Author's response

This document includes

- Point-by-point response to the reviews
- a list of all relevant changes made in the manuscript
- a marked-up manuscript version

Referee #1

Revision of manuscript: On soil textural classifications and soil texture-based estimations The proposed manuscript discusses the applicability of different soil texture representations using different textural fraction triplets in order to estimate soil properties. The manuscript addresses relevant questions in the scope of SE and present novel data. The scientific methodology is sound and already published elsewhere, but I think it could be clearly outlined. It is difficult to follow the manuscript methods without reading preview papers from the author. The manuscript is written in a fluent English with the presence of minor misspellings, the number and quality of the provided references is appropriate, and abstract provides a comprehensive and concise summary. Neverthe- less, there are some points that need clarification before publication:

General response We appreciate very much the overall positive opinion of this reviewer and specific comments that are helpful for the manuscript improvement.

Referee comment	Author's response	Author's change in the ma-
	1	nuscript
The scientific methodology is	As the Reviewer suggests, we	The following text was in-
sound and already published	can clarify the description of	cluded in the revised ma-
elsewhere, but I think it could	the part of the methodology	nuscript: "The set of textu-
be clearly outlined. It is diffi-	that is already published, i.e.	ral data, together with the
cult to follow the manuscript	the iterated function forma-	entropy self-similarity assum-
methods without reading pre-	lism.	ption, unequivocally determi-
view papers from the author.		ne the PSD (Martín and
		Taguas, 1998). Based on the
		theorem of Elton (Elton,
		1987), the mass of soil with
		size particles within an inter-
		val J , may be computed using
		the IFS as follows: (a) take
		any starting value x_0 in I , (b)
		choose, at random, an integer
		number <i>i</i> of the index set 1, 2,
		5, with probability p_i , and de-
		Bepeat the random experi-
		ment in (b) and suppose the
		new outcome is i and set
		$x_2 = \varphi_i(x_1)$. If x_0, x_1, \ldots, x_n
		is the sequence obtained in
		this way and m_n is the num-
		ber of x_i 's which fall in J , the
		ratio m_n/n , approaches the
		mass of the interval J as the
		number of iterations n goes to
		infinity. In practice, the esti-
		mation of mass in the interval
		J is achieved quickly."
1) Abstract—line 4 and Con-	We agree with the comment.	The exact number 6240 will
clusion— line 10 state that	The numbers should be the	be used throughout the revi-
6300 soil samples were used	same throughout the manus-	sed manuscript
as experimental data, but the	cript.	
Materials and Methods sec-		
tion state that " a to-		
included " (line 2 – page		
3) Are authors rounding the		
number 6240? If so it would		
be better to state something		
like around 6200 or circa 6200		
2) The first phrase of Ma- te-	The first phrase of the "Ma-	This phrase will be elimina-
rials and Methods is identical	terials and methods" section	ted in the revised manuscript
to the one presented at Mar-	is not only identical to the	-
tin et al (2017a) -reference of	one presented at Martin et al.	
the present manuscript. Is the	(2017a), it also does not pro-	
intention stated the reason	perly reflect the focus and ob-	
for the use of the dataset?	jective of the work described	
The same reason as given in	in this manuscript.	
Martin et al (2017a)?		

Referee comment	Author's response	Author's change in the ma-
		nuscript
3) Section 2.2 presents the	We agree with the Referee's	A reference to all possible tri-
formation of all possible tri-	suggestion	plets, which are included in
plets using seven fractions.		table 3, was included at the
Maybe authors could present		end of section 2.2
a table with such triplets or		
point to table 3 where triplets		
are presented.		
4) Section 3.1—from line 14	We agree with the Referee's	The second and the third co-
addresses table 1 results. The	suggestion	lumns in Table 1 will be swap-
stated results are confusing	248802000	ped to prevent the confusion
Are the standard triplets on		in the table explanation in
the central column and 3-2-2		the text Also in the table
triplets on the right column?		the name of the first column
Is it the other way around?		was changed from "5-1-1' tri-
What is 5.1.1 triplet indice		plot" to "standard '5 1 1' tri
tod on table 1?		plet to standard 5-1-1 th-
ted on table 1:		
5) Discussion section—phase	I ne sentence nas been repn-	"Between reflected" has been
on line 14 ("Rather).	rased.	changed to "reflected."
Please rephrase it, because it		
is not clear.		
6) Discussion section—phrase	The caption in Fig. 2 had two	The abbreviation "mkm" on
on line 19 ("The diameter	errors.	the vertical axis has been
."). Is figure 2 supposed to		changed to " $\%$ ", and the sa-
illustrate what it is stated? I		me abbreviation at the hori-
cannot see it in the figure.		zontal axis has been changed
		to "mm".
7) Page 6—line 28. Reformu-	We agree with the Referee's	Page 6—line 28 has been re-
late because clearly there is	suggestion	formulated to: "When analy-
something missing.		zing the utility of traditio-
		nal sand-silt-clay triplet for
		classifying soils by their hy-
		draulic properties, Twaraka-
		vi et al. (2010) concluded
		that "from a philosophical
		perspective, the research furt-
		her stresses the need to re-
		visit and reevaluate the re-
		sults from the past in order
		to successfully move ahead in
		to the future of soil physics"
		Using a set of fixed hour
		darios botwoon toxture free
		tiong has been a predictive
		approach in the next Can-
		approach in the past. Consi-
		deration of textural fraction
	3	boundaries as flexible para-
		meters that can be task and
		dataset specific can provide
		additional insights on the role
		ot texture in soil functioning
		and ecological services."

