José Domingos Albuquerque Aguiar

Characterization of soil microstructure using 3D X-ray tomographic images

Recife – PE July 2023



UNIVERSIDADE FEDERAL RURAL DE PERNAMBUCO PRÓ-REITORIA DE PESQUISA E PÓS-GRADUAÇÃO PROGRAMA DE PÓS-GRADUAÇÃO EM BIOMETRIA E ESTATÍSTICA APLICADA

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Concentration Area: **Modelagem e métodos computacionais.**

Advisor: **Ph.D. Borko Stosic** Co-advisor: **Ph.D. Tatijana Stosic**

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I dedicate this work to my parents for having invested in my education that made me get this far.

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"Perseverance is not a long race; it is many short races one after the other."

Walter Elliot

Abstract

Dozens of definitions of soil can be found in literature, ranging from the most straightforward concepts, where it is asserted, for example, that soil is a mixture of air, water, inorganic and organic heterogeneous solids. and microorganisms, to more complex concepts, where the soil is considered a living, fourdimensional natural Entity. However, regardless of the adopted definition, the importance of soil is unquestionable, as it provides nutrients for plant growth essential for human and animal nutrition. Moreover, history has frequently shown that its misuse can lead to poverty, hunger, drought, and ecological and economic disasters. This great importance given to soil generates a need for ongoing studies searching for methods and tools that contribute to new knowledge. A powerful tool that can observe the elements of soil in a non-destructive way is computed tomography (CT). Despite advances in the resolution of CT equipment and computer power, there is no consensus on data analysis methods that can reveal the complexity of all elements associated with 3D soil images, especially methods that do not require a threshold to segment images. In this context, this work employs two methods originally developed for the analysis of complex signals, Detrended Fluctuation Analysis (DFA) and Fisher-Shannon (FS), to bring a new understanding of the complexity of morphological properties of soil based on the analysis of 3D CT images. Up to date, these two methods have not been used in 3D image analysis. In this work, 3D soil tomographic images were analyzed using DFA in its original form and its generalization for 2D and 3D data. The results of DFA exponents were found to be smaller than 0.5 indicating antipersistence of local density fluctuations, which are consistently stronger (lower exponent value) for the sugar cane plantation sample, than for the Atlantic Forest. Furthermore, a new complexity measure is defined as the distance from the isocomplexity line in the normalized FS plane, which may be seen as a quantifier of soil degradation level. This novel approach resulted in a high grouping success rate (91.7%) between soil covered by native vegetation (Atlantic Forest) and soil that was the subject of the degradation process as the consequence of land use change (from native Atlantic Forest to sugarcane cultivation).

Keywords: X-Ray CT Scan Soil Samples. Detrended Fluctuation Analysis. Fisher-Shannon plane. Complexity. Land use change.

Resumo

Dezenas de definições de solo podem ser encontradas na literatura, desde os conceitos mais simples, onde se afirma, por exemplo, que o solo é uma mistura heterogênea de ar, água, sólidos inorgânicos e orgânicos, e microrganismos, até conceitos mais complexos, onde o solo é considerado uma Entidade natural viva e quadridimensional. No entanto, independentemente da definição adotada, a importância do solo é inquestionável, pois fornece nutrientes para o crescimento vegetal essenciais para a nutrição humana e animal. Além disso, a história tem mostrado frequentemente que seu mau uso pode levar à pobreza, fome, seca e desastres ecológicos e econômicos. Essa grande importância dada ao solo gera a necessidade de estudos contínuos em busca de métodos e ferramentas que contribuam para novos conhecimentos. Uma poderosa ferramenta que pode observar os elementos do solo de forma não destrutiva é a tomografia computadorizada (TC). Apesar dos avanços na resolução dos equipamentos de TC e na potência computacional, não há consenso sobre métodos de análise de dados que possam revelar a complexidade de todos os elementos associados às imagens 3D do solo, especialmente métodos que não necessitam de um limiar para segmentar imagens. Neste contexto, este trabalho emprega dois métodos originalmente desenvolvidos para a análise de sinais complexos, a Análise de Flutuação Destendenciada (DFA) e Fisher-Shannon (FS), para trazer uma nova compreensão da complexidade das propriedades morfológicas do solo com base na análise de imagens 3D de TC. Até o presente momento, esses dois métodos não foram utilizados na análise de imagens 3D. Neste trabalho, foram analisadas imagens tomográficas de solo 3D utilizando DFA em sua forma original e sua generalização para dados 2D e 3D. Os resultados dos expoentes da DFA foram menores que 0,5, indicando antipersistência das flutuações da densidade local, que são consistentemente mais fortes (menor valor do expoente) para a amostra do canavial do que para a Mata Atlântica. Além disso, uma nova medida de complexidade é definida como a distância da linha de isocomplexidade no plano normalizado do FS, que pode ser vista como um quantificador do nível de degradação do solo. Essa nova abordagem resultou em uma alta taxa de sucesso de agrupamento (91,7%) entre o solo coberto por vegetação nativa (Mata Atlântica) e o solo que foi objeto de processo de degradação como consequência da mudança de uso da terra (de Mata Atlântica nativa para o cultivo de cana-de-açúcar).

Palavras-chave: TC por raios X de amostras de solo. Análise de flutuação sem tendência. Plano de Fisher-Shannon. Complexidade. Mudança de uso do solo.

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Abbreviation list

1D	One-dimensional
2D	Two-dimensional
3D	Three-dimensional
AF	Atlantic Forest
CONAB	Companhia Nacional de Abastecimento
СТ	Computed tomography
DFA	Detrended Fluctuation Analysis
FIM	Fisher's information measure
FS	Fisher-Shannon
IBGE	Instituto Brasileiro de Geografia e Estatística
MFDFA	Multifractal Detrended Fluctuation analysis
PDF	Probability density function
SC	Sugarcane
SEP	Shannon Entropy Power

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1. General introduction

Dozens of definitions of soil can be found in literature, ranging from the most straightforward concepts, where it is asserted, for example, that soil is a heterogeneous mixture of air, water, inorganic and organic solids, and microorganisms (SPARKS, 2003), to more complex concepts, where the soil is considered a living, four-dimensional natural Entity (HARTEMINK, 2016). However, regardless of the adopted definition, the importance of soil is unquestionable, as it provides nutrients for plant growth essential for human and animal nutrition. Moreover, history has frequently shown that its misuse can lead to poverty, hunger, drought, and ecological and economic disasters (BEZDICEK; PAPENDICK; LAL, 2015). This great importance given to soil generates a need for ongoing studies searching for methods and tools that contribute to new knowledge.

A powerful tool that can observe the elements of an object, including soil, in a non-destructive way (JON *et al.*, 2022) is computed tomography (CT), which uses X-rays and computers to record two-dimensional images of multiple slices of an object (figure 1). These images can be assembled with the aid of a computer to form a threedimensional image of the scanned object (figure 2). The first recorded use of CT was in the medical field in 1971 with the tomography of a human head (HOUNSFIELD, 1973). The first recorded application of CT in the soil field was in 1982 with the analysis of the density of a soil sample (PETROVIC; SIEBERT; RIEKE, 1982). Although the first use of CT to record soil images is over 40 years old, interest in this research field continues with a growing trend, as can be seen from the graph (figure 3) of articles published using the Scopus database with the search terms "tomography and soil" on April 18th, 2023.

Using CT to scan soil samples provides data that can help understand some problems, such as degradation caused by changes in land use. In Brazil, a typical example of this problem occurs in the country's northeastern region with the conversion of areas of the Atlantic Forest biome into areas for sugarcane cultivation. Such conversion can negatively affect soil functions such as water storage and filtration, nutrient storage and recycling, carbon storage, and habitat for biological activity (RABOT *et al.*, 2018), directly influencing associated ecosystem services.



Figure 1. Four examples of 2D images (790x790 pixels) from a sugar cane plantation soil sample: (a) slice_001, (b) slice_100, (c) slice_395 and (d) slice_790.



Figure 2. 3D representation of a sugar cane plantation soil sample.

Despite advances in the resolution of CT equipment and computer power, there is no consensus on data analysis methods that can reveal the complexity of all elements associated with 3D soil images, especially methods that do not require a threshold to segment images. In this context, this work employs two methods originally developed for the analysis of complex signals, Detrended Fluctuation Analysis (DFA) and Fisher-Shannon (FS), to bring new understanding of the complexity of morphological properties of soil based on the analysis of 3D CT images. Up to date these two methods have not been used in 3D image analysis.



Figure 3. Publications using the terms "tomography" and "soil" from 1982 to 2022, according to the Scopus database.

