Netherlands Journal of Geosciences — Geologie en Mijnbouw | e1. doi: 10.1017/njg.2014.10

Modelling particle-size distributions from operator estimates of sediment particle-size

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Manuscript received: 2 December 2013, accepted: 13 April 2014

Abstract

Estimates of particle-size made by operators in the field and laboratory represent a vast and relatively untapped data archive. The wide spatial distribution of particle-size estimates makes them ideal for constructing geological models and soil maps. This study uses a large data set from the Netherlands (n = 4837) containing both operator estimates of particle-size and complete particle-size distributions measured by laser granulometry. Operator estimates are inaccurate and imprecise relative to measured laser data; only 16.68% of samples were successfully classified using the Dutch classification scheme for fine sediment. Operator estimates of sediment particle-size encompass the same range of percentage values as particle-size distributions measured by laser analysis. However, the distributions measured by laser analysis show that most of the sand percentage values lie between 0 and 1, so the majority of the variability in the data is lost because operator estimates are made to the nearest 1% at best, and more frequently to the nearest 5%. Operator estimates made by three technicians trained by the Geological Survey of the Netherlands are found not to be influenced by bias, rather they exhibit very similar levels of accuracy and precision. This study compares five different methods of modelling complete particle-size distributions from sparse data: (i) a four-part Pearson's probability distribution function, (i) a log-linear interpolation, (iii) a logit-linear interpolation, (iv) a logistic probability distribution function and (v) a logit constrained cubic-spline (logit-CCS) interpolation. The logit-CCS interpolation performed best across all the samples used, although the performance of all models was very similar for normal Gaussian, skewed and peaked distributions. Predictions for bimodal distributions using the Pearson's, logit-linear and logistic models are markedly less accurate than both log-linear and logit-CCS interpolation models. Although the logit-CCS interpolation model produces the best predictions of continuous particle-size distributions, the low accuracy and precision of operator estimates does not warrant the use of such a complex algorithm. Given this, it is suggested that a standard log-linear interpolation is the most effective means of modelling complete particle-size distributions from sparse data. Interpolation-based models are recommended over probability distribution functions because they allow for a greater degree of flexibility and will always honour the available input data.

Keywords: compositional data analysis, grain size distribution, operator estimates, particle-size distribution modelling, sediment texture

Introduction

Rationale

Estimates of sediment particle-size made in the field or laboratory by trained operators comprise the largest proportion of modern and archive lithological datasets. The estimation method relies on comparing known standards with field samples, both by visual inspection and by rubbing the sediment between thumb and fingers. Experienced operators are able to identify the relative proportions of gravel, sand, silt, clay and organic material in a sample (Fig. 1), as well as placing it in a soil classification category. Despite the clear potential for bias and inaccuracy, three-dimensional geological models and soil maps rely heavily on estimates of particle-size made from borehole cuttings, cores and exposures. The main reasons for this are (i) it is much less expensive to make estimates of sediment particle-size than to measure it in the laboratory, (ii) the high local variability of sediment particle-size means that it is better to spend time collecting a high number of low-quality samples rather than a low number of high-quality samples (Hengl et al., 2007), (iii) operator estimates are the only practical way to acquire textural

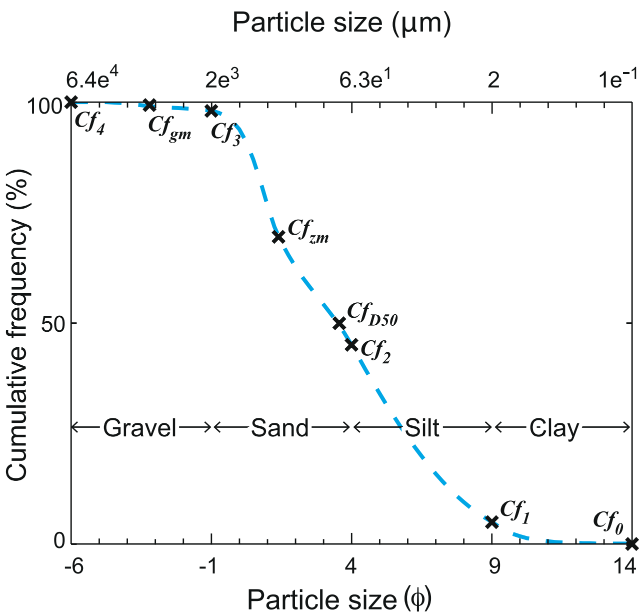

Fig. 1. Construction of a continuous cumulative frequency distribution (blue line) from operator estimates of sediment particle-size given as black crosses. The relative proportions of gravel, sand, silt and clay (Cf_0 to Cf_4) are calculated following Eq. 2. The cumulative percentage frequency for the distribution median (Cf_{D50}), the median of the gravel fraction (Cf_{gm}) and the median of the sand fraction (Cf_{zm}) are calculated following Eq. 3.

data for coarse sediments >50 mm in diameter (Church et al., 1987) without incurring the need to analyse very large samples (>100 kg), and (iv) sediment particle-size may be of relatively minor importance to subsurface exploration projects compared to the collection of geotechnical data.

Recent developments in geological modelling have made it possible to draw maps and build geological models of sediment particle-size using complete particle-size distributions, rather than separate textural categories (Walvoort & De Gruijter, 2001; Odeh et al., 2003; Roberson & Weltje, 2011; Lark et al., 2012). This approach offers a number of advantages over indicator kriging or sequential Gaussian simulation methods: (i) the quality of the data can be easily assessed, (ii) conversion from interpolated binary indicators (i.e. the presence or absence of different grain size categories) into particle-size distributions is avoided and (iii) the mathematical representation of sedimentary processes is simplified. In order to retain the advantages of using high-quality data alongside operator estimates of sediment particle-size when building a geological model it is necessary to both (i) model complete particle-size distributions from limited textural data and (ii) assess the error in operator estimates.

Existing modelling approaches

The huge potential for using operator estimates of sediment particle-size to model complete particle-size distributions has been widely recognised within the fields of soil science (Shirazi et al., 1988; Kozak et al., 1996; Skaggs et al., 2001), civil engineering (Fredlund et al., 2000; Fredlund & Houston, 2009) and mathematics (Dexter & Tanner, 1972; Barndorff-Nielsen, 1978; Fieller et al., 1992; Taguas et al., 2000). The majority of these studies have focused on summarising particle-size distributions using parametric function coefficients (e.g. mean, standard deviation, skewness), which provide convenient variables for spatial modelling (Meilianda et al., 2011). However, the errors involved in calculating distribution moments from limited textural data are often large for broad, skewed, peaked or multimodal distributions (Folk, 1966; Schlee & Webster, 1967; Weltje & Roberson, 2012). Furthermore, because moment methods are explicitly linked to one another, it is not possible to construct independent spatial models without running into serious mathematical difficulties. For these reasons the application of moment methods to modelling particle-size distributions is not recommended.