Referee comment	Author's response	Author's change in the ma-
	-	nuscript
8) Figure 1 b) would benefit	We agree with the Referee's	The '3-3-2' triplet is mentio-
from putting 3-2-2 triplet on	suggestion	ned in the Fig. 1. caption be-
the caption.		fore "(b)".
9) Table 2 - "being not diffe-	We agree with the Referee's	The Table 2 title was re-
rent"?	suggestion	formulated to "Percentage of
		samples for which simulated
		and measured particle size
		distributions are not different
		at the 0.05 significance level."
Attached PDF file with the	Thanks again for the tho-	All the misspellings were co-
minor misspellings found on	rough and constructive re-	rrected.
the manuscript:	view.	

Referee #2

The manuscript is generally well written and aims to test the hypothesis if the use of fraction sizes in triplets with a size boundaries range different from the USDA stan- dard textural fraction triplet 'sand-silt-clay' allows a more accurate reconstruction of the particle size distribution for estimate some soil parameters. The manuscript is well researched and subject of this work is relevant for the scope of Solid Earth and suf- ficiently novel and interesting to warrant publication. Abstract provide a concise and complete summary and the number and quality of references are appropriate. All sec- tions of the manuscript (introduction, materials and methods, results, discussion and conclusions) are explicit and developed in an appropriate way. However sometimes the text is confused and there are some inconsistencies that need clarification. In the specific comments, I provide a few indications that illustrate these concerns, which I consider as minor revisions, and after fixing these problems this will be a very good paper whose publication I recommend without reservation.

General response: We appreciate the general positive characterization and important specific comments in this review.

Referee comment	Author's response	Author's change in the ma-		
	riution 5 response	nuscript		
Abstract: line 4 – "ovpori	We agree with the Referee's	The mismatch in number of		
montal data for 6300 soil sam	suggestion	samples was corrected and		
mental data for 0500 son sam-	suggestion	6240 is used as suggested by		
pies. The same occurs in		0240 is used as suggested by		
the Conclusions section in li-		the Reviewer.		
ne 10 – "for 6300 predomi-				
nantly". In the Materials and				
Methods section, authors in-				
cluded a total of 6240 soil				
samples in this study after ap-				
plication of a selection crite-				
ria (described in Martin et al.				
(2017a)). I think it's better to				
put the same value of samples				
included in the study, which				
is 6240.				
Line 5. 6 – "original ones in	There is no discrepancy bet-			
25 and 85% of cases" but in	ween the content of the line			
Results section -; page 4 line	5.6 and line $4/31$ because the			
31 - "bigger than $97%$ of the	line 5.36 refers to to the 2 -			
total" Why this difference?	$2-2^{\circ}$ triplet and Page 4 line			
totar . Why this difference.	2^{-2} triplet, and 1 age 4 mic			
	3 -1-3' triplets			
Line 6 – The triplet 'sand-silt-	We agree with the Beferee's	The "silt-sand" in line 6 was		
and' must be 'sand silt elsy'	suggestion	abanged to "gilt alay"		
Diagonation: Line 10 "The	The line 10 in diagonation in	Arria titlea more changed, the		
Discussion: Line 19 – The	I ne line 19 in discussion in-	Axis titles were changed: the		
diameter. medium sand" (li-	deed contradicts to the con-	abbreviation "mkm" on the		
ne 21). It's difficult to under-	tempt of Fig. 2, because axis	vertical axis was changed to		
stand this phrase by looking	titles are wrong (the first Re-	"%", and the same abbrevia-		
at figure 2! Figure 2 should	viewer noted this error too).	tion at the horizontal axis was		
illustrate the phrase? It's not		changed to "mm".		
very clear!				
There is a PDF file attached	Once again, thanks to this	Spelling errors will be correc-		
with some misspellings found	Reviewer for very helpful re-	ted as suggested in the atta-		
on the manuscript.	view.	ched PDF file.		

Referee #3

The objective of this manuscript was to test the hypothesis that other fraction sizes in the triplets may provide better representation of soil texture for estimating some soil parameters. This is a interested topic and the authors has provided a profound and sound research on this. The English of this manuscript is fluent and easy to follow. In addition, this study was based on a large data set with 6300 soil samples. the previ- ous reviewers have provided valuable suggestions and comments for this manuscript. Therefore, I found this manuscript can be accepted for publication once the following comments are addressed. **General response:** We are grateful to the reviewer for the positive evaluation of the work and for stimulating comments.

Bibliography used

- Bird, N. R. A., Perrier, E., & Rieu, M. (2000). The water retention function for a model of soil structure with pore and solid fractal distributions. European Journal of Soil Science, 51(1), 55-63.
- Fredlund, M. D., Fredlund, D. G., & Wilson, G. W. (2000). An equation to represent grain-size distribution. Canadian Geotechnical Journal, 37(4), 817-827.
- Martín, MA., Taguas, FJ.: Fractal modelling, characterization, and simulation of particle-size distribution in soil. Proc. R. Soc. London A 454, 1457-1468 (1998)
- Martín, MA., Rey, JM., Taguas, FJ.: An entropy-based parametrization of soil textures via fractal modelling of particle-size soil distribution. Proc. R. Soc. London A 457, 937-947 (2001)
- Posadas, A. N., Giménez, D., Bittelli, M., Vaz, C. M., & Flury, M. (2001). Multifractal characterization of soil particle-size distributions. Soil Science Society of America Journal, 65(5), 1361-1367.

