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Application of the discordant outlier detection and separation system in the geosciences

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Basically, two main types of statistical methods – robust and outlier-based – are available for handling experimental data; we document here the application of the outlier-based method. Due to the unavailability of a suitable software system for statistically correct application of the outlier-based method, a new computer program, DODESSYS (*D*iscordant *O*utlier *D*etection and *S*eparation *S*YStem), was written for the application of 33 discordancy test variants to experimental data, constituting contaminated or uncontaminated normal statistical samples. We illustrate the application of the discordant outlier-based scheme by five specific examples; three include univariate data for which this procedure was specifically designed and two are for bivariate data for which this methodology can be easily adopted. We thus report new statistical information on two reference materials (granite G-2 and sediment IAEA-417), bryozoan species from eastern Oman, a new improved Na/K geothermometric equation, and a more significant correlation with water depth of the abundance of meiofauna from the Gulf of Mexico. Recently, two sets of multi-dimensional discrimination diagrams for basic as well as acid rocks have been proposed from statistically correct methodology of natural logarithm-transformation of element ratios; the diagrams also require that these ratios should be normally distributed. We present numerous examples of application of these new diagrams for inferring tectonic setting of Archaean to Recent rocks, both before and after testing the datasets for discordant outliers. We recommend that outlying observations should always be evaluated for their discordancy.

Keywords: outlier methods; discordancy tests; reference materials; univariate data; studentized residuals; geothermometric equation; discrimination diagrams

Introduction

The handling of experimental data constituting normal statistical samples requires estimation of both central tendency (location) and dispersion (scale) parameters, for which mainly two classes of statistical methods (robust methods and outlier-based methods) are available (Barnett and Lewis 1994; Miller and Miller 2005; Verma 2005; Verma and Quiroz-Ruiz 2006a). A ‘statistical sample’ here refers to an array of data or observations, irrespective of whether it is of univariate, bivariate, or multivariate type. Such samples may or may not be statistically contaminated – an issue that is not appropriately considered in most geoscience studies.

Robust methods have been claimed by Maronna *et al.* (2006) to be superior to the outlier-based methods, but the reasons are far from clear. These authors, in their short discussion (about 10 lines on pages 3–4 of Maronna *et al.* 2006), dismissed the outlier-based methods mainly on the grounds that the latter are characterized by subjective decision. Ironically, the same arguments of subjective judgements were earlier documented by Barnett and Lewis (1994) against the robust methods and by Verma (2005) against the trimmed and Winsorized central tendency

robust parameters. Therefore, instead of discussing which class of methods is superior in performance, we will concentrate on the statistically correct use of the outlier-based methods.

The outlier methods rely on the application of certain statistical tests, which were denominated discordancy tests by Barnett and Lewis (1994). These include Dixon tests (Dixon 1950, 1951, 1953), Grubbs tests (Grubbs 1950, 1969; Grubbs and Beck 1972), and skewness and kurtosis tests (see Barnett and Lewis 1994 and Verma 1997 for more details); the latter two tests have been shown to be very powerful for discordancy purposes (Ferguson 1961; Shapiro *et al.* 1968; Velasco and Verma 1998; González-Ramírez *et al.* 2009; Verma *et al.* 2009). We document here the use of these tests in international publications to ascertain that, contrary to the opinion of some experts such as Maronna *et al.* (2006), these tests are neither subjective nor outdated and should therefore be routinely used for handling data in all science and engineering fields, including geosciences.

Among these discordancy tests, the Dixon tests (Dixon 1950, 1951, 1953; Dean and Dixon 1951) have been very frequently cited in international journals (at least 1530

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citations) as confirmed (on 14 February 2011) in the ISI Web of Knowledge; some of the most recent ones (2009–2011) are the following references: Ceriotti *et al.* (2009) in clinical biochemistry, Chen *et al.* (2009) in three-dimensional imaging in medicine, Connor *et al.* (2009) in brain research, Daneshian *et al.* (2009) in nature protocols, Deglaire *et al.* (2009) in nutrition, Guimaraes *et al.* (2009) in measurement science and technology, Le and Papavassiliou (2009) in heat transfer, McCoy *et al.* (2009) in biotechnology, Obi *et al.* (2009) in applied ecology, Rajilic-Stojanovic *et al.* (2009) in environmental microbiology, Ribe (2009) in environmental management, Ross *et al.* (2009) in paediatrics, Rzeszowska-Wolny *et al.* (2009) in DNA research, Shah *et al.* (2009) in food chemistry, Tomy *et al.* (2009) in environmental science and technology, Van Donkelaar *et al.* (2009a) in neuroscience, Van Donkelaar *et al.* (2009b) in pharmacology, Coute *et al.* (2010) in proteomics, Kyle *et al.* (2010) in environmental biology, Pizzamiglio *et al.* (2010) in oncology, Schoepe *et al.* (2010) in skin pharmacology, Van Donkelaar *et al.* (2010) in medicinal chemistry, Zimmerman *et al.* (2010) in astronomy and astrophysics, and Basiye *et al.* (2011) in the study of RNA and DNA.

The Grubbs tests (Grubbs 1950, 1969; Grubbs and Beck 1972) have also been cited in numerous papers (at least 1240 citations) in international journals. The more recent publications are as follows: D'Errico (2009) in method testing, Ferreira *et al.* (2009) in soil analysis, Jain (2009) in quality assurance in clinical chemistry, Minguez *et al.* (2009) in medicinal and neuropsychiatric genetics, Mishra *et al.* (2009) in hydrologic engineering, Preiss *et al.* (2009) in chromatography, Von Freyberg *et al.* (2009) in glaucoma research, Xie *et al.* (2009) in medicinal chemistry, Bellaagh *et al.* (2010) in biology and zoology, Bretman *et al.* (2010) in behavioural ecology, Cooper *et al.* (2010) in educational research, Coute *et al.* (2010) in proteomics, Ebdrup *et al.* (2010) in psychiatry and neuroscience, McFadden and Hernandez (2010) in complementary therapies in medicine, Meade *et al.* (2010) in radiation research, Wywiał (2010) in applied mathematics, Young and Kimura (2010) in ophthalmology, and Krejza *et al.* (2011) in transcranial Doppler imaging.

Barnett and Lewis' authoritative book on outliers in statistical data, in its several editions and printings, for example, 1978, 1979, 1984, 1987, 1994, 1995, 1998, 2001, 2003, has been cited in more than 1740 papers published in international journals; some of the more recent ones include the following references: Backes *et al.* (2009) in pattern recognition and artificial intelligence, Begum *et al.* (2009) in shellfish research, Ferreira and Van Aarde (2009) in wildlife research, George *et al.* (2009) in data analysis techniques, Hernández-Martínez and Verma (2009) in soil–plant systems, Riaz and Saghir (2009) in statistical computation and simulation, Viscosi *et al.* (2009) in plant biosystems, Banerjee *et al.* (2010) in material science and technology, Keown *et al.* (2010) in psychology of

crime and law, Koufakou and Georgiopoulos (2010) in data mining and knowledge discovery, Lee and Hawkins (2010) in health research, Leng and Hong (2010) in applied mathematics, Liu *et al.* (2010) in educational and psychological measurement, Meloun *et al.* (2010) in mathematical chemistry, and Nelson *et al.* (2010) in bioelectrochemistry.

Instead of using isolated Dixon or Grubbs tests (Barnett and Lewis 1994), the outlier scheme based on multiple tests initially proposed and used by Verma (1997) as the multiple test method (MTM) for processing geochemical data was demonstrated to perform well for quality control of reference materials (Verma 1998; Verma *et al.* 1998; Guevara *et al.* 2001; Velasco-Tapia *et al.* 2001). More importantly, as documented in Verma (1998), Verma and Quiroz-Ruiz (2006a, 2008), and Verma *et al.* (2008b), the MTM performs better than the competitive methods, the two standard deviation method used by Gladney *et al.* (1990), the box and whisker plot (BWP) method practiced by Villeneuve *et al.* (2002, 2004), and the median absolute deviation (MAD-Z, robust) method applied by Xia *et al.* (2006 and unpublished), especially when the new, precise, and accurate critical values simulated by Verma and Quiroz-Ruiz (2006a, 2006b, 2008) and Verma *et al.* (2008b) are used with the MTM.

However, these competitive methods (two standard deviation, BWP, and MAD-Z) have been popular, because the application of the MTM involving a large number of tests (33 test variants listed in Table S1 in online supplementary material to this article; see also Barnett and Lewis 1994; Verma 1997, 2005; González-Ramírez *et al.* 2009; Verma *et al.* 2009) is cumbersome without the availability of a suitable computer program. Some of the earlier applications of these tests through spreadsheets had amounted to a month or more of dedicated work for data processing alone (Verma 1997, 1998). This may be the reason why in most papers only some discordancy tests, for example, Dixon type or Grubbs type, are being cited, whereas the more complicated but powerful skewness and kurtosis tests are seldom applied.

Computer programs to enable the application of discordancy tests were practically nonexistent as documented by Barnett and Lewis (1994). Later, about 12 years ago, a computer program (SIPVADE) was published by Verma *et al.* (1998), but it is now outdated for several reasons. The most important among them are that SIPVADE uses old, less precise, and sometimes even inaccurate critical values then available in the literature (Barnett and Lewis 1994; Verma 2005) and relies on linear interpolation of these values when for a given sample size n , the corresponding critical values were not tabulated. Both of these aspects have been shown to cause errors in the final statistical inferences (Verma and Quiroz-Ruiz 2006a, 2006b, 2008; Verma *et al.* 2008b; Verma 2009). Therefore, there is still an urgent need for a suitable computer program. The freely available software R (R Development Core Team 2009) cannot be considered competitive or

even appropriate for the application of discordancy tests, because it does not incorporate them but advocates for alternative robust procedures. Use of this software R has been suggested by Reimann *et al.* (2008) for environmental samples. However, a more objective way to prove that such robust procedures are superior to the discordant outlier approach of Barnett and Lewis (1994) or to the MTM of Verma (1997) and to convince the large number of users of Dixon and Grubbs tests (see above the citations in this section) would be to compare the application of the robust and outlier methods for a large number of simulated cases of contaminated statistical samples.