The DFA method is a tool typically used to analyze time series data to detect the presence of long-range correlations in non-stationary series. The advantage of DFA is that it can systematically eliminate trends of different orders (KANTELHARDT *et al.*, 2001). The DFA method was initially proposed by Peng et al (PENG *et al.*, 1994) in 1994 to analyze the organization of nucleotides in a DNA chain. Currently, several recent applications of DFA can be found in various areas of knowledge, such as physiology (BLOKHINA *et al.*, 2023; VAZ; SILVA; STERGIOU, 2023), climatology (KIRÁLY; JÁNOSI, 2005; MALLICK *et al.*, 2021; TATLI; DALFES, 2020), economics (KRISTOUFEK, 2019; MOHTI *et al.*, 2019), engineering (BOUNOUA; AFTAB; OMLIN, 2023; LIU; CHEN; ZHANG, 2020), sport (FERREIRA, 2018), and seismology (KATAOKA; MIYAGUCHI; AKIMOTO, 2021; SKORDAS; CHRISTOPOULOS;

SARLIS, 2020), among others. However, applications of DFA involving soil data are rare, among them three can be cited: the first that identifies active erosion sites (CAO *et al.*, 2020); another that analyzes patterns of water storage in soil (BISWAS; ZELEKE; SI, 2012); and the third that analyzes time series of radioactive elements in soil (RAFIQUE *et al.*, 2021). However, all three applications employ the multifractal version of DFA – Multifractal Detrended Fluctuation analysis (MFDFA), to analyze time series (RAFIQUE *et al.*, 2021) or one - dimensional spatial data (BISWAS; ZELEKE; SI, 2012; CAO *et al.*, 2020). In this work 3D soil tomographic images were analyzed using DFA in its original form and its generalization for 2D and 3D data (AGUIAR *et al.*, 2022).

The FS method is a statistical technique originated in information theory that consists of a joint analysis of Fisher's information measure (FIM) (FISHER, 1925), which quantifies the amount of organization (or order) in a signal, and Shannon entropy (SE) (SHANNON, 1948), which quantifies the degree of uncertainty (or disorder) (LOVALLO; PIERINI; TELESCA, 2012). Recent applications of the Fisher-Shannon method can be found in various areas of science, such as ecology (BA et al., 2020; TELESCA et al., 2022), economics (FERNANDES; DE ARAUJO; SILVA, 2022; KWAPIÉ et al., 2023), physics (DEHESA, 2023; MARTÍNEZ-FLORES, 2021), physiology (FUENTES et al., 2022) and climatology (DA SILVA et al., 2021) among others. However, applications of the Fisher-Shannon method in soil data are scarce. One of these few applications relates seismic microtremors to soil type through FS analysis (TELESCA et al., 2015) analysis but does not use soil tomographic images in the analysis. Another application is a partial result of this work, which quantifies the complexity of soil using FS of 3D tomographic images. In this work (STOSIC et al., 2022) the complexity of soil 3D tomographic images was analyzed through the application of FS method on the probability distribution of gray scale values of one dimensional columns extracted from 3D images.

Both methods DFA and FS were used to analyze 24 3D tomographic images extracted from soil samples from the Northeast region of Brazil, specifically in the state of Pernambuco between latitudes -7.84836 and -7.83519, and longitudes -34.9973 and -34.9935. Out of these images, 12 are from soil samples from the Atlantic Forest, and 12 are from sites where native vegetation of Atlantic Forest was replaced by sugarcane plantations.

The main objective of this work is to investigate complexity of morphological properties of soil under different land use. More specifically, it aims to:

- Apply the DFA method for 1, 2 and 3 dimensional data to 3D soil images to quantify long-range correlations (persistence of density fluctuation);

- To compare the performance of 1D, 2D, and 3D DFA methods to distinguish between soil properties under different land cover (Atlantic Forest and sugarcane plantations);

- Verify if the information quantifiers of 3D soil images obtained by the Fisher-Shannon method capture changes in land use;

- Quantify the complexity of soil samples in terms of distance from the isocomplexity line in the FS plane;

- Propose a new procedure for normalization of FS quantifiers for representation on the Fisher-Shannon information plane while preserving the Fisher Shannon complexity.

2. Detrended fluctuation analysis of three-dimensional data: application to soil X-ray CT scans

2.1 Abstract

In this work we compare three distinct schemes for Detrended Fluctuation (DFA) analysis of 3D N×N×N data sets: i) a N×N set of 1D DFA runs for each vertical line of length N, ii) a set of N 2D DFA runs for each of the N×N planes along the z direction, and iii) a single 3D DFA run. The objective of this work is twofold: i) to compare the performance of 1D, 2D and 3D DFA methods in terms of compatibility as well as the richness of obtained results, and ii) to demonstrate how these three complementary approaches shed new light on the complexity of the structure of the two real soil samples, through the analysis of grayscale high-resolution X-ray CT scan images.

Keywords: Detrended fluctuation analysis; three-dimensional data; X-ray CT scan soil samples.

2.2 Introduction

Analysis of three-dimensional data sets (images) has been gaining momentum over the years in diverse scientific and technological fields, with the advance of both technological data acquisition methods, and high-performance computational resources. A three-dimensional image may be composed in different ways, e.g. by merging satellite images acquired at successive time frames for a composite spatiotemporal analysis, but probably the most widespread applications stem from computed tomography (CT) scans.

The dramatic increase in the performance of CT scanners in terms of resolution and image quality has led to their widespread use principally in medicine, but applications in other fields of science and technology have also been experiencing a dramatic rise. On the other hand, the analysis of high-resolution images may pose computational challenges, as e.g., a 1000x1000x1000 resolution image is composed of one billion voxels (volume elements), represented by their gray scale values, that may turn out too demanding for many standard tools.

In this work, we explore the application of detrended fluctuation analysis (DFA) on 3D images to quantify long-range correlations at different scales, with an example of high-resolution soil CT scan images. The DFA method was introduced in 1994 by Peng et al (PENG *et al.*, 1994) to study correlations in non-stationary time series, and has been subsequently applied in diverse fields of science. More recently, a generalization of the DFA method was proposed by Gu and Zhou (GU; ZHOU, 2006), followed by only several applications up to date for 2D data sets, and to the best of our knowledge no applications have been published yet for 3D data. We consider here (and compare the results of) three distinct schemes for DFA analysis of NxNxN 3D soil samples: i) a NxN set of 1D DFA runs for each vertical line, ii) a set of N 2D DFA runs for each of the NxN planes along the vertical direction, and iii) a single 3D DFA run. The results of all three approaches are shown to be compatible.

The choice of soil CT scan images for the examples studied here stems from the fact that a deeper understanding of the physical, chemical and biological processes within soil depends on the quantification of heterogeneity and complexity of the spatial distribution of soil particles and aggregates (SCHLÜTER et al., 2018). X-ray CT scans have already been employed for quantification of the physical structure and spatial distribution of the pore space (HOUSTON et al., 2017), revealing extraordinary complexity of this system (FALCONER et al., 2012; JUAREZ et al., 2013; KATUWAL et al., 2015). The complexity of soil structure has also been assessed by using methods based on concepts from statistical physics such as fractals and multifractals (LUO; LIN, 2009; PERRET; PRASHER; KACIMOV, 2003; SAN JOSÉ MARTÍNEZ et al., 2010; WANG et al., 2016), information content (TORRE et al., 2020) and complex networks (CÁRDENAS et al., 2010; SAMEC et al., 2013). As there remains a lack of consensus on the appropriate poresolid CT threshold (GIBSON; LIN; BRUNS, 2006; TARQUIS et al., 2009; TORRE et al., 2020), it has also been suggested that grayscale soil images should be used for multifractal characterization of the soil structure, rather than thresholding (ROY; PERFECT, 2014; TORRE et al., 2018; TORRE; LOSADA; TARQUIS, 2018; ZHOU et al., 2010, 2011).

In this work, we analyze two 790x790x790 greyscale level X-ray CT scan images of real soil samples, from a sugar cane field, and a nearby Atlantic Forest site, in northeastern Brazil. The objective of this work is twofold: i) to compare the

performance of 1D, 2D and 3D DFA methods, and ii) to demonstrate how this approach sheds new light on the complexity of the structure of the two real soil samples. In the next section we describe the methodology, then we show the results with discussion, and finally we draw the conclusions.

2.3 Methodology

2.3.1 Detrended fluctuation analysis (1D DFA)

Detrended fluctuation analysis (DFA) was introduced by Peng et al. (PENG *et al.*, 1994) as a method for quantification of correlations in non-stationary time series (CHEN *et al.*, 2002; HU *et al.*, 2001; KANTELHARDT *et al.*, 2001). This method represents a modified root-mean-square analysis of a random walk, and has been subsequently successfully applied in a wide spectrum of areas, ranging from physiology (GOLDBERGER *et al.*, 2002; LI *et al.*, 2019), to geophysics (CURRENTI *et al.*, 2005), climatology (KIRÁLY; JÁNOSI, 2005; STOSIC; TELESCA; STOSIC, 2021), and finances (DE LIMA *et al.*, 2018; YAMASAKI *et al.*, 2005), to name just a few.