Referee comment	Author's response	Author's change in the ma-
		nuscript
1. when we use pipette met-	The Comment 1 requests	
hod or sieve method to test	the information about models	
the particle size distribution,	suitable to do reconstruct the	
we only get limited frac-	detailed particle size distri-	
tions. The authors used a self-	bution from a limited num-	
similarity model to recons-	ber of textural fractions con-	
truct the distribution of par-	tents. The self-similarity mo-	
ticle size distribution based	del of this work was chosen	
on the limited fractions. Ho-	mostly because the authors	
wever, I am wondering whet-	have an experience of working	
her there are other models to	with it, past applications of	
do this job? Why the authors	it appeared to be successful,	
selected this model? Have you	and a hypothetical physical	
or other studies compared dif-	explanation of its applicabi-	
ferent models?	lity can be put forward (Mar-	
	tin & Taguas, 1998; Martin	
	et al., 2005). There are other	
	models of particle size distri-	
	bution in soils based on sca-	
	ling hypothesis (Posadas et	
	al., 2001, Bird et al., 2000).	
	There exists a line of studies	
	in which the detailed parti-	
	cle size distribution is obtai-	
	ned by fitting various empi-	
	rical non-linear equations to	
	the data (Fredlund et al.,	
	2000). It should be interesting	
	to how this methodology may	
	work with textural triplets ot-	
	her than standard 'sand-silt-	
	clay' It may well be that the	
	efficiency of using various tri-	
	plets depends on/not only on	
	the task at hand – reconstruc-	
	tion of the detailed particle si-	
	ze distribution – but also on	
	the technique or model used	
	to perform the task.	
2. what kind of linear regres-	Comment 2 indicates the	The phrase "linear regession"
sions were used in this study,	need to clearly define the ty-	was chaged to "least squares
as well as the other statistical	pe of linear regression used in	linear regression".
methods, should be included	this work.	_
in the M&M section.		

Referee comment	Author's response	Author's change in the ma-			
		nuscript			
3. This manuscript tested the hypothesis for estimation bulk density. But people may be more curios about other properties like soil hydrau- lic properties. will this new law of particle size fractions will work fine for these pa- rameters? maybe the authors should include this in the dis- cussion.	This comment indicates that modified textural triangle may provide better inputs for pedotransfer functions to estimate soil hydraulic properties. This is definitely an exciting avenue for further research.	This was acknowledged in the article by changing page 6 paragraph to: "Usability of triplets other than standard ones indicate the opportu- nity of a more efficient use of existing results of textu- ral analysis. Although the- se results traditionally con- sist of seven fractions inclu- ding five fractions of sand, in the majority of applica- tions all sand fractions ha- ve been lumped together. For example, the overwhelming majority of pedotransfer fun- ctions in soil hydrology use the elements of the stan- dard triplet 'sand-silt-clay' (Pachepsky and Rawls, 2004). The use of different 'coarse- intermediate-fine' triplets in pedotransfer studies allows the use of available detailed data on fractions of sand and revisiting existing databases. Overall, application of nons- tandard textural triplets in development of pedotransfer functions presents an interes- ting avenue to explore."			

On soil textural classifications and soil texture-based estimations

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Abstract. The soil texture representation with the standard textural fraction triplet 'sand-silt-clay' is commonly used to estimate soil properties. The objective of this work was to test the hypothesis that other fraction sizes in the triplets may provide better representation of soil texture for estimating some soil parameters. We estimated the cumulative particle size distribution and bulk density from entropy-based representation of the textural triplet with experimental data for 6300-6240 soil samples. Results supported the hypothesis. For example, simulated distributions were not significantly different from the original ones

in 25 and 85 % of cases when the 'sand-silt-sandsand-silt-clay' and 'very coarse+coarse + medium sand - fine +very fine sand - silt+clay', were used, respectively. When the same standard and modified triplets were used to estimate the average bulk density, the coefficients of determination were 0.001 and 0.967, respectively. Overall, the textural triplet selection appears to be application- and data-specific.

10 1 Introduction

5

The particle size distribution is one of the essential controls of soil structure and functioning. Soil processes, properties and specific features are usually related to these distributions, commonly named soil texture. To express these relationships, the continuous particle size distributions are commonly replaced by their discrete representation with several textural fractions. The fractions are defined as particles within a range of sizes, e.g. medium sand, or fine silt, etc. Then the percentages of textural

15 fractions are used as attributes to classify soils and as predictors to estimate soil properties of parameters.

Different countries have employed different number of textural fractions and different ranges of sizes for each of the fraction. *Nemes et al.* (1999) reviewed definitions of textural fractions in 14 European countries and reported the number of ranges varying from three in Italy and France to 8 in the Netherlands and Germany, and 9 in Belgium. These authors also observed a large variability in size ranges. For example, while the minimum size of the second smallest fraction was 2 μ m in most cases,

- 20 the maximum size in such fraction varied from 6 μ m in Greece to 60 μ m in England and Wales. In 1967, the Committee of the Soil Science Society of America noted that the current system of particle size boundaries arose due to geographic accident (*Whiteside et al.*, 1967). The committee noted that there is "no narrowly definable natural particle size boundaries that would be equally significant in all soil materials" The authors noted that the boundary between clay and silt was originally set at 10 μ m, then changed to 5 μ m and finally established at 2 μ m (*Whiteside et al.*, 1967).
- There were indications that setting the boundaries between textural fractions might depend on the purpose of further textural data use as well as on the specifics of the dataset under consideration. *Twarakavi et al.* (2010) demonstrated that, soils are not

classified well from a hydraulic standpoint if the USDA textural fractions of sand, silt, and clay are used. They also noted that this conclusion is conditioned to the database used for the hydraulic classification evaluation. Reasons for selection of size boundaries varied. *Whiteside et al.* (1967) noted that for several reasons a scale based on 1 mm with subdivisions at 0.315 mm, 0.1 mm, etc. would seem to be the ideal scale for agricultural purposes, but advantages were not deemed to be sufficient to