Because no commercial software includes the application of all these discordancy tests, we prepared new software (see the next section for details) for applying the outlier-based methods to five case studies in geosciences. Besides, the usefulness of the discordancy tests has been further documented in the application of two new sets of multi-dimensional discrimination diagrams.

Identification and separation of discordant outliers: an essential task in experimental data handling by outlier-based methods

Under the outlier-based scheme, it is mandatory that discordant outliers be objectively identified before calculating the central tendency (mean or average) and dispersion (standard deviation) parameters from a set of observations (Barnett and Lewis 1994; Verma 2005). The presence of discordant outliers can seriously distort the above parameters (Barnett and Lewis 1994; Verma *et al.* 2009). Consequently, the identification and separation of such outliers from the statistical sample is an essential task. Interestingly, in numerous studies in geological, biological, and medical sciences, these discordant outlying observations when properly identified can also be separately interpreted (Barnett and Lewis 1994; Verma and Quiroz-Ruiz 2006b).

All these arguments led to the justification of a new computer program. We therefore developed DODESSYS software (*D*iscordant *O*utlier *D*Etection and *S*eparation *S*YStem), written in Java (for more details on this program see Figure S1, Table S1, and the text in online supplementary material to this article). The most precise and accurate critical values available for very large (up to 1000 and even more) sample sizes (Verma and Quiroz-Ruiz 2006a, 2006b, 2008; Verma *et al.* 2008b) make our new software much more appropriate and statistically accurate for this purpose.

This software will simplify the application of outlier-based methods for experimental data handling, hitherto being incorrect in numerous studies from the statistical point of view. In other words, many researchers use the mean and standard deviation as the estimates of central tendency and dispersion parameters, respectively, but do not take into account the basic assumption involved, viz., the experimental data must have been drawn from

a 'single' normal population without any statistical contamination from observations drawn from a different population. This practice of not ascertaining the validity of the basic assumption is statistically erroneous (Barnett and Lewis 1994; Verma 2005), but can be easily corrected through DODESSYS, available from any of the authors.

Application examples of MTM using DODESSYS software

The MTM has been applied or is applicable in a diversity of scientific and engineering fields, including all branches of earth sciences (see also Verma and Quiroz-Ruiz 2006a, 2006b, 2008; Verma *et al.* 2008b); corrosion research (Castrellon-Urbe *et al.* 2008); geochemometrics (Verma 2011); gas (CO₂) emissions from volcanoes (Sanci *et al.* 2010); geothermal research (Torres-Alvarado 2002; Díaz-González *et al.* 2008; Palabiyik and Serpen 2008; Pandarinath 2011); igneous rock geochemistry (Rodríguez-Ríos *et al.* 2007; Shekhawat *et al.* 2007; Rodríguez-Ríos and Torres-Aguilera 2009); mineralogy and mineral geochemistry (Colombo *et al.* 2007; Vargas-Rodríguez *et al.* 2008; Vattuone *et al.* 2008); magma genesis in active volcanoes (Torres-Alvarado *et al.* 2011); petroleum research (Salleh *et al.* 2007); pollution from mining operations (Gutiérrez-Ruiz *et al.* 2007; Méndez-Ortiz *et al.* 2007); proteomics research (Viner *et al.* 2009); quality control through reference materials (Velasco-Tapia *et al.* 2001; Verma 2004; Marroquín-Guerra *et al.* 2009; Pandarinath 2009a); sediment core studies (Pandarinath 2009b); sedimentary geochemistry (Kasper-Zubillaga and Zolezzi-Ruiz 2007; Jafarzadeh and Hosseini-Barzi 2008; Armstrong-Altrin 2009; Madhavaraju and Lee 2009; Madhavaraju *et al.* 2010; Najafzadeh *et al.* 2010); soil research (González-Márquez and Hansen 2009); stable isotope geochemistry (Nagarajan *et al.* 2008); viscosity estimates of drilling mud in geothermal and petroleum industries (Gómez-Arias *et al.* 2009); and water pollution and medical research (Ram *et al.* 2007; Obeidat *et al.* 2008; Heath *et al.* 2010).

Univariate data

Quality control through reference material granite G-2 from USA

As a specific example of univariate data, from Gladney *et al.* (1992) we compiled major and trace element data for the international geochemical reference material granite G-2 from the USA and processed them for possible discordant outliers using the default option of DODESSYS, that is, by applying 33 discordancy test variants. The individual identity of each method group (see Velasco-Tapia *et al.* 2001) was first maintained, and after ascertaining normal statistical samples (free from discordant outliers) for each group, they were combined and processed once again using DODESSYS. The results of initial and final statistics are

Table 1. Application of the new computer program DODESSYS to major (%m/m) and trace elements ($\mu\text{g/g}$) in international geochemical reference material granite G-2 and comparison with the earlier published statistics (Gladney *et al.* 1992).

Element	Initial statistics			Final statistics (this work)			Final statistics (literature)		
	n_{in}	x_{in}	s_{in}	n_{f}	x_{f}	s_{f}	n_{lit}	x_{lit}	s_{lit}
Si (%)	150	32.05	1.10	120	32.272	0.194	132	32.24	0.26
Ti (%)	169	0.295	0.055	150	0.2927	0.0220	154	0.293	0.022
Al (%)	157	8.16	0.61	139	8.143	0.173	142	8.14	0.17
Fe (%)	208	1.887	0.355	176	1.866	0.065	182	1.86	0.07
Mn (%)	178	0.0266	0.0065	156	0.02559	0.00426	155	0.0261	0.0036
Mg (%)	154	0.482	0.106	133	0.4605	0.0357	141	0.466	0.046
Ca (%)	167	1.432	0.243	131	1.4010	0.0450	147	1.40	0.06
Na (%)	159	3.016	0.308	130	3.025	0.079	141	3.03	0.10
K (%)	197	3.710	0.425	160	3.717	0.081	176	3.72	0.11
P (%)	95	0.0610	0.0167	76	0.0591	0.0048	84	0.0590	0.0060
H ₂ O ⁺ (%)	30	0.522	0.099	30	0.522	0.099	29	0.51	0.09
H ₂ O ⁻ (%)	34	0.122	0.063	32	0.112	0.051	31	0.11	0.04
Fe ₂ O ₃ (%)	41	1.081	0.178	41	1.081	0.178	38	1.07	0.14
FeO (%)	53	1.451	0.139	42	1.454	0.057	51	1.46	0.08
La	148	92.1	21.1	131	89.3	7.8	135	90	8
Ce	127	157.7	24.6	114	159.5	11.1	113	160	10
Pr	24	17.83	2.65	24	17.83	2.65	23	18	2
Nd	91	56.6	15.3	79	55.0	5.2	85	55	6
Sm	110	7.44	1.06	87	7.110	0.331	102	7.2	0.7
Eu	110	1.428	0.227	98	1.390	0.100	106	1.40	0.12
Gd	53	4.457	1.016	50	4.30	0.82	51	4.3	0.8
Tb	82	0.500	0.117	77	0.480	0.082	75	0.479	0.076
Dy	42	2.61	0.83	35	2.397	0.283	38	2.38	0.33
Ho	27	0.429	0.143	24	0.432	0.107	22	0.395	0.059
Er	20	1.215	0.430	17	1.082	0.238	19	1.14	0.29
Tm	24	0.232	0.138	20	0.188	0.090	20	0.182	0.079
Yb	103	0.836	0.222	88	0.762	0.120	98	0.80	0.17
Lu	85	0.1163	0.0387	73	0.1070	0.0182	76	0.108	0.020
Ag	19	0.075	0.152	16	0.0406	0.0137	16	0.040	0.014
As	18	0.64	0.90	15	0.415	0.281	12	0.26	0.09
Au	10	0.000995	0.000183	10	0.000995	0.000183	10	0.0010	0.00018
B	19	14.3	36.0	15	2.216	0.371	15	2.2	0.4
Ba	150	1833	300	130	1849	146	135	1840	150
Be	34	2.45	0.56	32	2.446	0.428	30	2.5	0.4
Bi	14	0.0497	0.0273	9	0.0360	0.0048	11	0.037	0.006
Br	7	0.238	0.139	7	0.238	0.139	7	0.240	0.140
C	26	234	75	26	234	75	25	227	67
Cd	21	0.0306	0.0168	19	0.0293	0.0146	19	0.027	0.013
Cl	28	82.5	40.1	22	65.4	20.5	24	69	24
Co	133	5.828	3.242	97	4.68	0.51	120	5	1.2
Cr	116	10.8	10.0	92	8.39	1.71	106	8.7	2.2
Cs	73	1.46	0.75	62	1.359	0.152	65	1.34	0.16
Cu	112	11.60	3.83	99	10.71	2.52	105	11	3
F	45	1279	240	30	1254	52	37	1280	80
Ga	59	22.77	4.21	59	22.77	4.21	56	23	4
Ge	15	1.103	0.319	15	1.103	0.319	15	1.1	0.32
Hf	58	7.95	0.97	57	7.92	0.94	52	7.95	0.69
Hg	33	0.31	1.45	31	0.0523	0.0150	30	0.051	0.014
In	9	0.0332	0.0058	7	0.03057	0.00257	8	0.032	0.004
Ir	7	0.000138	0.000252	6	0.000045	0.000049	6	0.00004	0.00005
Li	53	35.9	8.9	49	34.1	6.1	50	34	6
Mo	19	1.53	1.54	16	0.96	0.60	14	1.1	0.5
Nb	46	12.32	4.25	45	12.23	4.26	40	12	3
Ni	91	10.3	41.5	72	4.48	2.03	83	5.0	2.8
Pb	101	30.2	7.9	88	29.71	4.23	90	30	4
Rb	169	172.5	35.9	140	169.7	8.1	153	170	10
S	20	168	253	15	82.5	31.6	17	103	59
Sb	28	0.115	0.118	16	0.0644	0.0102	21	0.072	0.022

(Continued)

Table 1. (Continued).