As an alternative to fitting distribution functions, several attempts have been made to model particle-size distributions using customised parametric functions (Hwang et al., 2002; Silva et al., 2004; Wu & Jet-Chau Chang, 2009). For example, Skaggs et al. (2001) used a modified logistic function to predict distributions from three operator estimates: the clay mass fraction, the silt mass fraction and the very fine to fine sand mass fraction. A similar method was implemented by Gruijters et al. (2005), who used a combination of three arctan functions to define a cumulative frequency distribution from operator estimates of the silt fraction, the median particle-size of the sand fraction, the sand fraction and the gravel fraction. These types of predictive models rely on fine-tuning function coefficients to derive best-fit predictions for any given set of samples. Calculating optimal parameters usually involves one or more stochastic modelling steps and is therefore time-consuming.

The application of both standard and customised parametric distribution functions to large heterogeneous data sets is limited. Irrespective of how complex these functions are, they remain unable to successfully describe the full range of all particle-size distributions encountered in natural sediments, even when using a large number of discrete particle-size classes. In worst-case scenarios the model may not even honour the input data.

Interpolation of percentage-frequency values offers modelling flexibility, allowing all available data to inform the model without the need to produce a customised model for each data set. Interpolation functions also offer the considerable advantage over fitted distribution functions that all the input data will be honoured. In the past, interpolation methods used for particle-size distributions have suffered from a trade-off between over-simplification and the tendency to violate constant-sum and conservation of mass constraints (e.g. polynomial functions). A recent methodological study by Weltje & Roberson (2012) demonstrated that such issues could be overcome by transforming percentage-frequency data into the logit domain prior to the application of a constrained cubic-spline (CCS)

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algorithm. The model also uses an adaptive non-linear extrapolation algorithm to predict smoothly tapering distribution tails. The results presented by Weltje & Roberson (2012, their Figure 5) demonstrate that particle-size distributions measured by laser analysis could be modelled reliably using just four equiprobable particle-size categories.

Scope of this paper

The aims of this paper are to (i) quantify the accuracy and precision of operator estimates of particle-size, (ii) determine if operator bias is a significant factor, (iii) compare a range of different methods for modelling complete particle-size distributions from a small number of particle-size categories and (iv) demonstrate the application of the best method to modelling complete particle-size distributions from operator estimates of particle-size.

Methods

The data

This study uses an archive of high-quality sediment samples collected and maintained by the Geological Survey of the Netherlands. The *Top Integraal* database is a benchmark data set that contains lithological, hydraulic, geochemical and geotechnical measurements of the main lithofacies types in the Netherlands. The project aims to gather representative samples of the 27 geologically homologous areas identified by Vernes et al. (2010), with the overall objective of building a high-resolution geological model of the top 30–50 m of the Dutch subsurface. The 4855 particle-size distributions used by this project from the database are representative of aeolian, estuarine, fluvial, glacial, marine and lagoonal depositional environments found in the Netherlands.

The lithology of each sample was measured by passing the bulk sediment sample though a 2 mm sieve prior to laser diffraction. Laser diffraction was performed using a Fritsch Analysette 22 XL particle analyser (Fritsch GmbH, Idar-Oberstein, Germany). The particle-size distribution is described by 32 size categories ranging from 2000 to 0.1 μm.

In addition to laboratory analysis, each sample was also described by a trained laboratory technician according to the Dutch standard for sediment analysis (NEN5104 (Bosch, 2000, p. 38)). Operator estimates of the relative proportions of gravel, sand, silt, clay, shell material and organic matter were made, as well as estimates of the median particle-size of the sand fraction (one of six qualitative classes) and the gravel fraction (one of three qualitative classes).

Accuracy and precision of operator estimates

Operator estimates of sediment particle-size were made for four particles-size categories: gravel, sand, silt and clay. These correspond respectively with the following maximum particle-size boundaries: 63 mm, 2 mm, 63 μm and 2 μm. Error in operator estimates was calculated by comparing the *logratio* operator estimates of the relative proportions of gravel, sand, silt and clay with the *logratio* of those measured by laser analysis. The *logratio* function transforms percentile data into unconstrained real space, allowing mathematically robust analyses to be performed (Aitchison, 2003). The *logratio* transformation is an invaluable tool for the analysis of percentage frequency data, which otherwise are heavily biased because they exist in closed space, i.e. all data range between 0 and 100%. The *logratio* transform of particle-size distribution p is given as:

$$a = clr(p) = \left[\log\left(\frac{p_i}{g(p)}\right)\ldots\log\left(\frac{p_D}{g(p)}\right)\right] \qquad (1)$$

where a is the logratio transform of p, a D-part particle-size distribution, i is the i^{th} category and $g(p)$ is the geometric mean of particle-size distribution p. Each operator estimate considered here is a four-part particle-size distribution.

Accuracy is defined here as the median error ($\tilde{e}$) and precision as the standard deviation of the error (σ).

Operator bias

Operator estimates of the relative proportions of gravel, sand, silt and clay were made by three laboratory technicians each trained at the Geological Survey of the Netherlands. This study attempts to identify whether the operator estimates made were consistent between operators or if the estimates varied systematically with each operator. The existence of operator bias was assessed using a Wilcoxon rank-sum test to compare operator sub-populations of accuracy and precision scores. The Wilcoxon rank-sum test is a non-parametric test suitable for comparing different sized populations with non-Gaussian distributions.

Modelling particle-size distributions

The approach adopted in this study to converting visual estimates of sediment particle-size to a quantitative particle-size distribution is straightforward. The procedure is illustrated in Fig. 1 and described below (eqns 2 and 3). A D-part cumulative percentage-frequency distribution [X_1, Cf_1 … X_D, Cf_D] is calculated by the following series:

$$Cf_1 = P_l \qquad (2a)$$
$$Cf_2 = P_l + P_s \qquad (2b)$$
$$Cf_3 = P_l + P_s + P_z \qquad (2c)$$
$$Cf_4 = P_l + P_s + P_z + P_g \qquad (2d)$$

where P_l, P_s, P_z and P_g are, respectively, the relative contributions of clay, silt, sand and gravel. The particle-sizes corresponding to these cumulative frequency values are given as $X_1 \rightarrow X_4$, respectively, the largest particle-size in clay, silt, sand and gravel fractions, given here as 2, 630, 2000 and 64,000 μm (see Fig. 1). The precise values of X are dependent upon the sediment particle-size classification system used. While [X_4 , Cf_4] defines the upper limit of the distribution, it is also pragmatic to constrain the lower

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limit [X_0, Cf_0], where Cf_0 is zero and X_0 is a theoretical minimum particle-size. Given that the smallest particle detected by the Fritsch Analysette 22 XL is 13.25 φ (0.1 μm), X_0 is defined here as 14 φ (0.06 μm).