- 5 outweigh the radical departure from the existing textural classification. Also, physics-based reasoning influenced the selection of size boundaries between textural fractions. For example, the 2 μ m boundary for clay was chosen originally as 10 μ m, and then moved to 5 μ m. Around 1936 a switch of the clay limit from 0.005 to 0.002 mm was proposed based on the realization that at 0.002 mm a significant break in mineralogical properties of soil separates occurs (*Truog et al.*, 1936a, b) and that soil surveyors in the field tend to consider the 0.002 to 0.005 mm fraction as silt rather than clay (*Shaw and Alexander*, 1937).
- 10 One application of the data on textural fraction content is the reconstruction of the particle size distribution from the data on small number of fractions. *Martín and Taguas* (1998) proposed to use the hypothesis of self-similarity and iterated function formalism to generate the particle size distribution from small number of textural fractions. In applications of this technique, they used sand, silt, and clay fraction contents with size boundaries defined by the USDA textural classification. Another application of data on textural fractions is to compute the information entropy as the metric of the particle size heterogeneity
- 15 and derive the relationship between the bulk density (BD) and information entropy (IE) (*Martín et al.*, 2017a). Seven textural fractions were used in the latter work where a strong linear correlation between the respective average values was shown. This fact together with computational results obtained in (*Martín et al.*, 2017b), seemed to reinforce the entropy self-similarity approach which is used in the PSD reconstruction. Self-similarity, commonly expressed by scaling laws, actually means that the content of information obtained at the coarse scale keeps its average value at smaller scales (*Pastor-Satorras and Wagensberg*,
- 20 1998), which agrees with the driving idea of the PSD representation used.

The objective of this work was to test hypotheses that (a) the reconstruction of the particle size distribution can be more accurate if the textural fraction size boundaries will be changed from the USDA sand-silt-clay sizes to other size ranges, (b) a satisfactory relationship between the information entropy and packing density can be achieved with three textural fractions with boundaries between fraction change sizes other than in the USDA 'sand-silt-clay' triplet.

25 2 Materials and Methods

2.1 The dataset

The data set used to evaluate the influence of soil texture heterogeneity in soil bulk density values was extracted from the USKSAT database. This The USKSAT data base is comprised from journal publications and technical reports containing coupled data on Saturated Hydraulic Conductivity (Ksat), soil texture, bulk density, and organic matter content obtained across

30 the United States. Detailed information can be found in (*Pachepsky and Park*, 2015). We selected the dataset from Florida ((*Carlisle et al.*, 1978) and (*Carlisle et al.*, 1981)). This dataset is the largest of dataset in UKSAT obtained in the same laboratory with the same methods. The dataset was filtered to exclude samples for which data on seven textural fractions, or on bulk density were not available. Samples with inconsistent textural data (the sum of mass texture fractions not agreeing with

the total mass) were rejected. The selection criteria used in *Martín et al.* (2017a) were followed. Under these selection criteria, total of 6240 soil samples were included in the study. By USDA textural classes, sands, loamy sands, sandy loams, loams, silt loams, silts, sandy clay loams, clay loams, silt clay loams, sandy clays, and clays were represented by 3956, 570, 698, 27, 27, 4, 667, 26, 3, 118 and 144 samples.

5 2.2 Reconstruction of the particle size distributions from data on textural fraction content

The reconstruction of the particle size distribution (PSD) is based on the assumption that the entropy as the measure of heterogeneity of these distributions is preserved across the support scales (*Martín and Taguas*, 1998). Assuming the texture interval divided into k textural size ranges and that the respective textural fraction contents p_1, p_2, \ldots, p_k , $1 \le i \le k$, $\sum_{i=1}^k p_i = 1$ the Shannon Information Entropy (IE) (*Shannon*, 1948) is defined by

$$10 \quad \text{IE} = -\sum_{i=1}^{k} p_i \log_2 p_i \tag{1}$$

where $p_i \log p_i = 0$ if $p_i = 0$. The IE is a widely accepted measure of the heterogeneity of distributions (*Khinchin*, 1957). The IE values for three textural size classes range from 1 when only one fraction is present to $-\log_2 \frac{1}{3} = 1.585$ when all three fractions are represented equally.