For a random sequence of (positive and negative) increments (random walk steps), the implementation of the DFA algorithm is described as follows:

i) The original series x(i), i = 1, ..., N is integrated to yield

$$X(k) = \sum_{i=1}^{k} [x(i) - \langle x \rangle]$$
, $k = 1, 2, ..., N$

where $\langle x \rangle = \sum_{i=1}^{N} x(i)/N$ is the average. This step is necessary to transform the original series of random walk steps into a "profile" (series of the random walk displacements), and should be omitted if the actual data represent a profile, rather than steps.

ii) Next, the integrated series X(k) is divided into $N_n = [N/n]$ non-overlaping segments of length *n* (here [·] stands for the integer value of the argument), and in each segment $s = 1, ..., N_n$ the local trend $X_{n,s}(k)$ (linear or higher-order

polynomial least squares fit – termed DFA1, DFA2, DFA3,..., for polynomials of order 1,2, 3,..., respectively) is estimated and subtracted from X(k). In DFAm, trends of order m in the profile X(k), and of order m - 1 in the original record x(i) are eliminated.

iii) The detrended variance is now calculated as

$$F^{2}(n) = \frac{1}{nN_{n}} \sum_{s=1}^{N_{n}} \sum_{k=(s-1)n+1}^{sn} [X(k) - X_{n,s}(k)]^{2}.$$

iv) Repeating this calculation for different segment sizes provides the relationship between the fluctuation function F(n) and the segment size n. If long-term correlations are present in the original series, F(n) increases with n according to a power law

$$F(n) \sim n^{\alpha_1}.$$

The scaling exponent α is obtained as the slope of the linear regression of $\log F(n)$ versus $\log n$. The value $\alpha_1 = 0.5$ indicates the absence of correlations (white noise), $\alpha_1 > 0.5$ indicates the persistence of long-term correlations, meaning that large (small) values are more likely to be followed by large (small) values, while $\alpha_1 < 0.5$ indicates antipersistent long-term correlations, meaning that large values are more likely to be followed by large (small) antipersistent long-term correlations, meaning that large values are more likely to be followed by small values, and vice versa. The values $\alpha_1 = 1$ and $\alpha_1 = 1.5$ correspond to 1/f noise and Brownian noise (integration of white noise), respectively (PENG *et al.*, 1994), and values of $\alpha_1 > 1.0$ are obtained for fractional Brownian motion (when a series of displacements is integrated).

2.3.2 Detrended fluctuation analysis in two dimensions (2D DFA)

More recently, Guo and Zheng (GU; ZHOU, 2006) have generalized the above described one-dimensional DFA algorithm for higher dimensions. Up to date, there have been several implementations of this method (ALPATOV; VIKHROV; GRISHANKINA, 2013; ALVAREZ-RAMIREZ *et al.*, 2008; BARRERA *et al.*, 2010; LIU *et al.*, 2017; NIE *et al.*, 2015; VARGAS-OLMOS *et al.*, 2015; VELAZQUEZ-CAMILO *et al.*, 2010) in two-dimensions, for which the approach consists of the following steps.

- i) A self-similar surface represented by two-dimensional $N \times M$ matrix x(i,j), i = 1, ..., N and j = 1, ..., M is divided into $N_n \times M_n$ square non-overlapping segments of size $n \times n$, where $N_n = [N/n]$ and $M_n = [M/n]$.
- ii) In each segment indexed by $s = 1, ..., N_n$ and $t = 1, ..., M_n$, consisting of data points x(i,j) with i = (s-1)n + 1, ..., sn, j = (t-1)n + 1, ..., tn, data are integrated to produce the profile

$$X_{s,t}(k,l) = \sum_{i=1}^{k} \sum_{j=1}^{l} x ((s-1)n + i, (t-1)n + j) , \qquad k, l = 1, \dots, n$$

Note that the order of these two first steps has been reversed in comparison with the 1D DFA approach, but this is relevant only for multifractal generalization (GU; ZHOU, 2006), which is not being addressed here. Again, this step should be omitted if the actual data correspond to a profile rather than local fluctuations, in which case the profile segment simply consists of the data points $X_{s,t}(k, l) = x((s-1)n + k, (t-1)n + l)$, for k, l = 1, ..., n.

iii) Next, the local trend $\tilde{X}_{s,t}(k, l)$ is captured for each segment by least-squares fitting to a linear (or higher-order polynomial) bivariate function, and subtracted from $X_{s,t}(k, l)$ to find the residuals, from which the detrended variance is calculated for each segment as

$$F^{2}(s,t,n) = \frac{1}{n^{2}} \sum_{k=1}^{n} \sum_{l=1}^{n} \left(X_{s,t}(k,l) - \tilde{X}_{s,t}(k,l) \right)^{2}$$

It was shown in (GU; ZHOU, 2006) that linear interpolation of the form a + bk + cl works rather well.

iv) Finally, the fluctuation function F(n) at scale n is now calculated as

$$F(n) = \left\{ \frac{1}{N_n M_n} \sum_{s=1}^{N_n} \sum_{t=1}^{M_n} F^2(s, t, n) \right\}^{1/2}$$

v) As before, repeating this calculation for different segment sizes provides the relationship between the fluctuation function F(n) and the segment size n. If long-range correlations are present in the original data set, F(n) increases with n according to a power law

$$F(n) \sim n^{\alpha_2}$$

where the (2D DFA) scaling exponent α_2 is obtained as the slope of the linear regression of $\log F(n)$ versus $\log n$. It describes the long-range power-law correlation properties of the surface and can be seen as a measure of surface texture (or roughness). The value $\alpha_2 = 0.5$ corresponds to non-correlated surfaces, while $\alpha_2 > 0.5$ and $\alpha_2 < 0.5$ correspond to persistent and antipersistent correlations of the surface fluctuations (GU; ZHOU, 2006).

2.3.3 Detrended fluctuation analysis in three dimensions (3D DFA)

While the Guo and Zheng (GU; ZHOU, 2006) generalization in principle covers any dimension above unity, they mention that they have tested the approach on synthetic datasets, but they do not provide explicit formulas. Moreover, to the best of our knowledge no works have been published up to date for DFA analysis of threedimensional (or higher dimensional) data. It may be inferred from (GU; ZHOU, 2006) that for 3D, the approach consists of the following steps.

- i) A self-similar volume represented by a three-dimensional $N \times M \times P$ matrix x(i, j, k), i = 1, ..., N, j = 1, ..., M and k = 1, ..., P is divided into $N_n \times M_n \times P_n$ cubic non overlapping segments (boxes) of size $n \times n \times n$, where $N_n = [N/n]$, $M_n = [M/n]$ and $P_n = [P/n]$.
- ii) In each box segment indexed by $r = 1, ..., N_n$, $s = 1, ..., M_n$ and $t = 1, ..., P_n$, consisting of data points x(i, j, h) with indices i = (r - 1)n + 1, ..., rn, j = (s - 1)n + 1, ..., sn, and h = (t - 1)n + 1, ..., tn, data are integrated to produce the profile

$$X_{r,s,t}(k,l,m) = \sum_{i=1}^{k} \sum_{j=1}^{l} \sum_{h=1}^{m} x((r-1)n + i, (s-1)n + j, (t-1)n + h), \qquad k, l, m = 1, \dots, n$$

Again, this step should be omitted if the actual data correspond to a profile, rather than local fluctuations, in which case the profile segment simply consists of the data points $X_{r,s,t}(k,l,m) = x((r-1)n + k, (s-1)n + l, (t-1)n + m)$, for k, l, m = 1, ..., n.

iii) Next, the local trend $\tilde{X}_{r,s,t}(k, l, m)$ is captured for each segment by least-squares fitting to a linear (or higher-order polynomial) function of three variables, and subtracted from $X_{r,s,t}(k, l, m)$ to find the residuals, from which the detrended variance is calculated for each segment as

$$F^{2}(r,s,t,n) = \frac{1}{n^{3}} \sum_{k=1}^{n} \sum_{l=1}^{n} \sum_{m=1}^{n} \left(X_{r,s,t}(k,l,m) - \tilde{X}_{r,s,t}(k,l,m) \right)^{2}$$

In what follows, we shall apply linear interpolation of the form a + bk + cl + dm.

iv) Finally, the fluctuation function F(n) at scale n is now calculated as

$$F(n) = \left\{ \frac{1}{N_n M_n P_n} \sum_{r=1}^{N_n} \sum_{s=1}^{M_n} \sum_{t=1}^{P_n} F^2(r, s, t, n) \right\}^{1/2} .$$

v) Repeating this calculation for different segment sizes again provides the relationship between the fluctuation function F(n) and the segment size n. If long-range correlations are present in the original data set, F(n) increases with n according to a power law

$$F(n) \sim n^{\alpha_3}$$

where the (3D DFA) scaling exponent α_3 is obtained as the slope of the linear regression of $\log F(n)$ versus $\log n$. It describes the long-range power-law correlation properties of the surface and can be seen as of a measure of surface texture (or roughness). The value $\alpha_3 = 0.5$ corresponds to non-correlated volume, while $\alpha_3 > 0.5$ and $\alpha_3 < 0.5$ correspond to persistent and antipersistent correlations of the volume fluctuations.