Element	Initial statistics			Final statistics (this work)			Final statistics (literature)		
	n_{in}	x_{in}	s_{in}	n_f	x_f	s_f	n_{lit}	x_{lit}	s_{lit}
Sc	94	4.02	1.84	74	3.535	0.287	85	3.6	0.4
Se	7	0.072	0.063	7	0.072	0.063	7	0.072	0.063
Sn	24	23	102	23	1.85	0.79	23	1.8	0.8
Sr	177	475.6	73.5	143	470.9	27.4	155	473	34
Ta	53	0.889	0.151	48	0.868	0.096	48	0.88	0.10
Th	108	25.06	2.72	95	24.55	1.48	101	24.7	1.8
Tl	30	0.908	0.270	25	0.884	0.154	25	0.91	0.14
U	81	2.09	0.47	66	2.012	0.145	68	2.03	0.16
V	89	37.5	10.3	78	35.5	6.3	75	36	4
W	10	0.192	0.139	8	0.132	0.065	10	0.19	0.14
Y	54	11.645	4.066	46	11.18	2.16	47	11.3	2.2
Zn	109	89.2	34.0	97	85.2	7.6	100	86	8
Zr	104	295	65	87	309.7	27.9	98	309	35

Notes: The statistical results from this work are reported as rounded values (by retaining an extra significant digit) as suggested by Bevington and Robinson (2003) and Verma (2005). n_{in} , initial number of observations; x_{in} , initial mean; s_{in} , initial standard deviation; n_f , final number of observations (this work); x_f , final mean (this work); s_f , final standard deviation (this work); n_{lit} , final number of observations (literature); x_{lit} , final mean (literature); s_{lit} , final standard deviation (literature); literature refers to Gladney *et al.* (1992).

summarized in Table 1, which also includes the results reported by Gladney *et al.* (1992). These authors used the probably erroneous ‘two standard deviation’ method as documented by several workers (e.g. Barnett and Lewis 1994; Verma 1998; Verma and Quiroz-Ruiz 2006b; Hayes *et al.* 2007).

The initial sample size (number of data) for any given chemical element varied from 7 to 208 (Table 1). The final sample size from DODESSYS was from 6 to 176, whereas from Gladney *et al.* (1992) it was from 6 to 182 (Table 1).

The comparison of the MTM method (applied through DODESSYS) with that used by Gladney *et al.* (1992) is presented in Figure 1A for the differences in 99% confidence limits of the mean and in Figure 1B for the differences in mean values. The y -axis (‘CL%difference’) variable in Figure 1A is formulated such that when it results in positive values, 99% confidence limits (CLs) for literature values are higher than those for this work (DODESSYS), and vice versa. For the total of 71 chemical elements processed in this work, 45 elements showed positive CL%difference and 26 negative. If we arbitrarily consider that the CL%difference values outside the limits of about $\pm 10\%$ are significant, 28 elements showed positive values higher than $+10\%$ and 14 negative values lower than -10% . Also, for a better, more reliable estimate of the mean value, it is desirable that 99% CLs should be as low as possible, which is the case of more elements processed in this work than those reported in the literature (Figure 1A). Nevertheless, we must clarify that DODESSYS was applied at the strict 99% CL, whereas the ‘two standard deviation’ method used by Gladney *et al.* (1992) would, in theory, correspond to a less strict 95% CL. Therefore, for a more objective evaluation of DODESSYS, the literature

data compiled by Gladney *et al.* (1992) should have been processed by the ‘three standard deviation’ method.

Although apparently newer statistical results on central tendency and dispersion estimates for G-2 are also available from the literature at http://minerals.cr.usgs.gov/geo_chem_stand/pdfs/granite.pdf, the statistical method of data processing is unfortunately not known. Neither the individual measurements nor their numbers are reported in this Internet site. Furthermore, it appears that these ‘recommended’ or ‘information’ values are simply based on earlier compilations (Govindaraju 1989, 1994; Gladney *et al.* 1992). Therefore, the confidence limits of these literature values cannot be estimated and the Internet information cannot be objectively compared with the results of this work.

The mean values obtained from DODESSYS are also somewhat different from the literature mean values (Gladney *et al.* 1992). Although most results (64 elements) are within the arbitrarily set limits of $\pm 10\%$, 7 elements (Sm, S, W, Sb, Co, Ho, and Au; Table 1) showed very large differences (more than 40%; Figure 1B; for simplicity we have not identified the data points by element symbols, this can be easily checked in Table 1). Because reference materials such as G-2 are used in calibration of instruments, for example, X-ray fluorescence spectrometry (Guevara *et al.* 2005), and in quality control for other analytical methods such as liquid chromatography (e.g. Verma and Santoyo 2007), any differences in mean values will be important for such purposes. The differences in confidence limits will also be important for calibrations based on weighted least-squares linear regression models and for quantitative assessment of data quality (e.g. Meier and Zünd 1992; Santoyo and Verma 2003; Guevara *et al.* 2005; Asuero and González 2007).

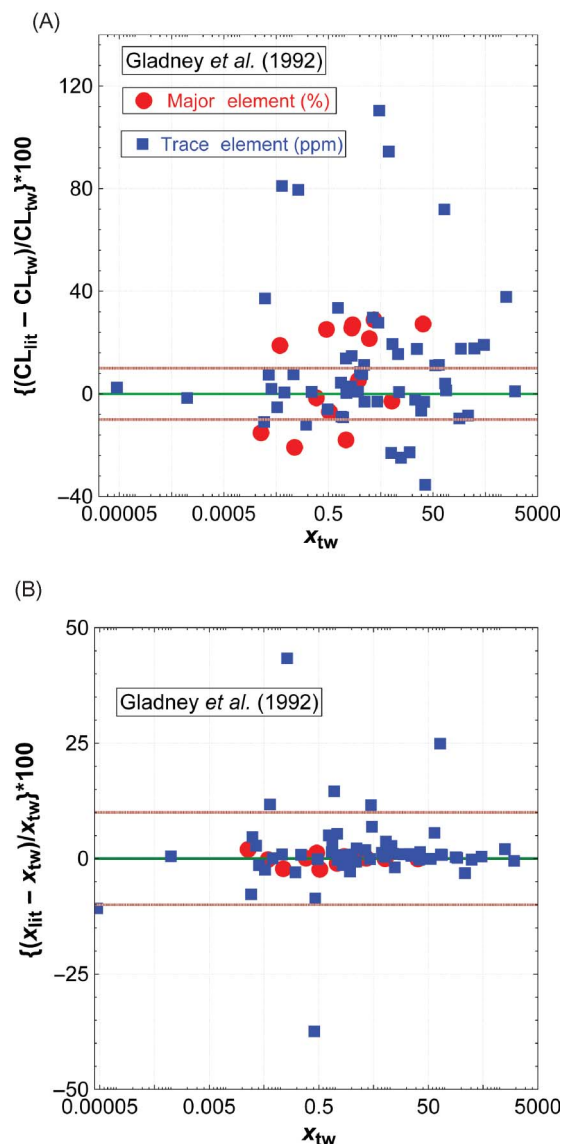


Figure 1. Application of DODESSYS to univariate data (major and trace elements) for geochemical reference material granite G-2 from USA (Gladney *et al.* 1992). The solid horizontal line represents zero difference in the y-axis variable, whereas the two dashed lines are for $\pm 10\%$ difference. (A) CL% difference (y-axis algorithm) for a given element versus its mean value estimated by DODESSYS. (B) Comparison of % difference of literature and DODESSYS mean values versus DODESSYS mean value.

Quality control through reference material sediment IAEA-417 from International Atomic Energy Agency

Similar to the above example, individual data for chlorinated pesticides and petroleum hydrocarbon compounds in sediment IAEA-417 were compiled from Villeneuve *et al.* (2002) who had used the BWP method to process their data. The results of DODESSYS software were compared with those of the BWP method (Table 2; Figure 2A and 2B) for 7 chlorinated pesticides and 24 petroleum hydrocarbons, which had at least 6 reported concentration data (6 being an arbitrary lower limit chosen for this comparison). Positive

CL% difference were obtained for 22 out of 31 compounds (Figure 2A), implying that, for most cases, DODESSYS provided lower CLs than the BWP. In fact, for 12 of these compounds the CL% difference values were very high ($> +10\%$), whereas for only two compounds were these values highly negative (below -10%). The literature mean values differed by more than 10% from those obtained by DODESSYS for seven compounds (HCB, EOM, nC17, rArom, Naph, phytane, and prist; Table 2 and Figure 2B).