- *Martín and Taguas* (1998) proposed a self-similarity model which allows generating the PSD from commonly available textural data which consist of mass percentages of small number of textural fractions. The driving idea of such proposal was that the heterogeneity that textural data show at the coarse scale - quantified in terms of Information Entropy - is also reproduced in a similar way inside any rescaled textural fractions at smaller scales (i.e. the heterogeneity of sieved fractions would resemble that observed at the coarse scale). From this single hypothesis, a mathematically precise representation of the PSD is then obtained by the iterated function formalism. A brief illustration of this technique for the case of three textural
- fractions looks as follows. Let us denote by I_1 , I_2 and I_3 the subintervals of sizes corresponding to the three size classes and p_1 , p_2 and p_3 the relative proportions of mass for the intervals I_1 , I_2 and I_3 , respectively. These proportions are treated as probabilities, $p_1 + p_2 + p_3 = 1$. Let φ_1 , φ_2 and φ_3 be the linear functions (similarities) which transform the whole size interval *I* into the subintervals I_1 , I_2 and I_3 , respectively. The set { $\varphi_1, \varphi_2, \varphi_3, p_1, p_2, p_3$ } is called an iterated function system (IFS) (*Barnsley and Demko*, 1985). The hypothesis of entropy self-similarity of the PSD states that the IE, now computed
- on the successive rescaled subintervals $\varphi_j(I_i) = I_{ij}$, $\varphi_k(I_{ij}) = I_{ijk}$,... and so on (i, j, k = 1, 2, 3), is scale-invariant. Then at each scale The set of textural data, together with the entropy self-similarity assumption, unequivocally determine the PSD (*Martín and Taguas*, 1998). Based on the theorem of Elton (*Elton*, 1987), the mass proportion of soil in an interval may be exactly computed (see *Martín and Taguas* (1998) for further details). of soil with size particles within an interval J, may be computed using the IFS as follows: (a) take any starting value x_0 in I, (b) choose, at random, an integer number i of the index
- 30 set 1, 2, 3, with probability p_i , and denote by x_1 the value $\varphi_i(x_0)$. Repeat the random experiment in (b), and suppose the new outcome is j, and set $x_2 = \varphi_j(x_1)$. If x_0, x_1, \dots, x_n is the sequence obtained in this way and m_n is the number of x_i 's which fall in J, the ratio m_n/n , approaches the mass of the interval J as the number of iterations n goes to infinity. In practice, the estimation of mass in the interval J is achieved quickly.

The reconstruction of distributions was performed using three size fractions - coarse, intermediate, and fine. The dataset contained experimental data on seven fractions - very coarse sand, coarse sand, medium sand, fine sand, very fine sand, silt, and clay. We used all possible triplets formed from seven textural fractions that were available. The symbols for triplet showed how the fractions were grouped. For example for the triplet '3-2-33-2-2' had "coarse" included very coarse sand, coarse sand

5 and medium sand, "intermediate" included fine sand and very fine sand , and "fine" included silt and clay; triplet '5-1-1' was the standard one where "coarse" included all five sand fractions, "intermediate" included silt, and "fine" included clay. Total of 15 triplets were available, a list of which can be found in table 3.

For all textural triplets we generated PSD and compared experimental particle size distributions (built from seven known fractions) with simulated ones. The Kolmogorov-Smirnov test has been applied to find the probability that that the samples are drawn from the same distribution

10 drawn from the same distribution.

2.3 Information Entropy/bulk density relation

Following Eq (1), the Information Entropy of soil texture is computed for all triplets in order to analyze how differences in the Information Entropy explain differences in the typical soil bulk density value of related soils. The range of information entropy values was divided into 10 subintervals of equal length. The mean bulk density value of soil samples binned into IE ranges was

15 computed for each of the subintervals. The <u>least squares</u> linear regression of the average information entropy vs. average bulk density value was computed.

3 Results and Discussion

3.1 Results

Examples of ternary graphs of showing locations of samples in the 'coarse-intermediate-fine' textural fraction content coordinates are shown in Figures 1a and 1b. The standard triangle in Figure 1a shows the majority of points in the left bottom corner. This reflects the fact that soils in the database are mostly coarse textured in terms of the USDA textural classification. The '3-2-2' textural triangle in the Figure 1b shows that the soil samples represent well both samples low in fines particles and samples low in coarse particles, whereas soils with low intermediate fraction contents are not represented well in the database. Table 1 shows total numbers of samples by the ranges of the IE values for standard and '3-2-2' triplets in Figure 1. The standard

25 triplet assigns small values of the information entropy to the majority of samples and thus interprets the majority of samples as heterogeneous. On the contrary, applying the '3-2-2' triplet leads to the conclusion that the majority of samples has a moderate level of textural heterogeneity.

The reconstruction of particle size distributions with the iterated function algorithm showed large difference between the applications different triplets. Data on the statistical difference between generated and measured distributions are shown in

30 Table 2 for all samples and for textural classes where the number of available samples exceeded 100. Triplets where the group of fines includes fine sand, silt and clay, i.e. '1-3-3', '2-2-3', '3-1-3' provide the best results. Results for fine textured soils

do not depend on the triplet because the proportions of coarse particles are small and do not affect results. The differences between triplets become more pronounced as the textures become coarser. The worst results are obtained for triplets '1-5-1, '2-4-1', and '5-1-1' having clay as a separate file fraction, Using the standard triplet '5-1-1' leads to absolutely worst results. The simulated and the experimental cumulative particle-size particle-size distributions are not statistically different at the 95%

5 probability level for 25% of soil samples when the standard triplet of fraction contents is used as input in the reconstruction of the PSD. Instead, when using the any of the triplets '1-3-3', '2-2-3' or '3-1-3' the percentage of soils whose simulated particle size distribution is not statistically different to the original one from the original is bigger than 97% of the total, for the same probability level.

Results of building linear regressions of Mean Information Entropy values versus mean bin bulk density values are shown in 10 Table 3. Different triplets cause different efficiency in estimating BD from IE by textural classes. Overall best relationships were found for sands. Efficiency of estimation was worse in textural classes where there was no single dominant fraction. The sandy clay and sandy clay loam classes provide examples of the above. Noticeably triplets with clay, silt, and fine sand combined in the fine fraction do not result in good R2- R^2 for non-sandy soils (Table 3). This is opposite to the PSD reconstruction where fines consisting of clay, silt, and very fine sand provide the best results (Table 2).