Depending on particular circumstances, the modelling process described above may require further adjustments peculiar to each data set. It is recommended that as much data as are available should be used to constrain cumulative-frequency distributions, rather than identifying a set of commonly available particle-size classes, as in Skaggs et al. (2001) for example. In addition, estimates of the median particle-size (D_{50}) can be directly inserted into the distribution series (Fig. 1). Median particle-size estimates for specific size fractions can also be inserted by assuming that cumulative frequency values are equidistant from both the upper and lower limits of the size fraction. For example, the cumulative frequency corresponding to the median particle-size of the sand fraction, the sand median (M_{63}), can be defined as:

$$Cf_3 = \frac{Cf_2 - Cf_3}{2} + Cf_3 \tag{3}$$

where Cf_{zm} is the cumulative frequency of the sand median. In some cases the introduction of additional input points may result in data conflicts. A common example would be when the estimated median grain size is not in agreement with estimates of gravel, sand, silt and clay proportions. Weltje & Roberson (2012) provide a solution using the Iman & Conover (1982) rank regression method, which uses a simple ranking method to reorder non-monotonically increasing data in cumulative percentage-frequency distributions.

Once a cumulative-frequency distribution has been constructed using all the available data, intermediate cumulative-frequency values can be predicted for any given set of particle-sizes using a suitable model. In this study a range of models are compared to establish which is most suitable for modelling continuous particle-size frequency distributions.

Model comparisons

Five different algorithms are used in this study to model particle-size distributions from sparse data: (i) a four-part Pearson's probability distribution function (Johnson et al., 1994), (ii) a linear interpolation of log-transformed cumulative-frequency distribution, (iii) a linear interpolation of a logit-transformed cumulative-frequency distribution after Bagnold & Barndorff-Nielsen (1980), (iv) a logistic function following Skaggs et al. (2001) and (v) Weltje & Roberson's (2012) constrained cubic-spline (logit-CCS) algorithm. Weltje & Roberson's (2012) algorithm is freely distributed as part of a Matlab toolbox, available at *http://particlesizetoolbox.wikipages.com*.

To allow unbiased comparisons to be made, each of the models (with the exception of the Gaussian distribution function) was run using the four particle-size categories defined by Skaggs et al. (2001): the relative proportions of clay, silt, very fine sand and fine sand. It should be noted that while the logistic model combines the proportions of very fine sand and fine sand into a single class, the three interpolation functions use these two classes independently. In contrast, the Pearson distribution function is run using the first four moments of each particle-size distribution (mean, standard deviation, skewness and kurtosis) calculated from measured laser analysis data (Folk & Ward, 1957).

Model performance was assessed by comparing the predicted distributions with those measured by laser analysis using the normalised distance (ND) statistic. The normalised distance between two logratio particle-size distributions **a** and **b** is given as:

$$ND_{(\mathbf{a},\mathbf{b})} = \frac{1}{D-1} \cdot \left[\sum_{D}^{i} \left(\frac{\ln b_i}{\sqrt[D]{b_1 \ldots b_D}} - \frac{\ln a_i}{\sqrt[D]{a_1 \ldots a_D}} \right)^2 \right] \tag{4}$$

where D is the number of particle-size categories, **a** is the logratio of a modelled distribution and **b** is the logratio of a distribution measured by laser analysis. Overall model accuracy is defined as the median ND score and model precision as the standard deviation of ND scores.

Results and discussion

Accuracy and precision of operator estimates

The accuracy and precision of operator estimates of sediment particle-size are presented as summary statistics (Table 1), box plots (Fig. 2), ternary diagrams (Fig. 3) and an additive logratio plot (Fig. 4). Table 1 and Fig. 2 both show that on average the relative proportions of gravel and sand were overestimated and correspondingly that the relative proportions of silt and clay were underestimated. Operator estimates were

Table 1. Median error and error variance of visual descriptions of sediment texture shown for each operator and for all samples.

	Operator 1		Operator 2		Operator 3		All samples	
	$\tilde{e}$	σ	$\tilde{e}$	σ	$\tilde{e}$	σ	$\tilde{e}$	σ
n	2557		311		360		4885	
$\tilde{N}D$	2.03		2.01		2.03		2.02	
Gravel	0.60	3.39	0.62	3.52	0.01	3.44	0.34	3.34
Sand	0.93	4.79	0.61	5.13	0.56	4.77	0.88	5.07
Silt	−0.18	2.71	−0.22	2.92	0.39	2.49	−0.13	2.90
Clay	−1.17	5.03	−0.91	5.16	−0.95	5.19	−1.02	5.08

Error is calculated as the difference between the log-ratio proportions of gravel, sand, silt and clay measured by laser analysis and estimated by visual description.
$\tilde{N}D$ is the median normalised compositional distance between operator estimates of the proportions of gravel, sand, silt and clay measured by laser analysis and estimated by visual description, a measure of overall operator accuracy.

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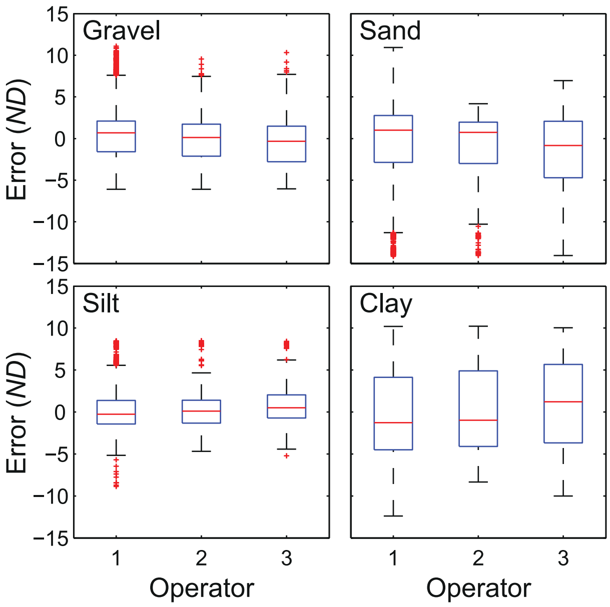

Fig. 2. Box-plots showing the distribution of error (ND) in operator estimates for relative proportions of: gravel, sand, silt and clay made by three different operators. The central mark is the median (accuracy), the edges of the box are the 25th and 75th percentiles, and the whiskers extend to the 99% confidence interval of the population. Outliers are plotted individually as red crosses. A Wilcoxon rank-sum test demonstrated that there was no significant difference between the accuracy or precision of operator estimates for different operators at a 95% confidence level.

least accurate and least precise when estimating the relative proportions of sand, followed by clay, gravel and silt. The comparatively high accuracy and precision of the gravel estimates may suggest that gravel particles can be identified relatively easily, although this could also reflect the low proportion of samples with gravel in them (<4%). The overall goodness-of-fit between the operator estimates and laser measurements was calculated using the ND statistic (eqn 4), giving a median value of 2.02 and a standard deviation of 1.55. The distribution of error is shown for each operator in Fig. 2 as a series of box plots. A piecewise one-sample Kolmogorov–Smirnov test indicated that none of the error populations are normally distributed ($p \approx 0$), so the median error $(\tilde{e})$ rather than the mean is used here as a measure of accuracy. The precision of operator estimates is given as the standard deviation of the error (σ) (see Table 1).