2.3.4 Soil samples

Soil samples were collected from a field cultivated with sugarcane and from a nearby native Atlantic Forest site, located in the state of Pernambuco, northeastern Brazilian region. The samples were obtained using a soil auger with an internal PVC cylinder of 7.5 cm height by 7.5 cm diameter, excavated by careful penetration with a cylinder coupled with a blade. After the insertion of the auger in the soil, the cylinders were carefully extracted to ensure the preservation of the original structure of the environment inside the PVC cylinders. The samples were then dried at 40°C to remove the water content, before the scanning tomography of the samples. The CT tomography was performed using a third-generation Nikon XT H 225 ST X-ray microtomography equipment with 150 kV voltage, 180 µA current, 500 ms exposure time, and a 45 µm resolution for voxels. A copper filter with a thickness of 0.5 mm was used to minimize low-intensity photons. After the scanning of the total cylinder volume in the preliminary acquisition, a subvolume of interest was defined and reconstructed using CTPro 3D XT 3.0.3 (Nikon Metrology NV) software. The central part of the cylinder was highlighted to avoid edge influence. The reconstructed 2D axial projections maintained the same spatial resolution of the acquisition of 45 µm, and were saved at a radiometric resolution (gray scale level) of 16 bits. The final volume was 790 stacks with 790 x 790 pixels, with an end volume of 790^3 = 493,039,000 voxels.

The voxel values of the CT scan images correspond to local sample density, and the sequence of values in any direction is interpreted here as the integrated series, that is, a profile with random (but correlated) increments. Therefore, in what follows, the integration step is omitted in all three versions of the DFA method. Moreover, the vertical (gravity) direction may be here considered as naturally preferential from a phenomenological point of view, but we have performed calculations in all three directions, and have found no significant anisotropy difference. Therefore, henceforth only the results in the vertical direction are reported.

2.4 Results and discussion

The 1D DFA method was applied here for 790x790=624,100 vertical soil sample lines of length 790, across the sample area, emulating a time series of observations of

a virtual observer, descending down the sample at constant speed, at all the different points of the cross-sectional area. The descriptive statistics, the histograms, and spatial distribution of the 1D DFA exponents for the two samples, are presented in table 1, figure 1 and figure 2, respectively. The 1D DFA exponent distributions are found to be statistically the same in all three directions (no anisotropy was observed).

	Minimum	1ºQuartile	Median	Mean	3ºQuartile	Maximum	Standard Deviation
Sugar cane	0.1141	0.2085	0.2255	0.2272	0.2440	0.4725	0.0272
Atlantic Forest	0.1534	0.2703	0.2907	0.2917	0.3119	0.5129	0.0311

Table 1. Descriptive statistics of DFA exponent values for the two samples.



Figure 1. 1D DFA exponent value histograms for the two samples.

It is seen from table 1 and figure 1 that fluctuations of soil density along the vertical direction are strongly antipersistent, with somewhat stronger pronounced antipersistence for the sugar cane sample, in comparison with the Atlantic Forest sample. The intricate spatial distribution of 1D DFA exponents displayed in figure 2 suggests that the local sugarcane soil fluctuations are somewhat more homogeneous than those of the Atlantic Forest.



Figure 2. Color coded DFA exponent values for a) sugarcane, and b) Atlantic Forest sample. The color coding scheme was chosen to emphasize the contrast among the samples, with bounds corresponding to ± 1.5 standard deviations of the composite sample, from the composite mean.

The 2D DFA method was then implemented for 790 vertical soil sample crosssections, of 790x790 voxels each. The descriptive statistics, the histograms, and vertical spatial distribution of the 2D DFA exponents for the two samples, are presented in table 2, figure 3, and figure 4, respectively.

	Minimum	1ºQuartile	Median	Mean	3ºQuartile	Maximum	Standard Deviation
Sugar cane	0.1625	0.1835	0.1911	0.1912	0.1978	0.2224	0.0119
Atlantic Forest	0.2538	0.2618	0.2672	0.2699	0.2750	0.3076	0.0113

Table 2. Descriptive statistics of 2D DFA exponent values for the two samples.

By comparing the results of the 1D DFA presented in table 1 and the 2D DFA presented in table 2, we can confirm that overall the two approaches are compatible: they both show stronger antipersistence of local density fluctuations for the sugar cane sample, in comparison with that of the Atlantic Forest sample, although for both samples the 1D DFA yields somewhat higher exponent values (less pronounced antipersistence), in comparison with the 2D DFA. Moreover, the 1D DFA explores the

vertical antipersistence of density fluctuations across the sample cross-section, revealing the intricate structure of this feature for the chosen projection.



Figure 3. 2D DFA exponent value histograms for the two samples.



Figure 4. 2D DFA exponent values for the two samples, as a function of depth.

Finally, the 3D DFA method yields only two exponent values of $a_3 = 0.2005$ for the sugarcane sample, and $a_3 = 0.2696$ for the Atlantic Forest, rather close to the means of the 2D DFA exponents given in table 2. Comparing all three methods, we can state here that all three yield rather similar results: all three methods indicate strong antipersistence of local density fluctuations, which are consistently stronger (lower exponent value) for the sugar cane sample, than for the Atlantic Forest.

In terms of computational effort and memory requirements, there is no significant difference among the three methods described here (all calculations were performed on an Intel I7-6700HQ processor, in an order of several hours). All three methods also arrive at rather similar quantitative measures of local fluctuation antipersistences, confirming the consistency of the current approach. On the other hand, the multiple 1D approach does seem to provide the most insight into the phenomenon (e.g. the homogeneity and/or the spatial distribution of the 1D DFA exponents observed in figure 2), while sacrificing the separation of the two samples, observed in Figs 1 and 3.

2.5 Conclusions

In terms of comparison of the three schemes of application of the DFA method for three dimensional datasets, we may conclude that the three considered approaches: i) an N×N set of 1D DFA runs for each vertical line of length N, ii) a set of N 2D DFA runs for each of the N×N planes along the vertical direction, and iii) a single 3D DFA run, all yield rather compatible results. More precisely, the 1D DFA yields somewhat higher DFA exponent values (indicate somewhat lower antipersistence) than those of the 2D and 3D DFA (which are practically the same), but the ranking of the results is preserved: sugar cane sample demonstrates lower exponent values (stronger antipersistence) than the Atlantic Forest sample, in all three cases. The fact that the 1D DFA exponent is somewhat higher may be seen as somewhat surprising, as one could well assume *a priori* that whatever antipersistence is observed in a onedimensional sample would be "weakened" when the analysis is extended to two or three dimensions. This could be explained by finite size scaling effects (the sheer sample size): in 1D DFA we are dealing with 624,100 samples of length 790, in 2D DFA there are 790 samples of size $790^2=624,100$, and for the 3D DFA there is a single sample of size 790³=493,039,000. Apparently, the 2D and the 3D samples are large enough to capture the full level of the relation among local density fluctuations, while the 1D DFA does not capture the full level of antipersistence, but it provides a more intricate description of the spatial distribution of antipersistecne of local density fluctuation. As all three approaches are similar in terms of necessary computational effort, we may conclude that all three should be used in unison, complementing the phenomenological picture.

Comparing the current study with previous works that have addressed fractal and multifractal properties of high resolution 2D and 3D CT scan soil samples (LUO; LIN, 2009; PERRET; PRASHER; KACIMOV, 2003; ROY; PERFECT, 2014; SAN JOSÉ MARTÍNEZ *et al.*, 2010; TORRE *et al.*, 2018; TORRE; LOSADA; TARQUIS, 2018; WANG *et al.*, 2016; ZHOU *et al.*, 2010, 2011), it should be emphasized here that all these works deal with the spatial arrangement of voxels. In (LUO; LIN, 2009; PERRET; PRASHER; KACIMOV, 2003; SAN JOSÉ MARTÍNEZ *et al.*, 2010; WANG *et al.*, 2016) thresholding is used to extract the information on pores, and then boxcounting is implemented to study fractal (LUO; LIN, 2009; PERRET; PRASHER; KACIMOV, 2003) and multifractal (SAN JOSÉ MARTÍNEZ *et al.*, 2010; WANG *et al.*, 2016) behavior. In (ZHOU *et al.*, 2010, 2011), Zhou et al. analyze 2D high resolution grayscale soil sample images, wherefrom partition function is constructed to examine multifractal behavior. In a follow-up of this work, Roy and Perfect (ROY; PERFECT, 2014) study 2D grayscale images

in terms of lacunarity and multifractal behavior. Finally, Torre et al (TORRE *et al.*, 2018; TORRE; LOSADA; TARQUIS, 2018) implement cube gliding on CT grayscale soil images to construct the partition function and therefrom derive the multifractal spectrum.

In the current work we adopt a rather different approach: we deal with local density fluctuations, that is, the density difference among neighboring sites (voxels). More precisely, consider a (tiny) observer that can freely hop from site (voxel) to site (another voxel), in one, two, or three dimensions. At each hop, the observer registers a change of density of the environment (voxel, at current experimental resolution). The question is: are these changes random? It turns out that they are not, instead, they are "antipersistent": small changes are more likely to be followed by large changes along the way (in one, two or three dimensions), and vice versa. Moreover, this antipersistence effect is more pronounced in the sugarcane soil sample than in the

Atlantic Forest sample. Whatever may be the practical implications of these phenomenological findings remains to be seen, but as such, we believe that the current work provides a complementary contribution to the understanding of this extremely complex phenomenon: the spatial arrangement of constituent soil particles.

Finally, it should be stressed here that the current approach of combining 1D, 2D and 3D DFA analysis for three-dimensional images is quite general, and can be applied in studies of diverse phenomena.