The best results by considering both sand and non sandy samples are obtained with triplets 2-4-1 and 3-3-1, i.e. triplets where fines are represented only by clays and there is a certain balance between the coarse and the intermediate fractions. Where this balance is not present (1-5-1 and 5-1-1) separation of clay in the fine fraction does not help. The standard triangle seems to work only for non sandy soils. Also, this triplet's IE relates well to the BD of sandy clays, sandy loams and sandy clay loams, but it gives unsatisfactory results for sands.

20 3.2 Discussion

The triplets having the fine fraction consisting of very fine sand, silt, and clay appeared to be superior in serving as the input for PSD reconstruction. One possible explanation is that mass size scaling is not scale-invariant across all particle sizes. Rather it has ranges particle sizes within which the power law scaling dependencies are applied and the boundaries between these ranges are between reflected by the modified textural triplet rather than by the original '5-1-1' sand-silt-clay triplet. Breaks in particle

- size distribution scaling were first highlighted by *Tyler and Wheatcraft* (1992) who noted that the strict fractal or self-similar behavior in soil PSDs is restricted to a narrow spectrum of soils found in nature. For the soils tested, the power law scaling was observed in only limited portions of their PSDs. Data on soils B to F from their work are shown in Figure 2. The diameter of the break in scaling varied between 100 μ m and 400 μ m and on average in this group of soils occurred at diameters of 220 μ m which is close to the boundary 250 mm between fine and medium sand. Later the break in scaling was demonstrated by
- 30 other authors, e.g. *Kravchenko and Zhang* (1998) who noted that "The critical particle size [radii M. A.] at which the fractal dimension values are changing, is about 100 to 200 μ m for most of the soils. The result is consistent with that reported in the literature (*Wu et al.*, 1993)"

Another reason for the better simulations of particle size distributions can be the better representation of the soil texture, i.e. distribution of samples by the ranges of IE where the majority of soil are found (Table 1). When the IE is computed with the

standard triplet a great amount of soils have low IE value (have unbalanced contents in respect to those texture fractions). This is-may be an obstacle for reconstruction of the PSD under the entropy self-similarity. In particular, because of the meaning of self-similarity itself, if the input contents are very unbalanced, it <u>eause-causes</u> a multiplicative effect of more unbalanced distribution in the "sub-fractions" at lower scales and probably a more unreliable simulation. On the contrary, in the case of

5 the modified triplet a great amount of soils have medium/high IE, which means that have more balanced contents in respect to the respective new fractions: a greater power of discriminating texture, texture based properties and of obtaining better PSD simulations are expected. This can be an interesting avenue to explore.

The large difference between the 'IE - Bulk density' relationships developed for different textural classes indicates that the IE computed for different triplets has the potential to reflect the effect of soil texture on particle packing in soils. The theoretical

10 analysis of *Assouline and Rouault* (1997) and *Martín et al.* (2017b) shows that the pore space arrangement can be related to the type of distribution of particles sizes. The IE parameter is related to packing but cannot reflect aggregation that is characteristic for soils where fine particles are present in substantial amounts. We note that when IE was computed using the seven texture fraction contents with the same database, the determination of coefficient of the regression 'average IE vs. average bulk density' was equal to 0.99 (*Martín et al.*, 2017b). Thus, results shows that the modified triplet provides almost the same information in respect to the bulk density values that the provided by the seven texture fractions altogether.

The best triplets were different for reconstruction of the particle size distributions and for establishing relationships between information entropy and bulk density after binning samples. Different triplets may be most informative to characterize results of fragmentation and sedimentation that manifest themselves in particle size distributions, and results of packing that manifest themselves in 'IE - BD' relationships. Finally, some process affecting the particle size distributions and 'IE - BD' relationships may not be elucidated by textural data only, aggregation and weathering being examples.

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The utility of textural fractions different from traditional sand-silt-clay triplet appears to have an application in the development of pedotransfer functions. Boundary of new fraction sizes can be parameters of pedotransfer functions along with the regression coefficients. *Nemes and Rawls* (2006) experimented with the boundary between silt and sand in the in the range from 20 μ m and 63 μ m and developed pedotransfer functions for water retention at -33 kPa and -1500 kPa matric potential

25 values. They could not point out the boundary size between silt and sand that would clearly provide better results in estimating the selected soil hydraulic properties. Our work indicates that the boundary may be moved to the range of much larger particle diameters.

Usability of triplets other than standard one indicates ones indicate the opportunity of a more efficient use of the existing results of textural analysis. Although these results traditionally consist of seven fractions including five fractions of sand, in the

30 majority of applications all sand fractions have been lumped together. For example, the overwhelming majority of pedotransfer functions in soil hydrology use the elements of the standard triplet 'sand-silt-clay' (*Pachepsky and Rawls*, 2004). The use of different 'coarse-intermediate-fine' triplets in pedotransfer studies allows the use of the available detailed data on fractions of sand and revisiting existing databases appears be. Overall, application of nonstandard textural triplets in development of pedotransfer functions presents an interesting avenue to explore.

When analyzing the utility of traditional sand-silt-clay triplet for classifying soils by their hydraulic properties, *Twarakavi et al.* (2010) concluded that "from a philosophical perspective, the research further stresses the need to revisit and reevaluate the results from the past in order to successfully move ahead into the future of soil physics". Using a set of fixed boundaries between texture fractions has been a productive approach in the past. Consideration of textural fraction boundaries as flexible parame-

5 ters that can be task and dataset specific can provide additional insights on the role of texture in soil functioning and ecological services.