The relative proportions of sand, silt and clay recorded by operator estimates and measured by laser analysis are compared by plotting both data sets on a traditional ternary diagram (Fig. 3B). The distribution of the operator estimates (black crosses) reflects that they are made to the nearest 5 to 1%. In spite of this limitation, the operator estimates exhibit a very similar range to the measured laser analysis data. However, because most of the data measured by laser analysis have relative proportions of sand >95% the similarity of the two data sets is difficult to see visually on a ternary diagram. This problem can be addressed by applying a logratio transform to the data,

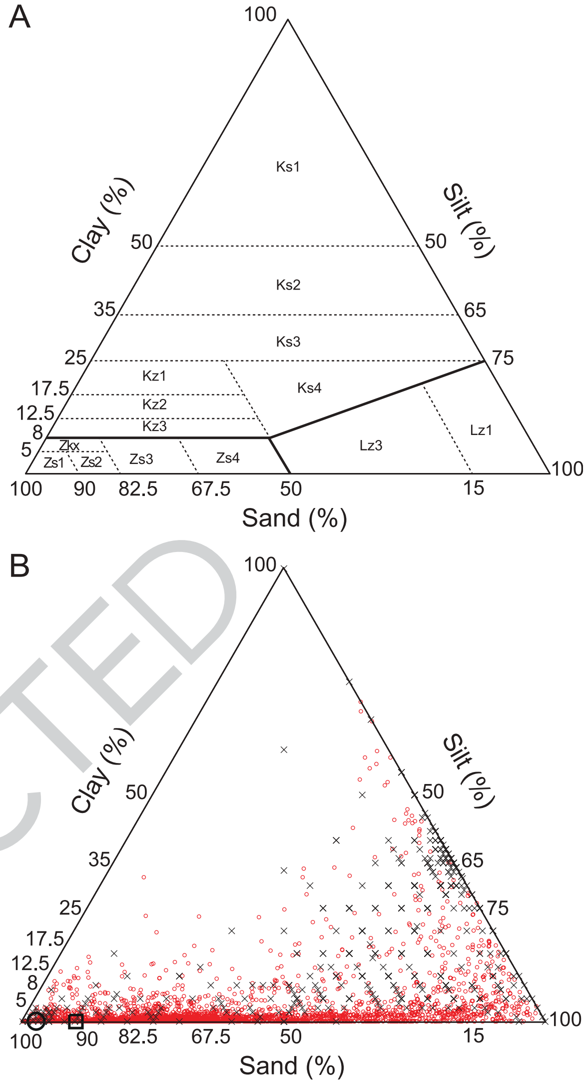

Fig. 3A. Ternary plot showing the Dutch sediment classification system for fine sediments (NEN5104). B. Ternary plot showing the relative proportions of sand, silt and clay measured by laser analysis (red circles) and estimated by operators (black crosses). The median compositions of both groups are indicated by a black square (laser analysis) and a black circle (operator estimates). Operator estimates replicate the full range of the measured data, but are limited in terms of their accuracy, i.e. they are made to the nearest 5–1%.

allowing the variability around the median (black square) to be seen with greater clarity (Fig. 4). Fig. 4 shows that there is a great deal of variability around the median of the laser measurements. In contrast, values recorded by operator estimates cluster very closely around the median, indicated by a black circle. Furthermore, the inability of operators to make estimates more accurate than 1% has a profound impact on modelling spatial trends in particle-size data because mathematically the relative difference between 0 and 1 is enormous.

The use of operator estimates has frequently been justified by the argument that they are more spatially representative of sedimentary environments than sparse laboratory samples.

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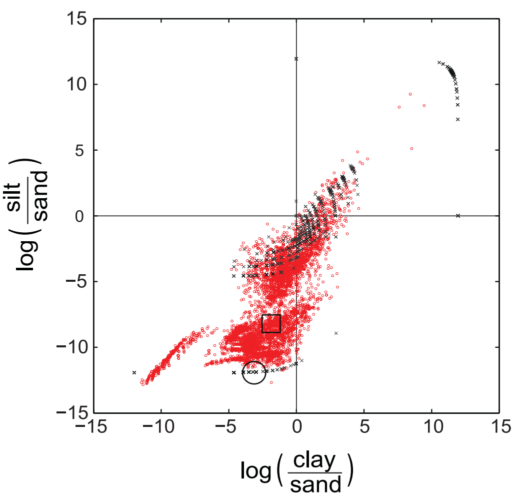

Fig. 4. Bivariate scatterplot showing the logratio of clay to sand against the logratio of silt to sand for all samples measured by laser analysis (red circles) and operator estimates (black crosses). The median compositions of both groups are indicated by a black square (laser analysis) and a black circle (operator estimates). Although operator estimates span the same range as the measured laser analysis data, they fail to characterise the majority of the data variability around the median in the lower left quadrant of the plot.

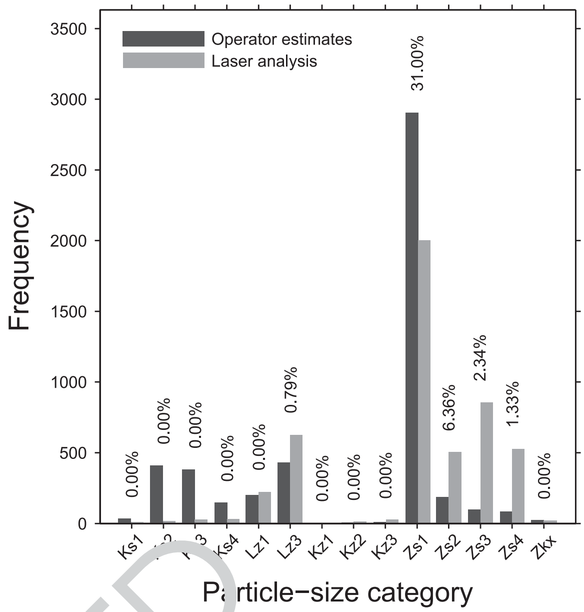

Fig. 5. Histogram comparing the classification of samples following the Dutch scheme for fine sediments (NEN5104) using operator estimates and laser analysis. The success rate of classifications made using operator estimates is given for each category as percentage scores. Note that many of these scores are zero because some samples have been placed in the wrong size category.

