in file organisation and spreadsheet format is essential for error-free execution of the code. Users only need to familiarise themselves with the code and structure once, while being able to work with datasets produced by different researchers. Moreover, the code is not tied to a specific instrument or manufacturer; the Munich procedure can improve the accuracy of p-XRF data universally, across specific materials or scientific disciplines. Therefore, this standardised approach can serve as a common reference point for p-XRF specialists across industries and professions.

By adhering to a standardised procedure and utilizing criteria that are comparable regardless of the instrument or material under study, discussions on instrument performance can be conducted consistently across diverse applications and research fields. The Munich Procedure therefore has the potential to establish a solid foundation for understanding the functionality and utility of p-XRF in greater detail by defining accuracy for chemical elements in a concise and directly comparable and reproducible manner (Fig 1 and 2). Sharing the data used to create coefcors (or calibration) following the Munich Procedure protocol, along with the related R-scripts and their output, through online repositories will offer direct access to essential information. This will provide transparent and consistent documentation, making it easier to understand the quality of the provided coefcors (or calibrations).

coefcor no.	a	b	r2	rSEE	SEE	RMS	start	end	CILR5	CIBS5	CILR95	CIBS95	out	outpct
coefcor I	1.0745	0	0.9471	7.6	5	1	37	110	1.047	1.0486	1.102	1.1025	11-14-24-17-15-25-20-8-10	30
coefcor II	1.0205	0	0.9538	7.04	5	0	39	119	0.9959	1.0008	1.0452	1.0418	12-15-2-18-7-25-26-21-5	29.03
coefcor III	1.0901	0	0.9716	5.4	4	1	37	107	1.0723	1.0711	1.1079	1.1064	13-16-20-26-14-27-6	21.88
coefcor IV	1.0242	5	0.9459	7.99	5	1	30	110	0.9439	0.955	1.1044	1.0891	13-16-6	6.45
coefcor ItoII	1.0333	0	0.9151	8.76	6	0	37	110	1.0066	1.0094	1.0601	1.0587	15	3.33
coefcor ItoIII	1.1006	-8	0.9151	9.3	7	0	37	110	0.9861	0.9973	1.2152	1.2395	15-17-20	10
coefcor IItoIII	0.9404	0	0.9509	6	4	1	39	119	0.9197	0.9216	0.961	0.9612	19-21-15-2-7-10-31-18	28.12
coefcor IIItoII	0.8401	13	0.9453	6.77	5	1	37	122	0.7643	0.7674	0.916	0.9369	2-7-18-23-6-16-10-21	25.81
coefcor IVtoIII	0.9598	4	0.9609	5.78	4	0	35	110	0.895	0.9042	1.0245	1.0177	16-26-20-14	12.5

Fig. 2: Table summarizing the criteria for linear regressions of Zn according to the Munich Procedure. The R script also provides the option of producing and comparing graphs as in Fig. 1 (data = coefcor I to IV (p-XRF to WD-XRF), coefcor ItoII, ItoIII, IItoIII, IIItoII, IVtoIII (instrument internal) [28,29])

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CRediT author statement
Schauer Michaela: Conceptualization, Methodology, Software, Formal Analysis, Data Curation, Writing – Original Draft, Visualization, Project administration, Funding acquisition. **Siegmund Frank**: Methodology, Supervision, Writing – Review & Editing. **Helfert Markus:** Resources, Supervision, Writing – Review & Editing. **Drake Brandon Lee:** Supervision, Writing – Review & Editing

Declaration of generative AI and AI-assisted technologies in the writing process
During the preparation of this work Michaela Schauer used DeepL Write, Deepl SE: https://www.deepl.com/write in order to better the wording. After using this tool, the text was reviewed and edited as needed. The authors take full responsibility for the content of the publication.

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Highlights

- The Munich Procedure, developed for p-XRF data, standardises coefficient corrections.
- It ensures consistent, reproducible data, benefiting specialists in various industries.
- The protocol, documented as R-Skript, enhances accuracy and transparency of p-XRF data.
- Establishing a common baseline fosters discussion and improves the overall understanding of p-XRF.

Graphical Abstract (for review)

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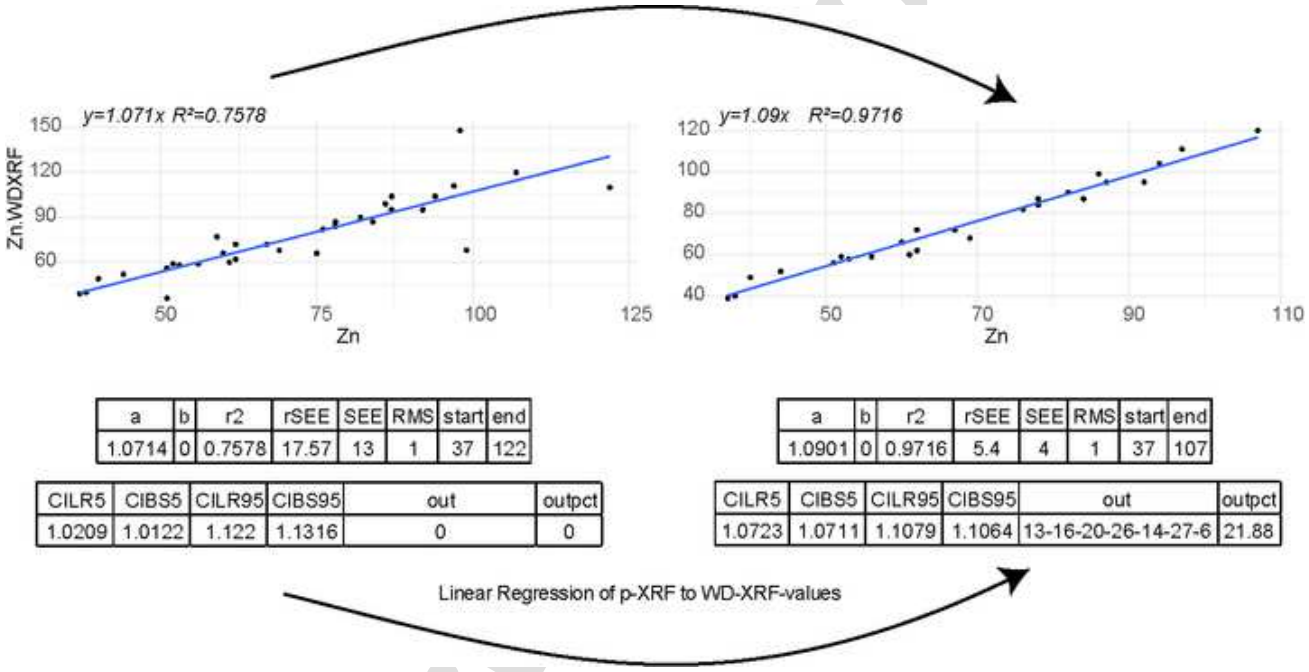

a	b	r2	rSEE	SEE	RMS	start	end
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a	b	r2	rSEE	SEE	RMS	start	end
1.0901	0	0.9716	5.4	4	1	37	107

CILR5	CIBS5	CILR95	CIBS95	out	outpct
1.0723	1.0711	1.1079	1.1064	13-16-20-26-14-27-6	21.88

Declaration of Interest Statement

Declaration of interests

X 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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