Data evaluation in palaeontology

Recently, Ernst *et al.* (2008) presented data on bryozoan species from eastern Oman and described several new species. They presented statistical data (number of samples from species, mean, standard deviation, coefficient of variation expressed as relative standard deviation (%), minimum, and maximum) on parameters such as aperture width, lunaria length, lunaria width, aperture spacing from centre to centre, diameter of vesicles, and number of vesicle per millimetre. These authors reported no prior statistical treatment of their data such as testing for potentially discordant outliers in these statistical samples, which is a basic requirement for using outlier-based central tendency and dispersion parameters of mean and standard deviation, respectively (Barnett and Lewis 1994). We decided to use DODESSYS to process the raw data (Ernst *et al.* 2008) by all single-outlier tests (Table S1). The results for only those parameters for which outlying observations were detected are presented in Table 3. For other parameters (not listed in Table 3) the DODESSYS results are the same as those summarized by Ernst *et al.* (2008). In all cases listed in Table 3, the initial and final statistics of the literature are the same as those presented by Ernst *et al.* (2008), because these authors had not applied any statistical tests to their data. In any geological discussion, the final statistics resulting from the detection and separation of one or sometimes two discordant outliers (Table 3) should be treated separately from the outlying observations. As expected, the final standard deviation values from DODESSYS are lower than the literature values. A comparison of the CL% difference and mean values is presented in Figure 3. It is interesting to note that the effect of a few (one or two) discordant outliers in small-sized samples such as those used in this study (5–30 in Table 3) seems to be greater on the dispersion estimates, viz., standard deviation and confidence limits (Figure 3A), rather than on the mean (Figure 3B).

This procedure of the correct use of outlier-based methods (Barnett and Lewis 1994; Verma 1997, 2005) is greatly facilitated by the availability of DODESSYS and would be of use in the evaluation of hypotheses related to significance tests of Student *t*, Fisher *F*, and ANOVA (Ebdon 1988; Jensen *et al.* 1997; Miller and Miller 2005; Verma 2005). These significance tests have the basic underlying assumption that the data in each statistical sample

Table 2. Results of chlorinated pesticides and petroleum hydrocarbons in IAEA-417 sediment reference sample from DODESSYS and comparison with literature statistics (Villeneuve *et al.* 2002).

Element	Initial statistics			Final statistics (this work)			Final statistics (literature)		
	n_{in}	x_{in}	s_{in}	n_f	x_f	s_f	n_{lit}	x_{lit}	s_{lit}
(a) Chlorinated pesticides									
HEOM	23	8.8	23.1	15	1.8	0.69	18	1.7	0.8
HCB	32	2.4	6.5	26	1.08	0.58	30	1.2	0.8
alphaHCH	6	2.2	4.6	5	0.282	0.191	5	0.28	0.19
Lindane	41	106	620	16	0.526	0.194	24	0.54	0.35
ppDDE	58	23	63	53	13.9	6.6	55	14	6.9
ppDDD	58	21.8	13.6	53	20.0	10.0	57	21	11
ppDDT	57	19.3	12.2	57	19.3	12.2	57	19	12
(b) Petroleum hydrocarbons									
EOM	16	10.7	27.6	12	1.90	0.87	14	1.7	1
Taliph	13	226	187	13	226	187	13	230	190
Raliph	13	57	89	9	13.5	5.2	9	14	5.2
UnAliph	10	233	150	10	233	150	10	230	150
nC17	16	404	630	12	227	133	14	200	140
Prist	14	423	630	11	222	139	14	420	630
nC18	15	409	720	12	209	160	14	230	200
Phytane	15	374	333	13	276	202	15	370	330
SAC14C34	17	17.9	24.7	15	9.5	6.8	15	9.5	6.8
RArom	14	186	426	10	53.6	23.1	12	48	25
Naph	27	555	1250	20	171	107	22	150	110
Phenan	45	4413	2870	39	3873	1210	43	3900	1500
2MPhenan	8	1239	1330	6	579	228	6	580	230
1MPhenan	14	492	460	12	318	145	12	320	150
Anthra	22	963	1270	17	662	189	20	630	240
Chrys	45	4659	4450	38	3759	1370	42	3600	1700
Fluoren	12	753	1810	9	227	56	11	230	110
Fluora	49	8740	5900	43	7676	2440	47	7700	3000
Pyren	48	7509	5100	41	6064	2010	43	6000	2200
BbFluora	18	5033	4270	13	3768	1400	17	4100	2000
BkFluora	15	1769	640	12	2037	295	12	2000	300
BaAnthra	42	3606	233	36	3218	940	40	3200	1200
BePyren	21	2845	1200	21	2840	1200	18	3000	830
BaPyren	44	2793	1230	44	2793	1230	44	2800	1200

Notes: The statistical results from this work are reported as rounded values (by retaining an extra significant digit) as suggested by Bevington and Robinson (2003) and Verma (2005).

n_{in} , initial number of observations; x_{in} , initial mean; s_{in} , initial standard deviation; n_f , final number of observations (this work); x_f , final mean (this work); s_f , final standard deviation (this work); n_{lit} , final number of observations (literature); x_{lit} , final mean (literature); s_{lit} , final standard deviation (literature).

under evaluation are normally distributed, that is, they have no statistical contamination. Importantly, this basic assumption can be easily checked from DODESSYS prior to the application of these tests.

Bivariate data

Residuals from regression equation of Na/K geothermometer

As an example of bivariate data, we used the recent work of Díaz-González *et al.* (2008) on new geothermometric equations. These authors compiled a large number of fluid analysis and well temperature data from geothermal wells around the world. After considerations of data quality as judged through 'charge-imbalance' of cations and anions in the fluid data and other criteria, these authors reported

a data base of 212 observations (see electronic supplement to Díaz-González *et al.* 2008).

For proposing a new geothermometric equation, it is customary that a regression equation be obtained through linear least-squares best-fit model (Fournier 1979). Verma and Santoyo (1997), in their attempt to improve the Na/K geothermometric equation of Fournier (1979) based on 36 observations, had applied the outlier-detection procedure for bivariate data proposed by Barnett and Lewis (1994). However, critical values or percentage points are available only for up to 100 observations – in statistical terminology only for sample sizes of 5(1)10(2)20(5)50(10)100, that is, 22 critical values between sample sizes of 5 and 100 – in a general linear model with normal error structure (see table 37 in Barnett and Lewis 1994). These values were reported to only two decimal places, and their correctness

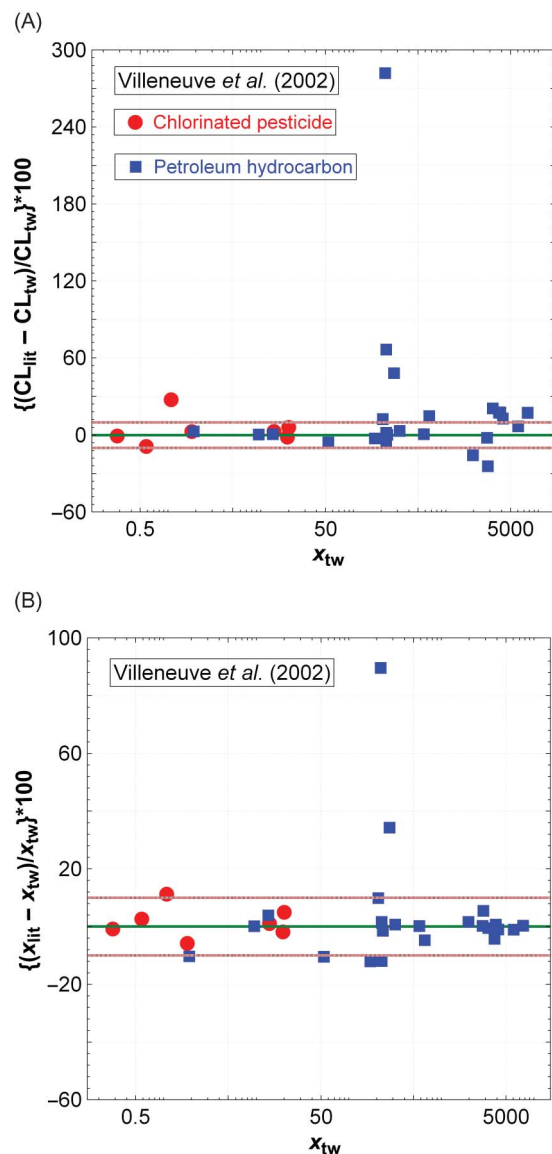


Figure 2. Application of DODESSYS to univariate data (chlorinated pesticides and petroleum hydrocarbons) for sediment reference material IAEA-417 from International Atomic Energy Agency (Villeneuve *et al.* 2002). The solid horizontal line represents zero difference, whereas the two dashed lines are for $\pm 10\%$ difference. (A) CL% difference (y -axis algorithm) for a given element versus its mean value estimated by DODESSYS. (B) Comparison of %difference of literature and DODESSYS mean values versus DODESSYS mean value.

has not been assessed from the modern point of view, which involves the estimation of standard error of the mean of critical values. These critical values therefore do not comply with the criteria proposed by Verma and Quiroz-Ruiz (2006a, 2006b, 2008) and Verma *et al.* (2008b) for reporting critical values of discordancy tests for univariate data, according to which a critical value should be reported to only those digits that are significant from its standard error. In other words, a dispersion parameter such as the standard

error of the mean dictates the number of digits to which a particular critical value can be reported (Verma 2005).