However, in this study rather than capturing geological heterogeneity operator estimates create a misleading characterisation. Inaccuracies in operator estimates are likely to result in geological inconsistencies and limit the extent to which spatial trends and hence sedimentary processes can be modelled owing to the introduction of noise; a high nugget effect in geostatistical terms. Small variations in particle-size distributions reflect changes in natural processes over space and time, including sediment deposition, erosion and mixing. The low resolution of operator estimates (<5%) restricts the extent to which the spatial trends in subsurface sediment particle-size can be modelled. This introduction of noise increases the overall uncertainty involved in geological modelling. Sediment samples were also classified according to the Dutch system for natural sediments (NEN5104 (Anonymous, 1989, 1990)) using both operator estimates and laser measurements of the relative proportions of sand, silt and clay (Fig. 3A). The Dutch classification system for fine sediment facies consists of 14 categories focused towards sand-rich facies. Comparing the two sets of results reveals that classifications made using operator estimates have an overall success rate of just 14%. The rate of successful classification is shown for each particle-size category, given as percentage values above each category (Fig. 5). Fig. 5 shows that the most precise operator estimates are made for silty sand particle-size categories, which also coincide with the largest number of samples. Of these, the category most precisely estimated is the slightly silty sand (Zs1), with a success rate of 31%. The other silty sand categories (Zs2, Zs3 and Zs4) have much lower classification success rates of 6.3%, 2.3% and 1.3%, respectively. The number of operator estimates for the silty clay categories (Ks1, Ks2, Ks3 and Ks4) is much higher than the number measured by laser analysis. At the same time the classification success rate of operator estimates for these categories is 0%. This suggests that it is very difficult to accurately estimate the relative proportions of clay and silt. These results are at odds with similar studies by Foss et al. (1975) and Post et al. (1986), who respectively reported 50% and 46% success rates in operator estimates using the USDA soil classification system. The comparatively low success rate possibly reflects the larger number of particle-size categories in the Dutch standard NEN5104 and its focus towards sand-rich categories. Operator estimates are typically made to the nearest 5%, hence differentiating between the four closely spaced categories Zs1, Zs2, Zkx and Zz3 can be problematic (Fig. 3A). Previous studies into operator estimates have shown that both accuracy and precision could be improved by training (Post et al., 1986, 2006). This suggests that investing in operator training could be a cost-effective means of improving the accuracy of geological models and soil maps.

It is appropriate at this stage to note that the NEN5104 classification system was developed for samples analysed by both sieve and pipette analysis (NEN5753 (Anonymous, 1994)). The uptake of laser granulometry technologies in laboratories has spawned an extensive literature dealing with conversion to and from this established standard. Conversion between these two analytical approaches is a necessary step because of the fundamental differences in the way that particle-size is measured. For example, laser granulometry relies on the diffraction

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and refraction of light through particles suspended in a flowing medium, while pipetting measures the concentration of sediment over time within a stationary water column. One of the impacts of these differences is that the clay fraction has a tendency to be overestimated by laser granulometry relative to sieve-pipette measurements. This is most often the result of platy clay minerals. The approach of most researchers to solving this issue has been to calculate a series of linear regression coefficients to convert percentage values measured by one technique to percentage values measured by the other (Konert & Vandenberghe, 1997; Beuselinck et al., 1998; Goossens, 2008). Roberson & Weltje (2014) use quadratic regression in combination with logratio-transformed data to address differences observed between sieve-pipette and laser measurements. This successfully avoids problems of predicting impossible percentage values, while allowing for a conversion method that incorporates data from adjacent size classes. The methods of Roberson & Weltje (2014) are used here to convert laser measurements to a sieve-pipette standard, using a replicate data set of 138 Dutch sediment samples (see Roberson & Weltje (2014) for further details). The converted laser data are then classified according to NEN5104 and compared to the classification made using operator estimates. The classifications made using the converted laser data indicate that the operator estimates have an accuracy of 16.68%. This negligible improvement can be explained by the comparative difference between operator estimates, sieve-pipette measurements and laser measurements. The median ND between operator estimates and laser measurements in this study is 2.02, while Roberson & Weltje (2014) calculate the median ND between sieve-pipette and laser measurements for their set of duplicate samples as 0.35.

Operator bias

The influence of operator bias was assessed using a Wilcoxon rank-sum test. The test indicated that there was no significant difference between the observations of the three different operators for each of the four parameters estimated (the relative proportions of gravel, sand, silt and clay) at a 95% confidence level. This statistic is supported by the consistent levels of operator accuracy (median ND, see Table 1), which are 2.03, 2.01 and 2.03 for operators 1, 2 and 3, respectively.

The number of samples processed by each operator is sufficiently large to exclude the possibility of any of them being under-represented (Table 1). However, the limited number of operators investigated by this study does not provide sufficient evidence to make generalisations about bias in operator estimates of sediment particle-size, particularly when all the operators worked in the same laboratory and received similar training. This limitation does not make the results of this test invalid, however, rather it demonstrates that operators at the Geological Survey of the Netherlands have all been trained to a consistent standard.

Model performance

This section compares the performance of five different models used to calculate complete particle-size distributions from limited percentage-frequency data. Data measured by laser analysis are used rather than operator estimates to remove the influence of operator error on the modelling process. The five different models compared are (i) a four-part Pearson's probability distribution, (ii) a log-linear interpolation, (iii) a logit-linear interpolation after Bagnold & Barndorff-Nielsen (1980), (iv) Skaggs et al.'s (2001) logistic probability distribution function and (v) Weltje & Roberson's (2012) logit-CCS interpolation algorithm.

The accuracy and precision of the particle-size distributions generated by each model are summarised respectively as the median ($\tilde{e}$) and standard deviation (σ) of the ND scores (Table 2). Median ND (accuracy) scores for all samples are very alike, ranging from 0.345 for the logit-CCS interpolation function to 0.459 for the log-linear model. Precision scores for each model are also comparable, ranging from 1.365 for the log-linear model to 1.524 for the four-part Pearson's model.

Model performance statistics for a range of different distribution types (Gaussian, skewed, peaked and bimodal) are also given in Table 2. These are illustrated for a series of randomly selected distributions in Fig. 6. The performance of the different models, on average, is very consistent for Gaussian, skewed and peaked (leptokurtic) distribution types. The logistic

Table 2. Comparison of different particle-size distribution model performances.