3. Quantifying soil complexity using Fisher-Shannon method on 3D X-ray CT scans

3.1 Abstract

The conversion of native forests into agricultural land, common in many parts of the world, poses important questions regarding soil degradation, demanding further efforts to understand better the effect of land use change on soil functions. With the advent of 3D Computed Tomography techniques and computing power, new methods are becoming available to address this question. In this direction, in the current work, we modify the Fisher-Shannon method, borrowed from information theory, to quantify the complexity of 12 3D CT soil samples from a sugarcane plantation and 12 samples from a nearby native Atlantic Forest northeastern Brazil. The distinction between the samples from the sugar plantation and the Atlantic Forest site is quite pronounced. The results at 91.7% accuracy were obtained considering the complexity of the Fisher-Shannon plane. Atlantic Forest samples are generally more complex than those from the sugar plantation.

Keywords: complexity, Fisher Shannon plane, land use change, X-ray CT scan soil samples.

3.2 Introduction

The degradation of soils due to land use changes driven by economic factors represents a major concern in many parts of the world for the foreseeable future. Land use change may adversely affect fundamental soil functions such as nutrient storage, diffusion and cycling, carbon storage and greenhouse gas emissions, erosion resistance, water storage, drainage, and filtration (BREUER; PAPEN; BUTTERBACH-BAHL, 2000; LABRIÈRE *et al.*, 2015; TELLES *et al.*, 2003; WILCKE *et al.*, 2002; WOHL *et al.*, 2012). Moreover, the biodiversity of forests may also be unfavourably affected by systematic land use change (FUJII *et al.*, 2018). On the other hand, poverty and population growth lead to an ever-increasing demand for indiscriminate natural

resources in developing countries. The demand for pasture, timber, firewood, and crops drives the conversion of tropical forests into agricultural land at an alarming rate. This situation dictates comprehensive studies on the impact of deforestation and land use conversion on soil quality in general. More precisely, the outstanding question is whether the cultivation of deforested land may lead to the permanent degradation of land productivity. The ecologically sensitive components of the tropical ecosystem may not buffer the effects of agricultural practices, see, e.g. (ISLAM; WEIL, 2000) and references therein. Therefore, a comprehensive assessment of soil properties is fundamental for the early detection and mitigation of adverse soil change effects.

The effects of land use change have been addressed mainly focusing on physical, chemical, and biological properties (ISLAM; WEIL, 2000; LEMENIH; KARLTUN; OLSSON, 2005; MAHARJAN *et al.*, 2017), while far fewer studies have been devoted to changes in soil structure (WANG *et al.*, 2019; ZHOU *et al.*, 2012). The latter governs its functions (RABOT *et al.*, 2018), and quantification of soil architecture can be seen as a key to better understanding the complex dynamical phenomena that govern these functions. Therefore, a comprehensive description and quantification of soil functions rely on an in-depth understanding of the characteristics such as the three-dimensional distribution of constituents, connectedness, hierarchical organization, and complexity.

While X-ray computed tomography (CT) has been advancing at an impressive rate over the last decades, it has also become a widespread tool for non-destructive 3D soil visualization and quantification, shedding new light on soil functions (HELLIWELL *et al.*, 2013). Diverse properties of soil that have not been previously amenable to analyses can now be assessed through CT scans, providing novel fundamental insights into soil functions (HELLIWELL *et al.*, 2013). These properties include isotropy, homogeneity, complexity, and hierarchical fractal (or multifractal) organization of soil constituents. They contribute to a deeper understanding of soil's physical, chemical, and biological processes (SCHLÜTER *et al.*, 2018). X-ray CT scans have already been studied to characterize the pores spatial distribution, revealing the extraordinary complexity of the pore space (GALDOS *et al.*, 2019; JUAREZ *et al.*, 2013; PIRES *et al.*, 2019; SANTOS *et al.*, 2020). The complexity of soil structure has also been addressed through methods based on concepts from statistical physics and information theory, such as fractals and multifractals (PERRET; PRASHER; KACIMOV, 2003; SAN JOSÉ MARTÍNEZ *et al.*, 2010; WANG *et al.*, 2016),

information content (TORRE *et al.*, 2020) and complex networks (CARDENAS *et al.*, 2010; SAMEC *et al.*, 2013). As a consensus has not yet been reached on the adequate threshold for separating pores from solids in CT scans (TARQUIS *et al.*, 2009), it has also been suggested that rather than thresholding, grayscale soil images should be used for multifractal characterization of the soil structure (ROY; PERFECT, 2014; TORRE *et al.*, 2018; TORRE; LOSADA; TARQUIS, 2018; ZHOU *et al.*, 2010, 2011).

Between 2000 and 2018, Brazil suffered a total reduction of 489,877 km² in the natural area of its six terrestrial biomes. Among them, the Atlantic Forest biome is the one with the highest percentage of degradation over time, as it covers the most industrialized and productive areas, in addition to having the highest demographic density in the national territory, housing about 49.3% of the urban areas of the country (IBGE, 2020). One of the crops that stands out in the Atlantic Forest biome is sugarcane, especially in the country's northeast region, where cultivation is present in eight of the nine states in the region. For the 2020/2021 harvest, an increase of 1.6% in the planted area and 4.1% in production were estimated compared to the previous sugarcane harvest in the northeastern region of Brazil (CONAB, 2020). The replacement of the native vegetation of the Atlantic Forest with sugarcane cultivation generates negative impacts on the physical attributes of the soil (BORDONAL et al., 2018; CASTIONI et al., 2018; CAVALCANTI et al., 2020; ORTIZ et al., 2017). These attributes control many soil functions, such as water retention and infiltration, gas exchange, resistance to erosion, nutrient dynamics, and root penetration (RABOT et al., 2018), and directly influence ecosystem services.

In this work, we investigate how land use change affects soil structure using information theory to quantify the complexity of soil 3D X-ray CT soil samples. For the first time, the Fisher-Shannon method (VIGNAT; BERCHER, 2003), introduced to jointly quantify the local and global properties of the probability density function of unidimensional signals, is applied in the context of soil complexity. In the current study, the "signals" are represented by a 790x790 set of 1D vertical lines of 790 greyscale values in X-ray CT scan images of soil samples from a sugarcane field and a nearby Atlantic Forest site in northeastern Brazil. For each image and each of these sequences, we calculate Shannon entropy power (SEP) and Fisher information measure (FIM) that quantify the disorder and structural organization of the signal's variation (MARTIN; PENNINI; PLASTINO, 1999). The joint FIM/SEP analysis is then performed through the Fisher-Shannon information plane (FS) through an innovative

normalization procedure to achieve a 91.7% level of accuracy of distinction between the sugar plantation and the Atlantic Forest samples.

3.3 Methodology

3.3.1 Soil samples

Twenty-four soil samples analyzed in this work were collected from sugarcane cultivation and a nearby native Atlantic Forest in the northeastern Brazilian region, Pernambuco. The site is between latitudes -7.84836 -7.83519, and longitudes - 34.9973 and -34.9935, as shown in figure 1. Two samples were collected at each site, at 10cm and 20cm depth.



Figure 1. Spatial distribution of sample sites, two samples were taken at each site, at 10 and 20cm depth.

The samples were collected using a soil auger with an internal PVC cylinder of 7.5cm height and 7.5cm diameter, excavated by careful penetration with a cylinder coupled with a blade. After the insertion of the auger in the soil, the cylinders were carefully extracted to ensure the preservation of the original structure of the environment inside the PVC cylinders. The samples were then dried at 40°C to remove the water content before the scanning tomography of the samples.

The CT tomography was performed using a third-generation Nikon XT H 225 ST X-ray microtomography with 150kV voltage, 180 μ A current, 500ms exposure time, and a 45 μ m resolution for voxels. A copper filter with a thickness of 0.5 mm was used to minimize low-intensity photons. After scanning the total cylinder volume in the initial acquisition, a sub-volume of interest was defined and reconstructed using CTPro 3D XT 3.0.3 (Nikon Metrology NV) software. The central part of the cylinder was highlighted to avoid edge influence. The reconstructed 2D axial projections maintained the spatial resolution of the acquisition of 45 μ m and were saved at a radiometric resolution (grayscale level) of 16 bits. The final volume was 790 stacks with 790 x 790 pixels, with an end volume of 790³= 493,039,000 voxels.

The voxel values of the CT scan images correspond to the local sample density. Considering the vertical (gravity) direction as naturally preferential from a phenomenological point of view, we perform calculations on 790x790=624,100 vertical lines of 790 grey-level values each for every sample.

3.3.2 The Fisher-Shannon method

The Fisher-Shannon method consists of a joint analysis of Fisher information measure (FIM), which quantifies the amount of organization (or order) in a signal, and Shannon entropy (SE) which quantifies the amount of disorder (VIGNAT; BERCHER, 2003). Fisher introduced the FIM concept in the statistical theory estimation (FISHER, 1925). It was subsequently used to describe physical systems (ESTAÑÓN *et al.*, 2020; FRIEDEN, 1990), as well as for time series analysis in geophysics (MORENO-TORRES *et al.*, 2018; SULEIMANOV; GUSEINOVA, 2019), ecology (BA *et al.*, 2020), astrophysics (LOVALLO; TELESCA, 2011), meteorology (PIERINI *et al.*, 2016; STOSIC; TELESCA; STOSIC, 2021), hydrology (DA SILVA *et al.*, 2021) and social science (LI *et al.*, 2020).