4 Conclusions

Having three textural size ranges, i.e. coarse, intermediate, and fine particle sizes, undoubtedly appears to be convenient for data presentation and textural class definition. Currently the coarse, intermediate, and fine fractions are identified as sand, silt, and

- 10 clay, respectively. However, it is not warranted that current sand, silt, and clay size ranges can provide the best representation of soil texture when these three size ranges are used for estimating soil properties. We hypothesized that the cumulative particle size distribution and soil bulk density can be more accurately estimated from the triplet 'coarse-intermediate-fine', if the boundaries of the coarse, intermediate, and fine size ranges will be different from those in the 'sand-silt-clay' triplet. The entropy-based representation of particle size distributions was used to convert the triplet particle size representations into
- 15 particle size distributions and to define ranges of soil textural heterogeneity. Experimental data on seven size fraction contents and bulk density for 6300 6240 predominantly coarse-textured soil samples were extracted from the USKSAT database

It appeared that the redefining the triplet 'coarse-intermediate-fine' may lead to a very substantial improvement of soil property estimates from soil textural data. Overall, the drastic improvement in predictions of both cumulative particle size distribution and mean bulk density for heterogeneity ranges occurred when the standard 'sand - silt - clay' triplet was replaced

- 20 with the modified textural triplet that was defined as very coarse, coarse, medium sand (coarse fraction), fine and very fine sand (intermediate fraction) and clay and silt (fine fraction). The modified triplet apparently provided more information about the particle size heterogeneity and particle packing. Different modified triplets provided the best inputs for different soil textural classes.
- Results of this work indicate that the detailed information about soil particle size distributions has the potential to enhance estimation of soil properties with soil texture as a predictor. Analyses of both existing and developing soil databases as well as the pedotransfer methodologies may benefit from exploring modifications of textural triangles. Compression of information on textural heterogeneity in textural triangles into a single entropy-based parameter may provide additional advantages.

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References

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- Assouline, S., and Y. Rouault (1997), Modeling the relationships between particle and pore size distributions in multicomponent sphere packs: Application to the water retention curve, *Colloids and Surfaces A: Physicochemical and Engineering Aspects*, 127(1-3), 201-210, doi:10.1016/S0927-7757(97)00144-1.
- 5 Barnsley, M. F., and S. Demko (1985), Iterated functions systems and the global construction of fractals, *Proc. R. Soc. Lon.*, A 399, 243-275, doi:10.1098/rspa.1985.0057.

Carlisle, V. W., R. E. Caldwell, F. Sodek, III, L. C. Hammond, F. G. Calhoun, M. A. Granger, and H. L. Breland (1978), Characterization Data for Selected Florida Soils, Univ. of Florida, Gainesville, Fla.

Carlisle, V. W., C. T. Hallmark, F. Sodek, III, R. E. Caldwell, L. C. Hammond, and V. E. Berkeiser (1981), Characterization Data For Selected

10 Florida Soils, Soil Conservation Service, University of Florida, Institute of Food and Agricultural Sciences, Soil Sciences Department, Soil Characterization Laboratory.

Khinchin, A. I., (1957), Mathematical Foundation of Information Theory. Dover Publications, New York.

Kravchenko, A., and R. Zhang (1998), Estimating the soil water retention from particle-size distributions: a fractal approach, *Soil Science*, 163(3), 171-179.

15 Elton, J. (1987), An ergodic theorem for iterated maps, J. Ergodic Theory Dynamical Syst. 7, 481-488

Martín, M. A., and F. J. Taguas (1998), Fractal modeling, characterization and simulation of particle-size distributions in soil, *Proc. R. Soc. Lond.*, A 454, 1457-1468, doi:10.1098/rspa.1998.0216.

Martín, M. A., M. Reyes, and F. J. Taguas (2017a), Estimating soil bulk density with information metrics of soil texture, *Geoderma*, 287, 66-70, doi:10.1016/j.geoderma.2016.09.008.

20 Martín, M. A., M. Reyes, and F. J. Taguas (2017b), An entropy-like parameter of particle size distributions as packing density index in complex granular media, *Granular Matter*, 19:9, doi:10.1007/s10035-016-0692-3.

Nemes, A., J. H. M. Wösten, A. Lilly, and J. O. Voshaar (1999), Evaluation of different procedures to interpolate particle-size distributions to achieve compatibility within soil databases, *Geoderma*, 90(3), 187-202, doi:10.1016/S0016-7061(99)00014-2.

Nemes, A., and W. J. Rawls (2006), Evaluation of different representations of the particle-size distribution to predict soil water retention,

25 *Geoderma*, 132(1), 47-58, doi:10.1016/j.geoderma.2005.04.018.

Pachepsky, Y. A., and W. J. Rawls (eds.) (2004), Development of Pedotransfer Functions in Soil Hydrology, Elsevier, Amsterdam.

Pachepsky, Y. A., and Y. Park, (2015), Saturated hydraulic conductivity of US soils grouped according to textural class and bulk density, *Soil Sci. Soc. Am. J.*, 79, 1094-1100, doi:10.2136/sssaj2015.02.0067.

Pastor-Satorras, R., and Wagensberg, J., (1998), The maximum entropy principle and the nature of fractals, *Physica A*, 251, 291-302, doi:10.1016/S0378-4371(97)00571-2.