	All samples		Gaussian		Skewed		Leptokurtic		Bimodal	
	$\tilde{e}$	σ	$\tilde{e}$	σ	$\tilde{e}$	σ	$\tilde{e}$	σ	$\tilde{e}$	σ
Pearson's	0.349	1.524	0.348	1.932	0.389	1.500	0.364	1.813	0.677	0.196
Log-linear	0.459	1.365	0.484	1.877	0.424	1.147	0.464	1.583	0.358	0.074
Logit-linear	0.417	1.376	0.362	1.887	0.481	1.149	0.410	1.590	0.776	0.174
Logistic	0.392	1.388	0.298	1.891	0.399	1.178	0.413	1.599	0.554	0.180
Logit-CCS	0.345	1.374	0.335	1.888	0.354	1.153	0.344	1.593	0.323	0.069

Model accuracy and precision are quantified as median and standard deviation of ND scores between modelled distribution and measured distribution. Model performance is summarised for all samples as well as a range of different distribution types, including normal Gaussian distributions, skewed distributions, leptokurtic (peaked) distributions and bimodal distributions.

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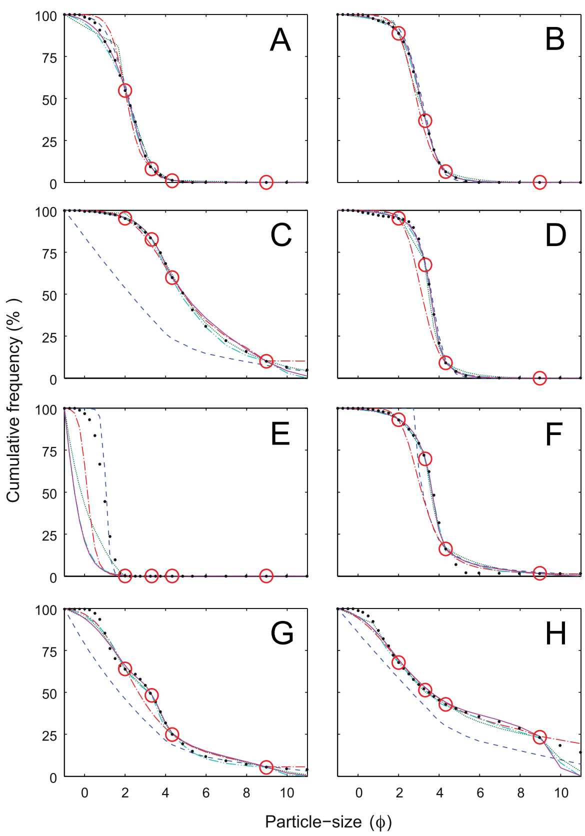

Fig. 6. Cumulative-frequency plots comparing distributions modelled from sparse input data (red circles) against measured distributions (black dots). The different algorithms used are (i) four-parameter Pearson's probability distribution function (blue dash), (ii) log-linear (green dot), (iii) logistic (red dot-dash), (iv) logit-linear (cyan dot-dash) and (v) logit-CCS (magenta solid). Models are shown for a range of distribution types: A, B, symmetric Gaussian distributions; C, fine skewed; D, coarse skewed; E, F, leptokutic (peaked); G, H, bimodal.

model in particular is a very accurate method for modelling normal Gaussian distributions ($\tilde{e}$ = 0.298).

However, when dealing with bimodal distributions, the performance of Pearson's, logit-linear and logistic models are markedly reduced, with median accuracy scores of 0.67, 0.78 and 0.55, respectively. The reduction in performance of the Pearson's model is expected, given that the model assumes unimodality. This means that markedly different distributions may be characterised by the same distribution moments. The relatively poor performance of the logit-linear model when predicting bimodal distributions is more difficult to account for, given the performance of the very similar logit-CCS model. The underlying cause lies in the linear extrapolation of the distribution tails in logit space. This leads to mathematical difficulties because logit values outside the range −7 to 7 (the equivalent of 0.1–99.9%) are often predicted, creating truncated distributions. The reduced performance of the logistic when dealing with bimodal distributions is also anticipated because of the fixed nature of the exponential function coefficients. While the form of the coefficients allows for skewed, peaked and broad distributions, no provision for bimodality is included (Fig. 6G).

In contrast, both log-linear and logit-CCS models show improved performance when predicting bimodal distributions (e.g. Fig. 6G). Median accuracy scores for log-linear and logit-CCS are improved to 0.36 and 0.32, respectively. The high performance of both of these models highlights the advantages of interpolation functions over probability distribution functions, i.e. fewer a priori assumptions about distribution shape are made. The contrast in performance between the logit-linear and logit-CCS models demonstrates the effectiveness of Weltje & Roberson's (2012) adaptive non-linear extrapolation algorithm (Weltje & Roberson, 2012, their eqn 11).

Model comparisons demonstrate that the logit-CCS interpolation algorithm is at present the best available method for modelling particle-size distributions from limited textural data. In addition to the higher levels of accuracy offered by the logit-CCS model, an interpolation-based approach offers the clear advantage that any size-frequency data can be used to build the distribution model, rather than relying on specific grain size classes. This makes the method considerably more widely applicable and furthermore avoids the need to condition empirical constants for specific particle-size fractions in the manner of Skaggs et al. (2001). It is worth noting that the interpolation method presented by Weltje & Roberson (2012) is considerably more complex than the standard log-linear approach and is currently only available as a Matlab function. In the absence of sufficient resources to run the logit-CCS algorithm, operators are advised to use the log-linear interpolation to model complete particle-size distributions, rather than alternative empirical functions.

Modelling particle-size distributions from operator estimates

The logit-CCS interpolation algorithm (Weltje & Roberson, 2012) was used to predict complete particle-size distributions (32 particle-size categories) from operator estimates of sediment particle-size taken from the data set of Dutch samples. The robustness of the predicted distributions are assessed by comparing them each to their respective particle-size distributions measured by laser analysis (Fig. 7). On average, modelled distributions are in better agreement with the distributions measured by laser analysis (median ND = 0.62) than the original operator estimates (median ND = 2.02). The accuracy of the Fritsch Analysette particle-sizer has been established previously by other studies (Jonkers et al., 2009; Weltje & Roberson, 2012). The results of this study indicate that distributions modelled using operator estimates are approximately six times less accurate than the Fritsch Analysette 22-XL system. Fig. 7 shows plots of eight randomly selected cumulative frequency distributions modelled from observer estimates plotted alongside their respective distributions measured by laser analysis. ND scores for the modelled distributions are shown for each plot. For samples