In spite of this potential weakness of the critical values for bivariate data, if we were dealing with somewhat greater than 100 observations, let us say up to 105 or 110, we might extrapolate the critical values and still obtain less precise, indicative critical values for the purpose of applying Barnett and Lewis (1994) outlier procedure to these bivariate data. For the extrapolation, the new regression procedure involving natural logarithm-transformation of the sample size recently proposed by Verma and Quiroz-Ruiz (2008) and Verma (2009) could be used. However, because the total number of 212 observations is far beyond the probably meaningful extrapolation range of presently available critical values, it is not advisable to apply this outlier procedure of bivariate data sets.

Nevertheless, given the less precise nature of these critical values for bivariate data (Barnett and Lewis 1994), instead of extrapolating the critical values to the sample size of 212, it is more appropriate to explore alternative procedures such as those proposed by Shoemaker *et al.* (1996) and Verma and Quiroz-Ruiz (2006b). The basic idea is to apply discordancy tests for univariate data to the studentized residuals of linear regression of 212 data of $\ln T$ and $\log(\text{Na}/\text{K})$ reported by Díaz-González *et al.* (2008). This data set is plotted in Figure 4A along with the ordinary linear least-squares regression line obtained from OYNYL computer program (Verma *et al.* 2006a). The difference between the actual y -axis $-\log(\text{Na}/\text{K})$ value and that predicted by the best-fit linear equation corresponding to the x -axis $-\ln T$ value for a given observation is called residual for a particular bivariate observation. All residuals for the 212 observations were thus calculated. These residuals were then studentized according to the procedure of Barnett and Lewis (1994, p. 322). This consists of dividing each residual by an unbiased estimate of standard deviation that corresponds to this particular residual (see pages 320–325 in Barnett and Lewis 1994). The distribution of these studentized residuals is shown in Figure 4B as a histogram plot.

The array of 212 studentized residuals was tested for discordant outliers using all 33 discordancy test variants (default option of DODESSYS). Nine discordant outliers were identified (filled circles in Figure 4C) and eliminated from the data array, thus reducing it to 203 observations. Distribution of the remaining data (203 studentized residuals) is shown in Figure 4D. The new regression line is also shown in Figure 4E.

The 203 studentized residuals were again tested by DODESSYS and two new discordant outliers were detected (filled squares in Figure 4E) and eliminated. Finally, the remaining 201 data were used for obtaining a new regression equation (Figure 4E) with the corresponding studentized residuals plotted in Figure 4F. These still newer studentized residuals were also tested for discordant outliers

Table 3. Application of DODESSYS to palaeontological (*Stenolaemate bryozoa*) data (Ernst *et al.* 2008).

Species	Parameter	Final statistics (this work)					Initial and final statistics (literature)						
		n_f	x_f	s_f	cv_f	min_f	max_f	n_{lit}	x_{lit}	s_{lit}	cv_f	min_f	max_f
<i>Fistulipora amplia</i>	Aperture width (mm)	19	0.2395	0.0155	6.472	0.216	0.264	20	0.24	0.022	9.124	0.22	0.31
<i>Fistulipora crescens</i>	Diameter of vesicles (mm)	10	0.0980	0.0134	13.673	0.085	0.125	11	0.09	0.019	20.555	0.05	0.13
<i>Hezagonella kobayashii</i>	Aperture spacing from centre to centre (mm)	18	0.3950	0.0381	9.645	0.32	0.50	20	0.41	0.059	14.288	0.32	0.55
<i>Hezagonella kobayashii</i>	Vesicles per 1 mm	4	9.00	1.15	12.778	8	10	5	10	2.049	20.912	8	13
<i>Sulcoretopora orientalis</i>	Aperture width (mm)	12	0.1505	0.0065	4.319	0.144	0.162	14	0.16	0.016	9.953	0.14	0.19
<i>Stenopora</i> sp.	Aperture spacing from centre to centre (mm)	14	0.2950	0.0129	4.373	0.28	0.32	15	0.30	0.023	7.664	0.28	0.37
<i>Streblotrypa katoi</i>	Axial zooecia width (mm)	4	0.1150	0.0058	5.017	0.11	0.12	5	0.11	0.010	8.866	0.10	0.12
<i>Streblotrypa</i> sp.	Aperture spacing across branch (mm)	23	0.3037	0.0245	8.067	0.24	0.35	24	0.31	0.034	10.933	0.24	0.42
<i>Streblotrypa germana</i>	Apertures per mm diagonally	4	6.75	0.57	8.503	6	7.2	5	7	0.600	8.696	6	7.5
<i>Rhabdomeson coniforme</i>	Aperture width (mm)	29	0.1847	0.0217	11.746	0.126	0.228	30	0.19	0.027	14.415	0.13	0.28
<i>Rhabdomeson coniforme</i>	Aperture spacing from centre to centre (mm)	19	0.3132	0.0167	5.328	0.29	0.35	20	0.32	0.022	6.973	0.29	0.36
<i>Rhabdomeson coniforme</i>	Microacanthostyle diameter (mm)	24	0.0544	0.0092	16.938	0.042	0.078	25	0.06	0.012	20.580	0.04	0.09
<i>Rhabdomeson latum</i>	Branch diameter (mm)	6	0.960	0.071	7.395	0.87	1.05	7	1.03	0.193	18.730	0.87	1.44
<i>Miniha rhomboidea</i>	Distance between branch (mm)	9	0.4862	0.0227	4.674	0.44	0.516	10	0.50	0.039	7.789	0.44	0.59
<i>Rectifenesitella ornatiformis</i>	Aperture width (mm)	11	0.1189	0.0085	4.674	0.11	0.14	12	0.12	0.012	10.014	0.09	0.14
<i>Kingopora?</i> sp.	Maximal chamber width (mm)	7	0.20214	0.00267	7.190	0.2	0.205	9	0.201	0.011	5.354	0.175	0.215
<i>Kingopora?</i> sp.	Obverse side node diameter (mm)	4	0.1238	0.0048	1.322	0.12	0.13	5	0.12	0.007	6.129	0.11	0.13
<i>Fenestellidae</i> sp.	Node diameter (mm)	9	0.0972	0.0137	3.868	0.0875	0.125	10	0.09	0.017	18.053	0.06	0.13

Notes: The statistical results from this work are reported as rounded values (by retaining an extra significant digit) as suggested by Bevington and Robinson (2003) and Verma (2005).

n_f , final number of observations (this work); x_f , final mean (this work); s_f , final standard deviation (this work); cv_f , final coefficient variation (this work); min_f , final minimal value (this work); max_f , final maximal value (this work); n_{lit} , final number of observations (literature); x_{lit} , final mean (literature); s_{lit} , final standard deviation (literature); cv_{lit} , final coefficient variation (literature); min_{lit} , final minimal value (literature); max_{lit} , final maximal value (literature); literature refers to Ernst *et al.* (2008).

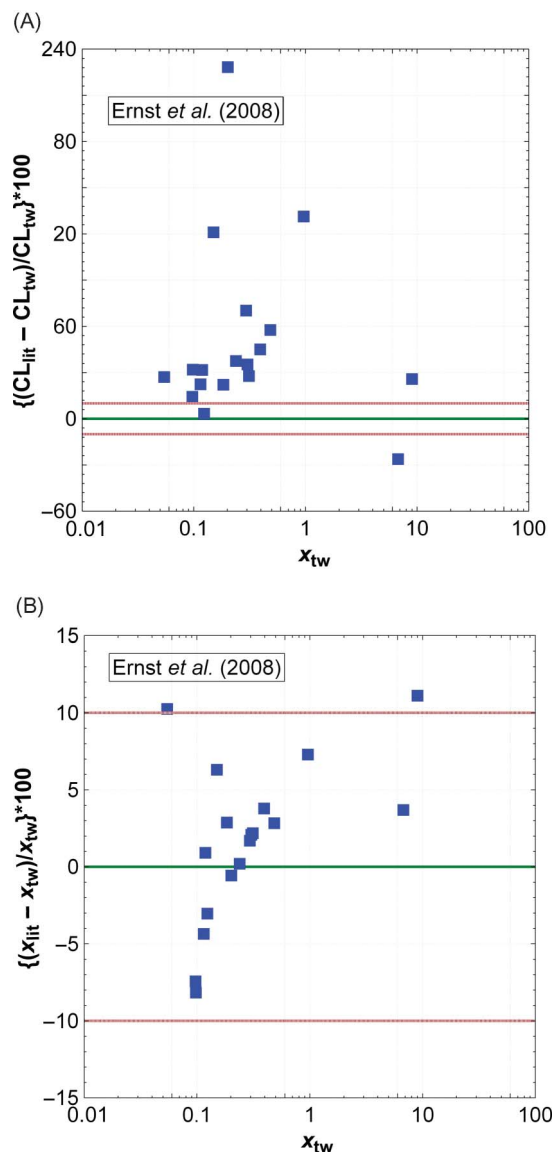


Figure 3. Application of DODESSYS to univariate palaeontological data on bryozoan species (Ernst *et al.* 2008). The solid horizontal line represents zero difference, whereas the two dashed lines are for $\pm 10\%$ difference. (A) CL%difference (y -axis algorithm) for a given element versus its mean value estimated by DODESSYS. (B) Comparison of %difference of literature and DODESSYS mean values versus DODESSYS mean value.

in the same way as done before. No discordant outliers were, however, observed, and these 201 observations now constitute the final data set. The total of 11 observations identified as discordant can also be checked for probable causes, whether geological or analytical, or both, that rendered them discordant with respect to the remaining 201 bivariate observations. The resulting geothermometric equation from these 201 observations should, in principle, be more reliable than most such existing equations (see Verma *et al.* 2008a for a compilation of such equations).