- Shaw, T. M., and L. T. Alexander (1937), A note on mechanical analysis and soil texture, *Soil Sci. Soc. Amer. Proc.*, 1, 303-304, doi:10.2136/sssaj1937.03615995000100000053x.
- Truog, E., J. R. Taylor, R. W. Pearson, M. E. Weeks, and R. W. Simonson (1936a), Procedure for special type of mechanical and mineralogical
 soil analysis, *Soil Sci. Soc. Amer. Proc.*, 1, 101-112, doi:10.2136/sssaj1937.03615995000100000013x.
 - Truog, E., J. R. Taylor, R. W. Simonson, and M. E. Weeks (1936b), Mechanical and mineralogical subdivisions of the clay separate of soils, *Soil Sci. Soc. Amer. Proc.*, 1, 175-179, doi:10.2136/sssaj1937.03615995000100000025x

Shannon, C. E., (1948), A mathematical theory of communication, I. Bell Syst. Technol. J., 27, 379-423.

- Twarakavi, N. K. C., J. Šimůnek, and M. G. Schaap (2010), Can texture-based classification optimally classify soils with respect to soil hydraulics?, *Water Resources Research*, 46(1), doi:10.1029/2009WR007939
- Tyler, S. W., and S. W. Wheatcraft (1992), Fractal scaling of soil particle-size distributions: analysis and limitations, *Soil Sci. Soc. Amer. J.*, 56(2), 362-369, doi:10.2136/sssaj1992.03615995005600020005x.
- 5 Whiteside, E. P., K. W. Flach, V. C. Jamison, W. D. Kemper, E. G. Knox, and A. C. Orvedal (1967), Considerations relative to a common particle size scale of earthy materials, *Soil Sci. Soc. Amer. Proc.*, 31(4), 579-584, doi:10.2136/sssaj1967.03615995003100040046x.
 - Wu, Q., M. Borkovec, and H. Sticher (1993), On particle-size distributions in soils, *Soil Sci. Soc. Amer. J.*, 57(4), 883-890, doi:10.2136/sssaj1993.03615995005700040001x.



Figure 1. Texture of soil samples in the database shown in the standard USA (a) and modified '3-2-2' textural triangles (b).



Figure 2. Scaling in cumulative particle mass of four soils studied by *Tyler and Wheatcraft* (1992)

Table 1. Total numbers of samples by ranges of the information entropy for two textural fraction triplets. The $\frac{2}{3}$ -2-2' triplet includes very coarse, coarse and medium sand (fraction 1), fine and very fine sand (fraction 2) and clay and silt (fraction 3); the standard triplet $\frac{2}{5}$ -1-1' includes sand (fraction 1), silt (fraction 2) and clay (fraction 3).

	Number of samples by information entropy ranges			
Range of the Information Entropy	standard '5-1-1' triplet	'3-2-2' triplet		
0.00-0.16	698	23		
0.16-0.32	1346	101		
0.32-0.48	1169	269		
0.48-0.64	754	407		
0.64-0.80	485	539		
0.80-0.96	499	772		
0.96-1.12	465	1172		
1.12-1.28	416	1250		
1.28-1.44	272	926		
1.44-1.60	136	781		

Textural triplet	Clay	Sandy clay	Sandy clay loam	Sandy loam	Loamy sand	Sand	All samples
115	100	100	82	45	37	8	27
124	100	100	97	83	76	51	64
133	100	100	100	100	100	97	98
142	100	100	98	84	57	15	40
151	100	100	84	32	5	1	19
214	100	100	97	84	78	53	66
223	100	100	100	100	100	100	99
232	100	100	100	95	79	28	52
241	100	100	93	59	38	8	31
313	100	100	100	100	100	100	100
322	100	100	100	99	94	77	85
331	100	100	99	90	79	55	68
412	100	100	100	100	100	82	88
421	100	100	100	100	100	83	89
511	97	100	99	78	0	0	25
N	144	115	660	685	565	3966	6224

Table 2. Percentage of samples with for which simulated and measured particle size distributions being are not different at the 0.05 significance level.

Triplet	Clay	Sandy clay	Sandy clay loam	Sandy loam	Loamy sand	Sand	All samples	All sands	Not sandy
115	0.633	0.076	0.426	0.725	0.520	0.509	0.571	0.567	0.035
124	0.579	0.085	0.817	0.807	0.797	0.908	0.915	0.899	0.167
133	0.695	0.143	0.460	0.463	0.111	0.448	0.932	0.854	0.445
142	0.432	0.037	0.027	0.024	0.318	0.799	0.412	0.772	0.590
151	0.762	0.345	0.219	0.630	0.789	0.433	0.125	0.663	0.742
214	0.682	0.177	0.834	0.894	0.545	0.919	0.824	0.868	0.239
223	0.713	0.141	0.337	0.517	0.682	0.942	0.786	0.978	0.474
232	0.604	0.275	0.004	0.053	0.803	0.931	0.960	0.959	0.748
241	0.837	0.256	0.305	0.689	0.743	0.756	0.891	0.933	0.897
313	0.594	0.482	0.053	0.767	0.496	0.963	0.823	0.964	0.508
322	0.388	0.055	0.000	0.216	0.777	0.968	0.909	0.968	0.704
331	0.878	0.164	0.312	0.872	0.822	0.966	0.967	0.971	0.790
412	0.361	0.077	0.080	0.603	0.546	0.307	0.943	0.873	0.731
421	0.701	0.161	0.019	0.438	0.061	0.308	0.833	0.865	0.774
511	0.703	0.812	0.814	0.873	0.542	0.372	0.000	0.218	0.745

Table 3. Determination of coefficients of regressions of for the average information entropy versus average bulk density for ten average entropy bins.