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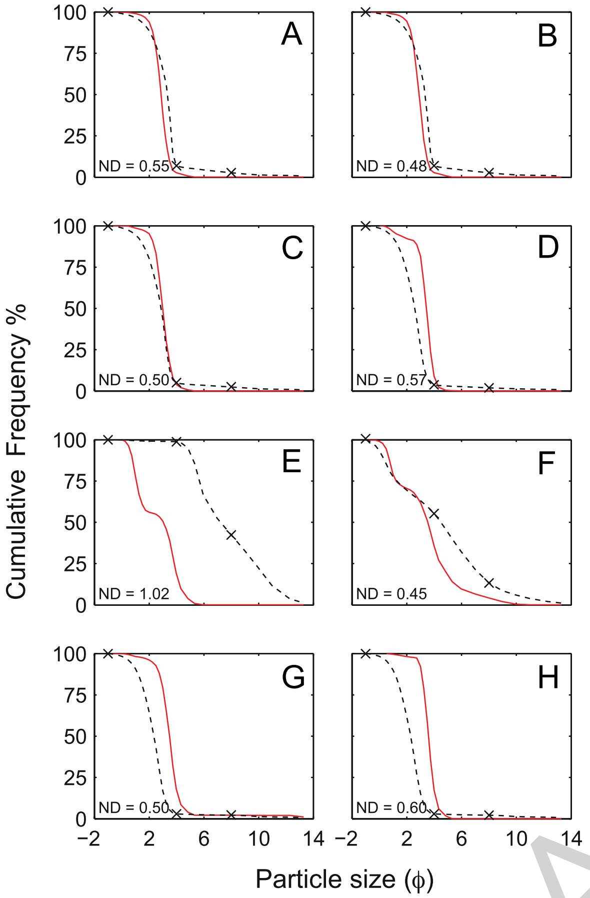

Fig. 7. Cumulative-frequency plots comparing particle-size distributions modelled from operator estimates (black dashed lines) with those measured by laser analysis (solid red lines). Note that for the modelled distributions shown operator estimates (black crosses) of the gravel fraction were zero and are not plotted. Samples were selected to show model performance for a range of distribution types: A, B, Gaussian; C, low standard deviation; D, high standard deviation; E, low skewness; F, high skewness; G, low kurtosis; H, high kurtosis. ND values indicate goodness-of-fit between the measured and predicted distributions. Lower scores indicate a better model fit.

where observer estimates are in good agreement with the data, the modelled particle-size distributions perform well (ND < 0.5). Conversely, if inaccurate input data are supplied, an inaccurate particle-size distribution model is predicted (Fig. 7E). Model performance is therefore dependent upon the capacity of operators to accurately estimate a range of particle-size classes. This limitation means that the application of relatively complex interpolation algorithms (e.g. the logit-CCS interpolation) to modelling particle-size distributions is unwarranted, as the operator estimates themselves are orders of magnitude less precise than the comparative performance of the different interpolation methods.

Conclusions

1. Comparisons of operator estimates of sediment particle-size with particle-size distributions measured by laser analysis show the former to be inaccurate and imprecise. Operator estimates yield a classification success rate of only 16.68% of samples using the Dutch classification of fine sediments. The classification success rate is probably limited by the large number of sand-rich classes in the Dutch system (NEN5104). Although operator estimates encompass the same range of percentage-frequency values measured by laser analysis, the heterogeneity of the estimated data does not match that of the measured data due to the limited accuracy of operator estimates, i.e. mostly the nearest 1–5%. Although this level of accuracy is excellent for operator estimates, it does not allow a geological modeller to capture the full variability of the data, hence many of the subtleties of sedimentary processes may be lost.
2. Operator bias is not a significant influence on estimates of sediment particle-size for the 4837 Dutch sediment samples analysed by three different operators. Although this is a relatively small number of operators compared to similar studies, the results demonstrate that the laboratory technicians at the Geological Survey of the Netherlands have been trained to a very similar standard.
3. Goodness-of-fit statistics (ND) show that for sediment samples from the Dutch shallow subsurface there is very little difference in performance between the five models used to predict complete particle-size distributions from sparse data: (i) a four-part Pearson's probability distribution function (Johnson et al., 1994), (ii) a linear interpolation of log-transformed cumulative-frequency distribution, (iii) a linear interpolation of a logit-transformed cumulative-frequency distribution after Bagnold & Barndorff-Nielsen (1980), (iv) a logistic function following Skaggs et al. (2001) and (v) Weltje & Roberson's (2012) constrained cubic-spline (logit-CCS) algorithm. ND scores also show that the performance of each of these models is not markedly affected by skewed or peaked distributions. However, the performance of Pearson's four-part probability distribution function, the logit-linear interpolation function and Skaggs et al.'s (2001) logistic function is reduced when dealing with bimodal distributions. In contrast, the performance of both the standard log-linear interpolation function and Weltje & Roberson's (2012) logit-CCS interpolation function is increased when predicting bimodal particle-size distributions. While, for a broad range of samples, both the probability distribution functions of Pearson and Skaggs et al. (2001) perform well, neither of these methods are able to accurately predict bimodal particle-size distributions. Of the five models used, the logit-CCS interpolation algorithm is the most consistently accurate model (Weltje & Roberson, 2012). Interpolation algorithms are considered to be much more practical than empirical distribution functions (Skaggs et al., 2001) as they are able to incorporate all available input data, rather than relying on a specific range of grain-size classes.
4. This study demonstrates a straightforward method for modelling complete particle-size distributions from operator estimates of sediment particle-size. However, the accuracy and precision

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of the modelled distributions are limited by the shortcomings of operator estimates. On average, predicted particle-size distributions are six times less accurate than corresponding laboratory analyses made by a Fritsch Analysette 22-XL. This large error margin demonstrates that relatively complex models (e.g. the logit-CCS interpolation) do not offer tangible improvements over the standard log-linear interpolation approach when making predictions of particle-size distributions from operator estimates.

Acknowledgements

The authors would like to thank the Geological Survey of the Netherlands for access to their sediment database. This research was conducted when SR was a post-doctoral research fellow at Delft University of Technology. The comments of Jeroen Schokker and two anonymous referees have helped to greatly improve the clarity of this manuscript.

References

Aitchison, J., 2003. A concise guide to compositional data analysis. *In:* Pawlowlsky-Glahn, V. and Barceló –Vidal, C. (eds). CODAWORK'03. Departament d'Informática i Matemática Aplicada, Universitat de Girona (Girona): p. 134.

Anonymous, 1989. NEN 5104:1989, Geotechnics: Classification of unconsolidated soil samples. Netherlands Normalization Institute (Delft): 24 pp.

Anonymous, 1990. NEN 5104:1989/C1, Geotechnics: Classification of unconsolidated soil samples. Netherlands Normalization Institute (Delft): 1 pp.

Anonymous, 1994. NEN 5753:1994, Soil: Determination of clay content and particle size distribution of soil samples by sieve and pipette. Netherlands Normalization Institute (Delft): 33 pp.

Bagnold, R. & Barndorff-Nielsen, O., 1980. The pattern of natural size distributions. Sedimentology 27: 199-207.

Barndorff-Nielsen, O., 1978. Hyperbolic distributions and distributions on hyperbolae. Scandinavian Journal of Statistics 5: 151-157.

Beuselinck, L., Govers, G., Poesen, J., Degraer, G. & Froyen, L., 1998. Grain-size analysis by laser diffractometry: comparison with the sieve-pipette method. Catena 32(3–4): 193-208.