The new improved Na/K geothermometer for the calculation of geothermometric temperature t in $^{\circ}\text{C}$ is given by Equation (1):

$$t = \frac{868.3 (\pm 12.7)}{\log\left(\frac{\text{Na}}{\text{K}}\right) + 0.8744 (\pm 0.0269)} - 273.15 \quad (1)$$

where the numbers in parentheses are the errors in the respective coefficients; and Na and K are the concentrations (in mg/kg) of these two elements in geothermal water samples. The error in the temperature resulting from the errors in the coefficients, as well as analytical errors in Na and K, can be estimated from Monte Carlo simulations practiced by Espinosa-Paredes *et al.* (2010) and Verma (2011).

Residuals from regression of microfaunal abundance–depth relationship

Baguley *et al.* (2006) determined abundances of 21 meiofauna taxa in a total of 586 samples from 51 stations in the northern Gulf of Mexico and inferred a significant linear correlation between $\log(\text{meiofauna abundance})$ (in units of 'N 10 cm $^{-2}$ ' used by Baguley *et al.* 2006, see their Table 2) and water depth (Figure 5A). We obtained the following statistical information on these data: $n = 51$, $r = -0.81086$; inferred to be significant at 99% CL (for critical values see Bevington and Robinson 2003, or Verma 2005). We then used DODESSYS and applied all single-outlier tests to studentized residuals of these bivariate data (histogram plot in Figure 5B) and observed two discordant outliers (filled circles in Figure 5C), which were separated because these two data can (and probably should) be interpreted separately. The new regression line ($n = 49$, $r = -0.86206$; also significant at 99% CL) is shown in Figure 5C and the corresponding residuals as a histogram plot in Figure 5D. No more outliers were detected as discordant. This example highlights the usefulness of DODESSYS for bivariate data in environmental sciences.

Applications of DODESSYS to new multi-dimensional discrimination diagrams

In an altogether different field of tectonomagmatic discrimination diagrams using linear discriminant analysis (Agrawal *et al.* 2004, 2008; Verma *et al.* 2006b; Agrawal and Verma 2007; Verma 2010), DODESSYS under the option of single-outlier tests (Table S1) has proved useful for improving the quality of newer diagrams recently proposed by Verma and Agrawal (2011) and Verma *et al.* (2011). The multivariate technique of linear discriminant analysis used in proposing discrimination diagrams requires that the natural logarithm-transformed element-ratio parameters be normally distributed, which was ascertained by Verma and Agrawal (2011) and Verma *et al.*

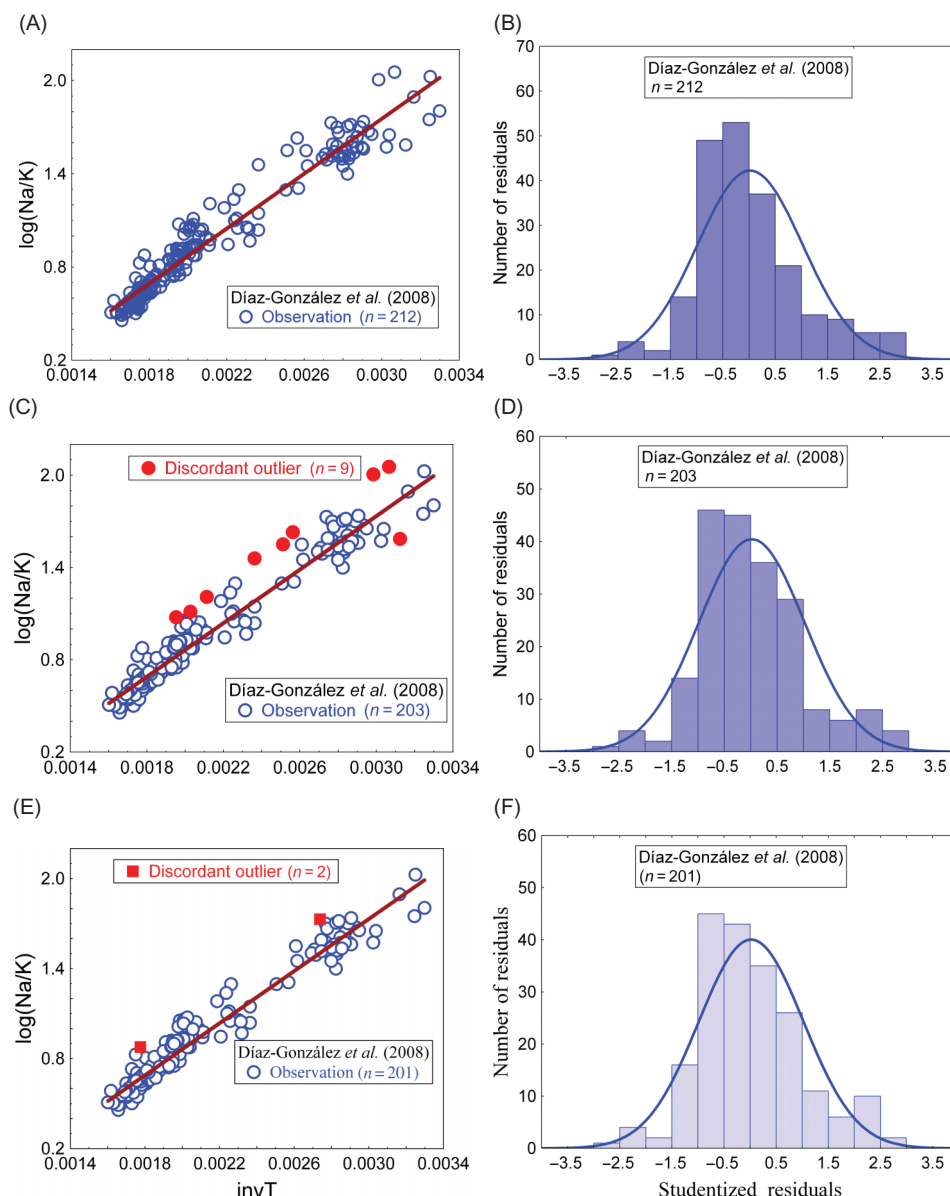


Figure 4. Application of DODESSYS to bivariate data from fluid geothermometry (Díaz-González *et al.* 2008). The x -axis is $\text{inv}T$ – the inverse of fluid temperature in Kelvin; the y -axis is $\log(\text{Na}/\text{K})$ – logarithm of the ratio of Na and K concentration data in geothermal fluids. (A) Linear regression of all 212 bivariate observations. (B) Histogram of the 212 studentized residuals calculated from the linear regression in (A). (C) Linear regression of the remaining 203 bivariate observations with the 9 discordant observations indicated by filled circles. (D) Histogram of the 203 studentized residuals calculated from the linear regression in (C), for which 9 outlying observations were excluded. (E) Second round of application of DODESSYS which detected 2 discordant outliers indicated by filled squares and linear regression of the remaining 201 bivariate data. (F) Histogram of the 201 studentized residuals calculated from the linear regression in (E) for which 2 outlying observations (filled squares) were excluded. The third round of application of DODESSYS detected no outlying observations as discordant.

(2011) from the application of discordancy tests. The main achievement of this procedure was enhanced success rates for both sets of diagrams.

The condition that the natural logarithm-ratio parameters represent samples from normally distributed populations should also be fulfilled for application data.

Therefore, to illustrate this rather novel application of DODESSYS we compiled geochemical data for basic and ultrabasic rocks as well as acid rocks from several localities around the world and processed these log-ratios (immobile element ratios for Verma and Agrawal 2011; major element ratios for Verma *et al.* 2011) for possible discordant

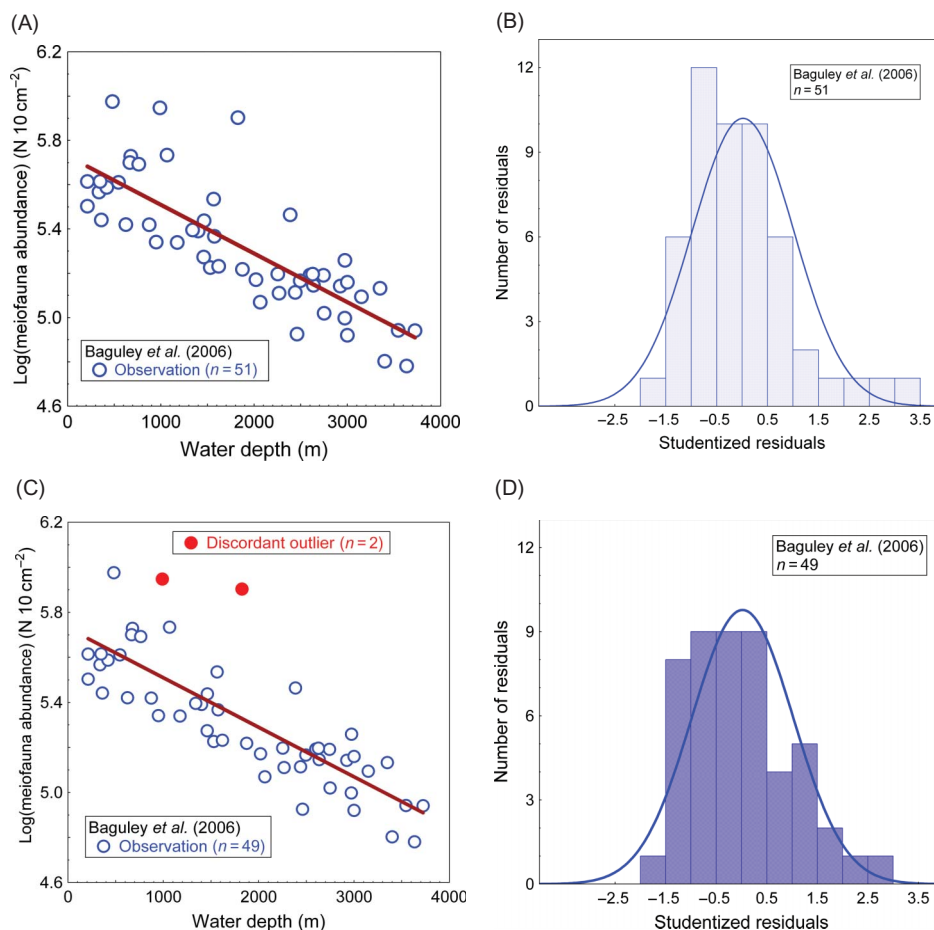


Figure 5. Application of DODESSYS to bivariate data of logarithm of meiofauna abundance versus water depth relationship (Baguley *et al.* 2006). (A) Linear regression of all 51 bivariate observations. (B) Histogram of the 51 studentized residuals calculated from the linear regression in (A). (C) Linear regression of the remaining 49 bivariate observations with the two discordant outliers indicated by filled circles. (D) Histogram of the 49 studentized residuals calculated from the linear regression in (C), for which the two outlying observations were excluded. The second-round of application of DODESSYS detected no outlying observations as discordant.