For a continuous one-dimensional variable *X* with probability density function (PDF) f(x), the Fisher information measure I_X is defined as (LI *et al.*, 2020)

$$I_x = \int_{-\infty}^{\infty} \left(\frac{\partial}{\partial x} f(x)\right)^2 \frac{1}{f(x)} dx \quad , \tag{1}$$

and Shannon entropy H_X as

$$H_x = -\int_{-\infty}^{\infty} f(x) \log f(x) dx \quad . \tag{2}$$

The Fisher information measure thus describes the local properties of the PDF, while the Shannon entropy describes its global properties (LI *et al.*, 2020). The shape of the PDF is reflected in these measures, as the FIM assumes high values if the PDF is narrow and low values if the PDF is broad, while SE attains high values for a broad PDF and low values for a narrow PDF.

Instead of Shannon entropy, it is often more convenient (ANGULO; ANTOLÍN; SEN, 2008) to use the quantity called Shannon entropy power (SEP), defined by

$$N_x = \frac{1}{2\pi e} e^{2H_x} (3)$$

The product $C_X = N_X \cdot I_X$ satisfies "isoperimetric inequality" $N_X \cdot I_X \ge 1$ (where equality holds for the Normal distribution), demonstrating that FIM and Shannon entropy are intrinsically related and can be jointly used to characterize the nonstationary behavior of complex signals. The product $N_X I_X$ is called Fisher Shannon complexity (FSC) and can be used as the statistical measure of complexity of the signal under study (DEMBO; COVER; THOMAS, 1991). The joint FIM/SEP analysis is performed through the Fisher Shannon information plane (FS), where Shannon entropy power N_X is used for the horizontal axes, and Fisher information measure I_X is taken for the vertical axis variable (VIGNAT; BERCHER, 2003). The signal is mapped to the point with coordinates (N_X, I_X) which can lie anywhere in the FS plane where the "isoperimetric inequality" $N_X I_X \ge 1$ is satisfied. The distance from the "isocomplexity" line $N_X I_X = 1$ can be used as a measure of the complexity of the signal (LI *et al.*, 2020).

As the above measures depend only on the PDF, Fisher-Shannon analysis can be implemented for real-world datasets corresponding to complex systems through nonparametric density estimation, avoiding parametric assumptions on the distribution. One possibility is using histograms with the discretized version of (1) and (2). However, in this work, we implement kernel density estimation, which is more reliable (TELESCA; LOVALLO, 2017) in the current case. The Kernel density estimator of the PDF is given by (RAYKAR; DURAISWAMI, 2006)

$$\hat{f}_M(x) = \frac{1}{Nb} \sum_{i=1}^N k\left(\frac{x - x_i}{b}\right) \quad , \tag{4}$$

where b > 0 is the so-called bandwidth parameter, *N* is the length of the signal, and K(u) is the kernel function, a continuous symmetric function that satisfies $K(u) \ge 0$ and $\int_{-\infty}^{+\infty} K(u) du = 1$. The most widely used is the Gaussian kernel $k(u) = (2\pi)^{-1/2} exp (-u^2/2)$ yielding

$$\hat{f}_M(x) = \frac{1}{Nb\sqrt{2\pi}} \sum_{i=1}^N e^{-\frac{(x-x_i)^2}{2b^2}} \quad .$$
(5)

3.4 Results and discussion

The I_x , N_x and C_x values were calculated for each of the 624,100 vertical lines of length 790 for all the 24 CT scan images and for the 790 horizontal planes of 790x790=624,100 voxels each, and for the full 790³= 493,039,000 voxel images. After extensive testing with different combinations of quantities and distribution measures that can be extracted from these calculations, we have found that the first option of considering the set of vertical lines for each sample yields the best distinction between the sugar cane and the Atlantic Forest samples. The descriptive statistics (minimum, maximum, quartiles, mean, and standard deviation) of the I_x , N_x and C_x values of vertical lines are presented in Tables I, II and III, respectively, and the distribution of the values in the 790x790 plane for all samples are presented in Figs. 2, 3 and 4.

	min	Q1	Q2	Q3	max	mean	stdev	
Atlantic forest								
AF1-10	4.24E-06	6.07E-06	6.50E-06	7.01E-06	1.62E-05	6.62E-06	8.67E-07	
AF2-10	3.53E-06	6.79E-06	7.52E-06	8.40E-06	1.76E-05	7.70E-06	1.29E-06	
AF3-10	3.65E-06	6.28E-06	6.89E-06	7.64E-06	1.79E-05	7.05E-06	1.09E-06	
AF4-10	3.31E-06	6.54E-06	7.14E-06	7.89E-06	1.69E-05	7.34E-06	1.19E-06	
AF5-10	4.13E-06	7.13E-06	7.90E-06	8.81E-06	2.02E-05	8.08E-06	1.36E-06	
AF6-10	3.79E-06	9.58E-06	1.07E-05	1.19E-05	2.59E-05	1.08E-05	1.86E-06	
AF1-20	4.51E-06	7.46E-06	8.14E-06	8.86E-06	1.46E-05	8.20E-06	1.03E-06	
AF2-20	3.32E-06	8.10E-06	9.02E-06	1.01E-05	1.78E-05	9.15E-06	1.47E-06	
AF3-20	3.45E-06	7.63E-06	8.37E-06	9.20E-06	1.74E-05	8.47E-06	1.19E-06	
AF4-20	3.93E-06	7.47E-06	8.20E-06	9.04E-06	1.58E-05	8.31E-06	1.18E-06	
AF5-20	3.69E-06	7.33E-06	8.18E-06	9.21E-06	1.82E-05	8.37E-06	1.50E-06	
AF6-20	4.08E-06	8.11E-06	9.08E-06	1.02E-05	1.82E-05	9.22E-06	1.54E-06	
			Suga	rcane				
SC1-10	4.91E-06	8.15E-06	8.76E-06	9.40E-06	1.45E-05	8.80E-06	9.37E-07	
SC2-10	3.24E-06	8.35E-06	9.35E-06	1.05E-05	2.02E-05	9.47E-06	1.60E-06	
SC3-10	3.57E-06	9.05E-06	9.78E-06	1.05E-05	1.61E-05	9.81E-06	1.13E-06	
SC4-10	4.52E-06	9.02E-06	9.77E-06	1.06E-05	1.71E-05	9.83E-06	1.16E-06	
SC5-10	4.01E-06	9.22E-06	1.01E-05	1.10E-05	1.82E-05	1.01E-05	1.31E-06	
SC6-10	3.67E-06	1.07E-05	1.17E-05	1.27E-05	1.94E-05	1.17E-05	1.45E-06	
SC1-20	5.11e-06	1.03e-05	1.11e-05	1.19e-05	1.72e-05	1.11e-05	1.15e-06	
SC2-20	3.51E-06	8.54E-06	9.36E-06	1.02E-05	1.81E-05	9.43E-06	1.30E-06	
SC3-20	3.46E-06	9.87E-06	1.07E-05	1.15E-05	1.78E-05	1.07E-05	1.24E-06	
SC4-20	3.96E-06	7.93E-06	8.71E-06	9.57E-06	1.72E-05	8.81E-06	1.26E-06	
SC5-20	3.71E-06	9.17E-06	1.01E-05	1.11E-05	1.79E-05	1.01E-05	1.43E-06	
SC6-20	6.56E-06	1.27E-05	1.41E-05	1.56E-05	2.68E-05	1.42E-05	2.17E-06	

Table 1. Descriptive Statistics of Fisher Information Measure I_x .