Bosch, J.H.A., 2000. Standaard Boor Beschrijvingsmethode. Technical Report NITG 00-141-A, Nederlands Instituut voor Toegepaste Geowetenschappen: TNO: 106 pp.

Church, M.A., McLean, D. & Wolcott, J., 1987. River bed gravels: sampling and analysis. *In:* Sediment Transport in Gravel-Bed Rivers. John Wiley and Sons (New York): pp. 43-88.

Dexter, A. & Tanner, D., 1972. Packing densities of mixtures of spheres with log-normal size distributions. Nature 238(80): 31-32.

Fieller, N., Flenley, E. & Olbricht, W., 1992. Statistics of particle size data. Journal of the Royal Statistical Society. Series C (Applied Statistics) 41(1): 127-146.

Folk, R., 1966. A review of grain-size parameters. Sedimentology 6(2): 73-93.

Folk, R. & Ward, W., 1957. Brazos River bar [Texas]: a study in the significance of grain size parameters. Journal of Sedimentary Research 27(1): 3-26.

Foss, J., Wright, W. & Coles, R., 1975. Testing the accuracy of field textures. Soil Science Society of American Proceedings 39: 800-802.

Fredlund, D. & Houston, S., 2009. Protocol for the assessment of unsaturated soil properties in geotechnical engineering practice. Canadian Geotechnical Journal 46(6): 694-707.

Fredlund, M., Fredlund, D. & Wilson, G., 2000. An equation to represent grain-size distribution. Canadian Geotechnical Journal 37(4): 817-827.

Goossens, D., 2008. Techniques to measure grain-size distributions of loamy sediments: a comparative study of ten instruments for wet analysis. Sedimentology 55(1): 65-96.

Gruijters, S., Maljers, D. & Veldkamp, J., 2005. 3D interpolation of grain size distributions in the upper 5 m of the channel bed of three lower Rhine distributaries. Physics and Chemistry of the Earth, Parts A/B/C 30(4–5): 303-316.

Hengl, T., Toomanian, N., Reuter, H. & Malakouti, M., 2007. Methods to interpolate soil categorical variables from profile observations: Lessons from Iran. Geoderma 140(4): 417-427.

Hwang, S., Lee, K., Lee, D. & Powers, S., 2002. Models for estimating soil particle-size distributions. Soil Science Society of America Journal 66(4): 1143-1150.

Iman, R. & Conover, W., 1982. A distribution-free approach to inducing rank correlation among input variables. Communications in Statistics – Simulation and Computation 11(3): 311-334.

Johnson, N.L., Kotz, S. & Balakrishnan, N., 1994. Continuous Univariate Distributions, Vol.1. Wiley-Interscience (New York).

Jonkers, L., Prins, M., Brummer, G., Konert, M. & Lougheed, B., 2009. Experimental insights into laser diffraction particle sizing of fine-grained sediments for use in palaeoceanography. Sedimentology 56(7): 2192-2206.

Konert, M. & Vandenberghe, J., 1997. Comparison of laser grain size analysis with pipette and sieve analysis: a solution for the underestimation of the clay fraction. Sedimentology 44(3): 523-535.

Kozak, E., Sokołowska, Z., Stępniewski, W., Pachepsky, Y.A. & Sokołowski, S., 1996. A modified number-based method for estimating fragmentation fractal dimensions of soils. Soil Science Society of America Journal 60(5): 1291-1297.

Lark, R., Dove, D., Green, S., Richardson, A., Stewart, H. & Stevenson, A., 2012. Spatial prediction of seabed sediment texture classes by cokriging from a legacy database of point observations. Sedimentary Geology 281: 35-49.

Meilianda, E., Alfian, D. & Huhn, K., 2011. Sediment grain-size distribution analysis at the shallow sandy shelf of the North Sea using multivariate geostatistics. Procedia Environmental Sciences 7: 317-322.

Odeh, I., Todd, A. & Triantafilis, J., 2003. Spatial prediction of soil particle-size fractions as compositional data. Soil Science 168(7): 501-515.

Post, D., Huete, A. & Pease, D., 1986. A comparison of soil scientist estimations and laboratory determinations of some Arizona soil properties. Journal of Soil and Water Conservation 41(6): 421-424.

Post, D., Parikh, S., Papp, R. & Ferriera, L., 2006. Evaluating the skill of students to determine soil morphology characteristics. Journal of Natural Resources and Life Sciences Education 35: 217-224.

Roberson, S. & Weltje, G., 2011. 3D modelling of particle-size distributions in the shallow subsurface: Zeeland, The Netherlands. Proceedings of the International Association of Mathematical Geologists Congress, Salzburg 1: 708-718.

Roberson, S. & Weltje, G.J., 2014. Inter-instrument comparison of particle-size analysers. Sedimentology 1-18.

Schlee, J. & Webster, J., 1967. A computer program for grain-size data. Sedimentology 8(1): 45-53.

https://doi.org/10.1017/njg.2014.10 Published online by Cambridge University Press

Shirazi, M., Boersma, L. & Hart, J., 1988. A unifying quantitative analysis of soil texture: improvement of precision and extension of scale. Soil Science Society of America Journal 52: 181-190.

Silva, E., Lima, J., Rodrigues, L. & Azevedo, J., 2004. Comparison of mathematical models for fitting particle-size distribution curves. Pesquisa Agropecua' ria Brasileira 39(4): 363-370.

Skaggs, T., Arya, L.M., Shouse, L. & Mohanty, P., 2001. Estimating particle-size distribution from limited soil texture data. Soil Science Society of America Journal 65(4): 1038-1044.

Taguas, F., Martin, M. & Perfect, E., 2000. Simulation and testing of self-similar structures for soil particle-size distributions using iterated function systems. Developments in Soil Science 27: 101-113.

Vernes, R.W., Bosch, A.J., Harting, R., de Heer, E. & Griffioen, J., 2010. Towards a physical and chemical characterization of the shallow subsurface of the Netherlands. *In:* Ghose, R., Hassanizadeh, M., Leijnse, T. & Rijnarts, H.H.M. (eds). Proceedings of the First International Conference on Frontiers in Shallow Subsurface Technology. European Association of Geocientists & Engineers (Delft): 224 pp.

Walvoort, D. & De Gruijter, J., 2001. Compositional kriging: a spatial interpolation method for compositional data. Mathematical Geology 33(8): 951-966.

Weltje, G. & Roberson, S., 2012. Numerical methods for integrating particle-size frequency distributions. Computers and Geoscience 44: 156-167.

Wu, C. & Jet-Chau Chang, K., 2009. Evaluation of the gray model gm (1, 1) applied to soil particle distribution. Soil Science Society of America Journal 73(6): 1775.

https://doi.org/10.1017/njg.2014.10 Published online by Cambridge University Press