outliers. The results are presented separately for the diagrams for basic and ultrabasic magmas (Verma and Agrawal 2011) and acidic magmas (Verma *et al.* 2011). For simplicity, only the numbers of samples (and not the success rates) are tabulated; furthermore, the inapplicable diagram is also identified for each case study.

Immobile element-based diagrams for basic and ultrabasic magmas

The results are shown in Figures S2A-E and S3A-E and summarized in Tables 4 and 5. As stated earlier, the appropriate log-ratio values for basic magmas (including ultrabasic magmas when present) were processed for the identification and separation of discordant outliers. No outliers were detected as discordant for samples from Kambalda (Australia), Adola (Ethiopia), and Gadwal (India) areas

(Table 4); the same was the case for Punta Orvili (Sardinia), Posada valley and Punta de li Tulchi (Sardinia), Balikun area (China), and New Georgia group (Solomon Islands) areas (Table 5).

An arc setting was inferred for Kambalda (~2700 Ma), Adola (~825 Ma), and Solomon Islands (~6–0 Ma), Gadwal greenstone belt (~2600 Ma), and Posada valley (~453 Ma), and ocean island setting for Punta Orvili (~453 Ma) and Balikun area (~286 Ma).

For Kalgoorlie (Australia), Lomza (Poland), Faroe Islands (North Atlantic Ocean), and Westerwald (Germany), one discordant outlier was detected for each area, whereas for North Caribou and Wawa greenstone belts (Canada) two outliers were detected as discordant in each case (Tables 4 and 5; Figures S2 and S3). The inferred tectonic settings for these areas were as follows: mid-ocean ridge for Kalgoorlie (~2690 Ma) and Lomza

Table 4. Application of DODESSYS to the set of five discriminant function multi-dimensional diagrams (Verma and Agrawal 2011) for basic and ultrabasic rocks from Precambrian terranes (see Figure 6A–6E).

Locality; magma type; age; reference; inferred tectonic setting	Figure type	Total number of samples	Number of discriminated samples				
			Within-plate				
			IAB (1)	CRB+OIB (2+3)	CRB (2)	OIB (3)	MORB (4)
Kambalda, western Australia; basic; Archaean (~2700 Ma); Arndt and Jenner (1986); island arc.	1-2+3-4 1-2-3 1-2-4 1-3-4 1-3-4 2-3-4 ^a	5 5 5 5 5 5 ^a	5 5 5 5 5 –	0 – – – – 4 [1]	– 0 0 – 0 –	– 0 – 0 0 0	0 – 0 0 0 5
Kalgoorlie greenstone belt, Yilgarn craton, western Australia; basic and ultrabasic; Archaean (~2675–2710 Ma); Bateman <i>et al.</i> (2001); mid-Ocean ridge.	1-2+3-4 1-2-3 ^a 1-2-4 1-3-4 2-3-4	32 32 ^a 32 32 32	11 20 12 10 –	4 [1] – – – –	– 5 [1] 4 [1] – 0	– 6 – 6 [1] 4 [1]	16 – 15 15 27
Adola, southern Ethiopia; basic and ultrabasic; Neoproterozoic (765–885 Ma); Wolde <i>et al.</i> (1996); island arc.	1-2+3-4 1-2-3 1-2-4 1-3-4 2-3-4 ^a	7 7 7 7 7 ^a	5 6 5 4 –	0 – – – –	– 0 0 – 0	– 1 0 1 1	2 – 2 2 6
Gadwal greenstone belt, eastern Dharwar craton, South India; basic; Archaean (~2700–2500 Ma); Manikyamba <i>et al.</i> (2005); mid-Ocean ridge.	1-2+3-4 1-2-3 ^a 1-2-4 1-3-4 2-3-4	7 7 ^a 7 7 7	7 0 0 1 –	– – – – –	– 0 0 – 0	– 0 – 0 0	– – 7 6 7
Lomza orthoamphibolite, NE Poland; ultrabasic and basic; Palaeoproterozoic (~1800 Ma); Krzeminska <i>et al.</i> (2005); mid-Ocean ridge.	1-2+3-4 1-2-3 ^a 1-2-4 1-3-4 2-3-4	12 12 ^a 12 12 12	3 [1] 4 [1] 3 [1] 3 [1] –	0 – – – –	– 7 0 – 0	– 0 – 0 0	8 – 8 8 11 [1]
North Caribou greenstone belt, northwestern Superior Province, Canada; basic; Archaean (~3000 Ma); Hollings and Kerrich (1999); island arc.	1-2+3-4 1-2-3 1-2-4 1-3-4 2-3-4 ^a	15 15 15 15 15 ^a	13 [2] 13 [2] 13 [2] 13 [2] –	0 – – – –	– 0 0 – 0	– 0 – 0 0	0 – 0 0 15
Wawa greenstone belt, Superior Province, Canada; basic and ultrabasic; Archaean (~2700 Ma); Polat <i>et al.</i> (1999); island arc.	1-2+3-4 1-2-3 1-2-4 1-3-4 2-3-4 ^a	50 50 50 50 50 ^a	36 41 37 34 –	6 [2] – – – –	– 1 5+2 – 3	– 6 [2] – 7 [2] 7 [2]	6 – 6 7 38

Notes: Figure type refers to the tectonic fields being discriminated where the tectonic group numbers are as follows: 1, IAB; 2, CRB; 3, OIB; 4, MORB.
^aInapplicable results and diagrams; boldface italic font shows the expected tectonic settings; the number of samples enclosed in [] are the discordant outliers detected by DODESSYS.

Table 5. Application of DODESSYS to the set of five discriminant function multi-dimensional diagrams (Verma and Agrawal 2011) for basic and ultrabasic rocks from Precambrian terranes (see Figure 7A–7E).

Locality; magma type; age; reference; inferred tectonic setting	Figure type	Total number of samples	Number of discriminated samples				
			Within-plate				
			IAB (1)	CRB+OIB (2+3)	CRB (2)	OIB (3)	MORB (4)
Punta Orvili, Variscan belt, NE Sardinia; basic; Middle-Ordovician (~453 Ma); Cruciani <i>et al.</i> (2010); ocean island.	1-2+3-4 1-2-3 1-2-4 ^a 1-3-4 2-3-4	6 6 6 ^a 6 6	0 0 0 0 –	6 – – – –	– 0 6 – 0	– 6 – 6 6	0 – 0 0 0
Posada valley and Punta de li Tulehi, Variscan belt, NE Sardinia; basic; Middle-Ordovician (~453 Ma); Cruciani <i>et al.</i> (2010); mid-ocean ridge.	1-2+3-4 1-2-3 ^a 1-2-4 1-3-4	5 5 ^a 5 5	1 5 1 1	0 – – –	– 0 0 0	– 0 0 0	4 – 4 4
Balikun area, east Tianshan, central Asian orogenic belt, China; basic; Permian (~288–284 Ma); Yuan <i>et al.</i> (2010).	2-3-4 1-2+3-4 1-2-3 1-2-4 ^a 1-3-4 2-3-4	5 9 9 9 ^a 9 9	– 0 0 0 0 –	– 6 – – – –	0 0 6 – 0	0 – 9 – 9	5 3 – 3 0 0
Faroe Islands, North Atlantic Ocean; basic; Palaeogene (~56–55 Ma); Søager and Holm (2009); ocean island.	1-2+3-4 1-2-3 1-2-4 ^a 1-3-4 2-3-4	13 13 13 ^a 13 13	0 0 0 0 –	12 – – – –	– [1] 12 – 0	– 12 12 12 12	[1] – [1] [1] [1]
Central European volcanic province, Westerwald region, Germany; ultrabasic and basic; Tertiary (30–10 Ma); Haase <i>et al.</i> (2004); ocean island.	1-2+3-4 1-2-3 1-2-4 ^a 1-3-4 2-3-4	21 21 21 ^a 21 21	0 0 0 0 –	20 [1] – – – –	– 6 [1] 20 [1] – –	– 14 – 20 [1] 12	– 0 0 0 0
New Georgia group, Solomon Islands, Pacific Ocean; basic; Neogene (6–0 Ma); Schuth <i>et al.</i> (2004); island arc.	1-2+3-4 1-2-3 ^a 1-2-4 1-3-4 2-3-4	23 23 23 23 23 ^a	22 23 22 22 –	0 – – – –	– 0 – – 1	– 0 – 0 0	1 – 1 1 22

Notes: Figure type refers to the tectonic fields being discriminated where the tectonic group numbers are as follows: 1, IAB; 2, CRB; 3, OIB; 4, MORB. ^aInapplicable results and diagrams; boldface italic font shows the expected tectonic setting; the number of samples enclosed in [] are the discordant outliers detected by DODESSYS.