Table 2. Descriptive Statisti	s of Shannon entrop	y power N_x .
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	min	Q1	Q2	Q3	max	mean	stdev	
Atlantic forest								
AF1-10	1.24E+05	2.14E+05	2.37E+05	2.62E+05	4.10E+05	2.39E+05	3.53E+04	
AF2-10	7.07E+04	1.84E+05	2.11E+05	2.39E+05	6.14E+05	2.13E+05	4.03E+04	
AF3-10	7.43E+04	1.92E+05	2.17E+05	2.44E+05	6.00E+05	2.20E+05	3.99E+04	
AF4-10	9.73E+04	1.85E+05	2.09E+05	2.37E+05	6.23E+05	2.15E+05	4.63E+04	
AF5-10	8.54E+04	1.76E+05	2.03E+05	2.34E+05	3.88E+05	2.06E+05	4.05E+04	
AF6-10	5.55E+04	1.04E+05	1.30E+05	1.65E+05	4.34E+05	1.38E+05	4.11E+04	
AF1-20	7.64E+04	1.30E+05	1.45E+05	1.62E+05	3.72E+05	1.48E+05	2.40E+04	
AF2-20	6.30E+04	1.22E+05	1.39E+05	1.60E+05	7.27E+05	1.43E+05	3.08E+04	
AF3-20	5.92E+04	1.25E+05	1.41E+05	1.58E+05	9.73E+05	1.44E+05	2.84E+04	
AF4-20	7.90E+04	1.40E+05	1.58E+05	1.82E+05	3.96E+05	1.64E+05	3.44E+04	
AF5-20	6.98E+04	1.47E+05	1.72E+05	2.03E+05	5.56E+05	1.78E+05	4.29E+04	
AF6-20	5.91E+04	1.18E+05	1.36E+05	1.58E+05	5.51E+05	1.39E+05	2.98E+04	
			Suga	rcane				
SC1-10	7.31E+04	1.19E+05	1.29E+05	1.41E+05	3.03E+05	1.31E+05	1.71E+04	
SC2-10	6.34E+04	1.40E+05	1.72E+05	2.13E+05	9.73E+05	1.79E+05	5.13E+04	
SC3-10	6.82E+04	1.06E+05	1.16E+05	1.29E+05	8.74E+05	1.20E+05	2.02E+04	
SC4-10	6.50E+04	1.05E+05	1.15E+05	1.28E+05	4.23E+05	1.17E+05	1.82E+04	
SC5-10	6.23E+04	1.02E+05	1.14E+05	1.31E+05	4.34E+05	1.20E+05	2.60E+04	
SC6-10	5.43E+04	8.70E+04	9.63E+04	1.08E+05	7.01E+05	9.86E+04	1.63E+04	
SC1-20	6.05E+04	9.01E+04	9.72E+04	1.05E+05	3.58E+05	9.84E+04	1.22E+04	
SC2-20	5.79E+04	1.12E+05	1.26E+05	1.43E+05	1.05E+06	1.30E+05	2.68E+04	
SC3-20	5.88E+04	9.36E+04	1.02E+05	1.12E+05	1.10E+06	1.04E+05	1.54E+04	
SC4-20	6.46E+04	1.24E+05	1.39E+05	1.57E+05	4.46E+05	1.43E+05	2.69E+04	
SC5-20	5.79E+04	1.00E+05	1.12E+05	1.27E+05	5.15E+05	1.17E+05	2.52E+04	
SC6-20	3.83E+04	7.48E+04	8.49E+04	9.66E+04	2.19E+05	8.69E+04	1.72E+04	

	min	Q1	Q2	Q3	max	mean	stdev	
Atlantic forest								
AF1-10	1.05E+00	1.36E+00	1.51E+00	1.72E+00	4.30E+00	1.58E+00	3.22E-01	
AF2-10	1.02E+00	1.36E+00	1.53E+00	1.79E+00	4.61E+00	1.63E+00	3.89E-01	
AF3-10	1.03E+00	1.33E+00	1.46E+00	1.65E+00	4.13E+00	1.54E+00	3.11E-01	
AF4-10	1.03E+00	1.30E+00	1.44E+00	1.68E+00	5.08E+00	1.58E+00	4.53E-01	
AF5-10	1.02E+00	1.35E+00	1.54E+00	1.84E+00	4.69E+00	1.65E+00	4.22E-01	
AF6-10	1.01E+00	1.14E+00	1.32E+00	1.64E+00	5.48E+00	1.47E+00	4.74E-01	
AF1-20	1.01E+00	1.12E+00	1.17E+00	1.24E+00	2.29E+00	1.19E+00	1.00E-01	
AF2-20	1.01E+00	1.14E+00	1.21E+00	1.33E+00	4.13E+00	1.29E+00	2.69E-01	
AF3-20	1.01E+00	1.11E+00	1.16E+00	1.23E+00	4.13E+00	1.20E+00	1.61E-01	
AF4-20	1.01E+00	1.18E+00	1.27E+00	1.40E+00	3.58E+00	1.34E+00	2.55E-01	
AF5-20	1.01E+00	1.22E+00	1.34E+00	1.55E+00	4.85E+00	1.47E+00	4.17E-01	
AF6-20	1.01E+00	1.13E+00	1.21E+00	1.31E+00	2.71E+00	1.25E+00	1.68E-01	
			Suga	rcane				
SC1-10	1.01E+00	1.09E+00	1.12E+00	1.17E+00	2.00E+00	1.14E+00	7.35E-02	
SC2-10	1.01E+00	1.29E+00	1.50E+00	1.91E+00	4.44E+00	1.68E+00	5.32E-01	
SC3-10	1.01E+00	1.08E+00	1.12E+00	1.20E+00	3.55E+00	1.16E+00	1.19E-01	
SC4-10	1.01E+00	1.08E+00	1.11E+00	1.17E+00	2.38E+00	1.14E+00	9.14E-02	
SC5-10	1.01E+00	1.08E+00	1.12E+00	1.21E+00	3.79E+00	1.19E+00	2.29E-01	
SC6-10	1.00E+00	1.07E+00	1.11E+00	1.17E+00	2.87E+00	1.14E+00	1.02E-01	
SC1-20	1.00E+00	1.05E+00	1.07E+00	1.10E+00	1.97E+00	1.08E+00	5.51E-02	
SC2-20	1.01E+00	1.10E+00	1.16E+00	1.25E+00	4.03E+00	1.20E+00	1.43E-01	
SC3-20	1.01E+00	1.05E+00	1.08E+00	1.12E+00	4.82E+00	1.10E+00	6.40E-02	
SC4-20	1.01E+00	1.14E+00	1.20E+00	1.28E+00	3.19E+00	1.23E+00	1.34E-01	
SC5-20	1.01E+00	1.08E+00	1.12E+00	1.19E+00	3.36E+00	1.15E+00	1.27E-01	
SC6-20	1.00E+00	1.11E+00	1.18E+00	1.27E+00	2.73E+00	1.20E+00	1.28E-01	

Table 3. Descriptive Statistics of Fisher-Shannon complexity C_x .

In order to address the distance from the iso-complexity line $N_X I_X = 1$ as a measure of the complexity of the vertical sample lines (LI *et al.*, 2020), it should be noted that the scales of Shannon entropy power with an average of $\langle N_x \rangle = 1.497 \times 10^5$ and Fisher Information with average $\langle I_x \rangle = 9.307 \times 10^{-6}$ differ in orders of magnitude, while the average the Fisher-Shannon complexity $\langle C_x \rangle = 1.317$ is of the order of unity. If the projection of a point (N_X , I_X) in the FS plane presented in figure 5a to the nearest point on the "isocomplexity" line is denoted by (N_{X0} , I_{X0}), then the displacement of Shannon Information $\Delta I_X \equiv I_X - I_{X0}$ turns negligible in comparison with the displacement of Shannon entropy power $\Delta N_X \equiv N_X - N_{X0}$, and by minimizing the distance to the iso-complexity line, the points are projected vertically down to the isocomplexity line, and the Euclidean distance is practically reduced to ΔN_X , with no influence of ΔI_X .



Figure 2. Spatial distribution of the I_x values in the horizontal projection plane for each sample. Pixels are colour-coded in blue below two standard deviations from the global average and red for values above two standard deviations. A spectrum of colors is used for values in between, as per the colour bar.



Figure 3. Spatial distribution of the N_x values in the horizontal projection plane for each sample. Pixels are colour-coded in blue below two standard deviations from the global average and red for values above two standard deviations. A spectrum of colors is used for values in between, as per the colour bar.



Figure 4. Spatial distribution of the C_x values in the horizontal projection plane for each sample. Pixels are colour-coded in blue below two standard deviations from the global average and red for values above two standard deviations. A spectrum of colors is used for values in between, as per the colour bar.

To mitigate this fact, here we introduce a novel normalization procedure for the variables N_X and I_X . More precisely, first, we identify the maximum value N_{Xmax} among all the samples, and we scale all the sample values as $N'_X = N_X/N_{Xmax}$ and $I'_X = I_X N_{Xmax}$, thus **preserving** the $C_x \equiv N_X I_X$ complexity values. Distance from a point (N'_X, I'_X) to a projection point (N'_{XI}, I'_{XI}) on the isocomplexity plane is now given by

$$d = \sqrt{(N'_X - N'_{XI})^2 + \left(I'_X - \frac{1}{N'_{XI}}\right)^2} , \qquad (6)$$

and setting the derivative of *d* concerning N'_{XI} to zero to find the closest point (N'_{X0}, I'_{X0}) yields the fourth-order polynomial expression for $x \equiv N'_{X0} \equiv 1/I'_{X0}$

$$x^4 - x^3 N'_X + x I'_X - 1 = 0 \quad , \tag{7}$$

which is solved numerically for all samples. The results of this novel procedure are presented in figure 5b, and the distances scatterplot from the iso-complexity plane is presented in figure 6.



Figure 5 a) Scatterplot of the original (N_X, I_X) value pairs, and b) a scatterplot of the normalized values (N'_X, I'_X) , together with projections (N'_{X0}, I'_{X0}) to the closest point on the iso-complexity line.

The Sugarcane sample's complexity, quantified by the distance from the isocomplexity line (figures 4 and 5), is generally lower than those of the Atlantic Forest samples, exhibiting large fluctuations between the alternative values from samples taken at 10cm and 20cm depth. The complexity values are presented in Table IV.