(~1800 Ma), arc for North Caribou (~3000 Ma) and Wawa (~2700 Ma), and ocean island for Faroe Islands (~55 Ma) and Westerwald region (~20 Ma). As can be seen in Tables 4 and 5 and Figures S2 and S3, the discordant outliers generally plot outside the field of the inferred tectonic setting, in which most of the samples from a given area plot. Thus, if we calculate the success rates, the identification and separation of outlying observation(s) would generally increase the reliability of the inferred tectonic settings, because in most cases we would obtain higher success rates when the outlying observation(s) is (are) not considered. For example, for Lomza area (Table 4), the success rate for the inferred MORB setting for all samples (8 samples correctly discriminated from 12 samples, amounting to about 67%) would increase from about 67% to about 73% (8 out of 11 samples) as a result of the application of DODESSYS. More importantly, the use of DODESSYS will help us comply with the basic assumption of multivariate technique of linear discriminant analysis.

Major element-based diagrams for acid magmas

The results are shown in Figures S4A–S4E and summarized in Table 6. The discordancy tests did not identify any outlying observation as discordant for Kinwat (India, ~2230 Ma), External crystalline massif of the Alps (France, Italy, and Switzerland, ~300 Ma), Balikun (Tianshan, China, ~286 Ma), and Central Anatolian crystalline belt (Turkey, ~74 Ma). For all these regions, collision tectonic setting was inferred (Table 6, Figure S4A–S4E). On the other hand, one outlier was detected as discordant for North Caribou greenstone belt (Canada, ~3000 Ma) as well as Adola (Ethiopia, ~825 Ma). For these areas, continental and island arc settings were, respectively, inferred.

It is important to note that the tectonic inference of arc setting for North Caribou and Adola confirms the consistency of these two sets of diagrams (Verma and Agrawal 2011; Verma *et al.* 2011), even though the first set is based on immobile elements in basic and ultrabasic magmas and the second relies on major elements in acid magmas.

Table 6. Application of DODESSYS to the set of five discriminant-function-based multi-dimensional discrimination diagrams (Verma *et al.* 2011) to acid rocks from six different regions of the world (see Figure 8A–8E).

Locality; magma type; age; reference; inferred tectonic setting	Figure type	Total number of samples	Number of discriminated samples				
			IA+CA (1+2)	IA (1)	CA (2)	CR (3)	Col (4)
North Caribou greenstone belt, northwestern Superior Province, Canada; acid; Archaean (~3000 Ma); Hollings and Kerrich (1999); continental arc.	1+2–3–4	6	4 [I]	0	–	–	1
	1–2–3	6	–	1 [1]	3	1	–
	1–2–4	6	–	2	1	–	2 [1]
	1–3–4 ^a	6 ^a	–	3	–	–	2 [1]
	2–3–4	6	–	–	5 [I]	0	0
Kinwat, Nanded and Yeotmal districts, Maharashtra (India); acid; Palaeoproterozoic (2385–2074 Ma); Banerjee and Shivkumar (2010); collision.	1+2–3–4	49	2	–	–	10	37
	1–2–3 ^a	49 ^a	–	1	6	42	–
	1–2–4	49	–	2	3	–	44
	1–3–4	49	–	4	–	13	32
	2–3–4	49	–	–	4	10	35
Adola, southern Ethiopia; acid; Neoproterozoic (765–885 Ma); Wolde <i>et al.</i> (1996); island arc.	1+2–3–4	9	5 [I]	–	–	2	1
	1–2–3	9	–	4 [I]	1	3	–
	1–2–4	9	–	3 [1]	0	–	5
	1–3–4	9	–	4 [I]	–	3	1
	2–3–4	9	–	–	6 [I]	2	0
External crystalline massifs of the Alps, France, Italy and Switzerland; acid; Palaeozoic (305–295 Ma); Debon and Lemmet (1999); collision.	1+2–3–4	11	0	–	–	1	10
	1–2–3 ^a	11 ^a	–	0	4	7	–
	1–2–4	11	–	0	2	–	9
	1–3–4	11	–	–	–	2	9
	2–3–4	11	–	–	0	2	9
Balikun area, east Tianshan, central Asian orogenic belt, China; acid; Permian (~288–284 Ma); Yuan <i>et al.</i> (2010); collision.	1+2–3–4	24	0	–	–	10	14
	1–2–3 ^a	24 ^a	–	0	10	14	–
	1–2–4	24	–	0	8	–	16
	1–3–4	24	–	0	–	10	14
	2–3–4	24	–	–	0	10	14
Central Anatolian crystalline complex, Turkey; acid; Permian (~80–67 Ma); Ilbeyli <i>et al.</i> (2004); collision.	1+2–3–4	13	2	–	–	1	10
	1–2–3 ^a	13 ^a	–	0	2	11	–
	1–2–4	13	–	0	7	–	6
	1–3–4	13	–	0	–	3	10
	2–3–4	13	–	–	1	1	11

Notes: Figure type refers to the tectonic fields being discriminated where the tectonic group numbers are as follows: 1, IA; 2, CA; 3, CR; 4, Col.

^aInapplicable results and diagrams; boldface italic font shows the expected tectonic setting; the number of samples enclosed in [] are the discordant outliers detected by DODESSYS.

Other applications

DODESSYS should be of much use for estimating statistical parameters for a large number of 'traditional' reference materials, for example, such as those reported by Dybczynski *et al.* (1991, 1998) and Balaram *et al.* (1995), or compiled by Gladney and Roelandts (1987), Govindaraju (1989, 1994), Potts *et al.* (1992), and Imai *et al.* (1996), among others.

It is also possible that most users of analytical instruments are not aware of the fact that the software may include discordancy tests that 'filter' the data for statistical contamination before providing the output to the user. An example of such an application of Dixon tests was documented by Dougherty-Page and Bartlett (1999). We suggest that DODESSYS with its single-outlier variant can be easily programmed with such instrumental data-procuring software, because the skewness and kurtosis tests as well as certain types of Grubbs tests, not generally used, can be more powerful than the Dixon tests (e.g. Velasco and Verma 1998; Verma *et al.* 2009).

A recent study (Verma *et al.* 2009) involving geochemical reference materials and X-ray fluorescence spectrometry calibrations provides another application of bivariate data, in which the MTM of Verma (1997) was successfully applied. Other types of bivariate data, for example, the rainfall data reported by Yadava *et al.* (2007), can also be processed in a similar way, and statistically valid conclusions could be drawn.

In combination with other computer programs such as SolGeo (Verma *et al.* 2008a) for estimating geothermometric temperatures and OYNYL (Verma *et al.* 2006a) for ordinary and weighted linear least-squares (York and New York types) regressions, DODESSYS would be of much use for handling geochemical, geothermometric, and many other kinds of experimental data.

Finally, we may stress that although only univariate and bivariate examples are specifically presented for illustration purposes in this work, the method should, in theory, be applicable to multivariate and time-series data. In such cases, after a proper model or function fitting, the studentized residuals will have to be computed and processed by DODESSYS as done for the two bivariate examples presented in this work.

Future work

As shown in the present article the new software DODESSYS can be used for numerous other applications than just the quality control in many fields of science and engineering.

Analytical data from different techniques should be combined only if all individual statistical samples are drawn from a single (or equivalent) population, for which significance tests, viz., Student *t*, Fisher *F*, and ANOVA, have proved indispensable (Verma 1998, 2009). These tests

will be programmed in a second version of DODESSYS. Log-transformed regression equations can be used to advantage, instead of critical value tables, for a more efficient programming and faster program running operations (Verma and Quiroz-Ruiz 2008; Verma 2009). Finally, the experimental data in different fields of science and engineering would be better handled by input files specifically designed for a given application; this work will be the focus of our future efforts.

DODESSYS should make the provision for applying the discordancy tests at CL different from 99% used in this work, for example, 95% practiced in the area of chemistry (Miller and Miller 2005), which would require additional programming work.

On the other hand, it will be worthwhile to explore the relative efficiency of these discordancy tests and their variants for different types of statistical samples drawn from normal populations. The comparison of single-outlier discordancy tests for geochemical reference data bases and their usefulness for the calibration of X-ray fluorescence spectrometry have been recently documented by Verma *et al.* (2009), whereas a more complete comparison of all 33 test variants for handling geochemical data is also published by González-Ramírez *et al.* (2009). This kind of work for different areas of science and engineering may eventually provide guidelines on the use of the discordancy tests individually programmed in DODESSYS. Probable answers to the question of which discordancy test(s) is (are) more appropriate for an application might thus be eventually put forth.

DODESSYS is freely available from any of the authors to any scientist interested in correctly using the outlier-based methods for processing experimental data.

Conclusions

We have prepared a new first-version computer program DODESSYS and have successfully demonstrated its applicability and usefulness for identifying discordant outliers in both univariate and bivariate geochemical, geothermometric, ecologic, and palaeontologic data sets. The usefulness of discordancy tests for multi-dimensional discrimination diagrams is also well documented in this work. Numerous other applications of DODESSYS have also been noted. Future work should concentrate on the improvement of DODESSYS in order to make it more useful in all areas of science and engineering.

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Supplementary material

Figures S1–S4, Table S1, and description of DODESSYS can be found in the online version of this article at the website of the journal.

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