Figure 6 The distances scatterplot from the iso-complexity line, in the order of samples from south to north.

Sugarcane							
SC1-10	SC2-10	SC3-10	SC4-10	SC5-10	SC6-10		
0.0676	0.2899	0.0696	0.0619	0.0825	0.0531		
SC1-20	SC2-20	SC3-20	SC4-20	SC5-20	SC6-20		
0.0342	0.0951	0.0420	0.1144	0.0714	0.0660		
Atlantic forest							
AF1-10	AF2-10	AF3-10	AF4-10	AF5-10	AF6-10		
AF1-10 0.3290	AF2-10 0.3198	AF3-10 0.2961	AF4-10 0.3022	AF5-10 0.3179	AF6-10 0.1799		
AF1-10 0.3290 AF1-20	AF2-10 0.3198 AF2-20	AF3-10 0.2961 AF3-20	AF4-10 0.3022 AF4-20	AF5-10 0.3179 AF5-20	AF6-10 0.1799 AF6-20		

Table 4. Complexity (distance from the isocomplexity plane).



To demonstrate the validity of this novel approach, we show in figure 7 the 3D images of the two samples with the lowest and highest complexity, respectively.

Figure 7. Samples SC1_20 with d=0.0342 (left), and AF1_10 with d=0.329 (right), at a threshold of 1500 Hounsfield units.

The current approach, without arbitrary parameters (e.g., threshold), yields results that agree well with a visual observation (as seen in figure 5) and provides a precise quantitative measure of the samples' complexity. The usefulness of this approach for quantifying soil degradation should be tested in future studies in the natural environment and controlled laboratory experiments.

Finally, to test the discriminative power of the current approach, we implement here the fitting of values from table 4 to a logistic function, where a categorical variable of zero value is attributed to the sugarcane samples and unit value to the Atlantic Forest samples, with results shown in figure 8.

Considering logistic regression as a binary classifier, the threshold of d=0.0952 separates the two groups of samples, with only two samples (SC2-10 and SC4-20) falling into the wrong category. It should be noted here that the k-means method does not produce meaningful results in this case because of the difference in the variance of the d values of the two groups, which is much smaller for the sugarcane samples than for the Atlantic Forest samples.



Figure 8. Fit to a logistic function. The vertical dashed line represents the threshold d = 0.0952.

Observing the images of I_x , N_x and C_x of the spatial distribution of these samples in Figs. 2, 3 and 4 reveals that the origin of the strikingly high value of d =0.290 for sample SC2-10 stems from the pronounced values of Shannon entropy power N_x . This entropy, in combination with Information, measures values I_x yield Fisher-Shannon complexity C_x for each of the 624,100 vertical lines, somewhat similar to those of the Atlantic Forest samples. Therefore, a correct grouping of 22 out of 24 samples (91.7%) is attained, demonstrating the power of the current novel nonparametric approach.

3.5 Conclusions

Overall, we can claim that the Fisher-Shannon complexity captures the morphological changes induced by land-use change relatively well. More precisely, the sugarcane field sites lie in an area converted from an Atlantic Forest to a plantation.

The subsequent cultivation activities have brought about changes in the soil morphology. While the results are not entirely consistent regarding depth and/or position, the 91.7% grouping success rate may be considered relatively high, where the discrepancies may be attributed to some yet unknown particularities of these sites.

The approach introduced in the current work does not use arbitrary parameters. It provides a rather precise quantitative complexity measure, which may be seen as a quantifier of soil degradation level. Finally, the novel normalization procedure of variables for representation in the Fisher-Shannon information plane, preserving the Fisher-Shannon complexity, may be helpful for general time series and image analysis.

4. Final considerations

In this work two methods, originally used for the analysis of complex signals, Detrended Fluctuation Analysis (DFA) and Fisher-Shannon method (FS), were applied for the first time in the context of innovative analysis of 3D tomographic images of soil. The methods were adapted for image analysis in general, in this case 3D CT images of soil samples from undisturbed sites covered by Atlantic Forest and sites that undergo soil degradation due to land cover change (replacement of native Atlantic Forest vegetation by sugarcane).

Each 3D image contains NxNxN gray level voxel values (N=790) so 1D DFA was applied on NxN vertical lines of length N, 2D DFA on N planes of size NxN along the vertical direction, and 3D DFA on the whole NxNxN dataset. In all cases the values of DFA exponents were found to be smaller than 0.5 indicating antipersistence of local density fluctuations, which are consistently stronger (lower exponent value) for the sugar cane plantation sample, than for the Atlantic Forest.

The FS method was applied on NxN vertical lines of length N (N=790) for 24 3D soil images (12 samples from Atlantic Forest and 12 samples from sugarcane plantation, obtained at 10cm and 20 cm depth). For each vertical line the FS information quantifiers Shannon entropy and Fisher information measure were calculated, and a novel method is introduced here for their proper normalization, preserving the Fisher Shannon complexity. In this way a complexity measure is defined as the distance from the isocomplexity line in the normalized FS plane, which may be seen as a quantifier of soil degradation level. This novel approach resulted in a high grouping success rate (91.7%) between soil covered by native vegetation (Atlantic Forest) and soil that was the subject of degradation process as the consequence of land use change (from native Atlantic Forest to sugarcane cultivation).

To achieve the proposed objectives in this work, two programs were developed in C programming language, one that implements the DFA (1D, 2D, and 3D) and the other that implements the FS method, both suitable for 3D tomographic image data from soil samples. While each image is composed of 790x790x790 16-bit voxels, totaling 986,078,000 bytes, on one of the computers used in data processing with an I7-7700HQ 2.80GHz processor with 16 GB of RAM, the processing time for each image in the DFA method was relatively short, approximately 90 seconds. The processing time for each image using the FS method on the same computer was relatively high, around 5 hours. For this reason, parallel processing of 4 images simultaneously was implemented in the case of the FS method.

The results of this work showed that some methods that are used for the analysis of one-dimensional signals can be adapted for the analysis of 2D and 3D images. The suggestion for future work for investigation of soil degradation by analysis of 3D tomographic images from undisturbed and disturbed sites are the use of Multifractal detrended fluctuation analysis (MFDFA) in its original 1D form and its 2D and 3D generalization. Along the information of persistency of density fluctuations obtained by DFA, MFDFA also provides the information about the dominance of large/small fluctuations and the degree of signal multifractality (trough the set of parameters of the multifractal spectrum) and these properties could be used as a "fingerprint" of analyzed images. Other methods such as Visibility Graph and Recurrence Plot (together with Recurrence quantification analysis) that provide the set of quantitative measures that describe signal complexity could also be tested for image analysis in general.

In summary, considering the continuous advent of non-invasive X-ray tomographic methods over the last decades, together with the exponential growth of accessible computer power, the spectrum of techniques from other fields of knowledge (such as complex systems theory, information theory, complex networks and statistical physics) that may be adapted for soil sample analysis is rapidly growing, promising novel complementary insights into the intricate structure of soil. The current work should be therefore understood as a contribution in this direction, where two wellknown methods originally used for the analysis of complex signals were adapted for this purpose.

5. Supplementary information

Sample	Land use	Depth (cm)	Soil type	Latitude	Longitude
AF1-10	Atlantic Forest	10	Spodosol	-7.84791	-34.99660
AF2-10	Atlantic Forest	10	Argisol	-7.84562	-34.99575
AF3-10	Atlantic Forest	10	Spodosol	-7.84396	-34.99542
AF4-10	Atlantic Forest	10	Latosol	-7.84084	-34.99511
AF5-10	Atlantic Forest	10	Latosol	-7.83650	-34.99666
AF6-10	Atlantic Forest	10	Latosol	-7.83527	-34.99729
AF1-20	Atlantic Forest	20	Spodosol	-7.84791	-34.99660
AF2-20	Atlantic Forest	20	Latosol	-7.84562	-34.99575
AF3-20	Atlantic Forest	20	Latosol	-7.84396	-34.99542
AF4-20	Atlantic Forest	20	Latosol	-7.84084	-34.99511
AF5-20	Atlantic Forest	20	Latosol	-7.83650	-34.99666
AF6-20	Atlantic Forest	20	Latosol	-7.83527	-34.99729
SC1-10	Sugarcane	10	Spodosol	-7.84836	-34.99551
SC2-10	Sugarcane	10	Argisol	-7.84583	-34.99483
SC3-10	Sugarcane	10	Spodosol	-7.84441	-34.99428
SC4-10	Sugarcane	10	Latosol	-7.83860	-34.99346
SC5-10	Sugarcane	10	Latosol	-7.83610	-34.99610
SC6-10	Sugarcane	10	Latosol	-7.83519	-34.99612
SC1-20	Sugarcane	20	Spodosol	-7.84836	-34.99551
SC2-20	Sugarcane	20	Argisol	-7.84583	-34.99483
SC3-20	Sugarcane	20	Spodosol	-7.84441	-34.99428
SC4-20	Sugarcane	20	Latosol	-7.83860	-34.99346
SC5-20	Sugarcane	20	Latosol	-7.83610	-34.99610
SC6-20	Sugarcane	20	Latosol	-7.83519	-34.99612

Table 1: Characteristics and coordinates of soil samples.

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