- The Structure of Chaos: An Empirical Comparison of Fractal Physiology
 Complexity Indices using NeuroKit2
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Abstract

Complexity quantification, through entropy, information and fractal dimension indices, is 21 gaining a renewed traction in psychopsyiology, as new measures with promising qualities 22 emerge from the computational and mathematical advances. Unfortunately, few studies 23 compare the relationship and objective performance of the plethora of existing metrics, in turn hindering reproducibility, replicability, consistency, and restults clarity in the field. In 25 this study, we systematically compared 125 indices of complexity by their computational 26 weight, their representativeness of a multidimensional space of latent dimensions, and 27 empirical proximity with other indices. We propose that a selection of indices, including 28 ShanEn (D), MSWPEn, CWPEn, FuzzyMSEn, AttEn, NLDFD, Hjorth, MFDFA (Width), 29 MFDFA (Max), MFDFA (Mean), SVDEn, MFDFA (Increment), might offer a complimentary choice in regards to the quantification of the complexity of time series. 31

32 Keywords: chaos, complexity, fractal, physiology, noise

Word count: 2587

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36 Introduction

Complexity is an umbrella term for concepts derived from information theory, chaos
theory, and fractal mathematics, used to quantify unpredictability, entropy, and/or
randomness. Using these methods to characterize physiological signals (a subfield
commonly referred to as "fractal physiology," Bassingthwaighte et al., 2013) has shown
promising results in the assessment and diagnostic of the state and health of living systems
Goetz (2007).

There has been an exponential increase in the number of complexity indices in the
past few decades (A. C. Yang & Tsai, 2013). Although these new procedures are usually
mathematically well-defined and theoretically promising, limited empirical evidence is
available to understand their similarities and differences (Lau et al., 2021; A. C. Yang &
Tsai, 2013). Moreover, some of these methods are resource-intensive and require long
computation times. This complicates their application with techniques that utilise high
sampling-rates (e.g., M/EEG) and makes them impractical to implement in real-time
settings - such as brain-computer interfaces (Manis et al., 2018; "Refined Composite
Multiscale Dispersion Entropy and Its Application to Biomedical Signals," 2017). As such,
having empirical data about the computation time of various complexity indices would
prove useful, for instance to objectively guide their selection, especially in contexts where
time or computational resources are limited.

Additionally, the lack of a comprehensive open-source and user-friendly software for computing various complexity indices likely contributes to the limited availability of empirical comparison (Flood & Grimm, 2021a). Indeed, most complexity indices are only described mathematically in journal articles, with reusable code seldom made available, therefore limiting their further application and validation (Flood & Grimm, 2021a; A. C.

- Yang & Tsai, 2013). To address this gap, we added a comprehensive set of
 complexity-related features to NeuroKit2, a Python package for physiological signal
 processing (Makowski et al., 2021). This submodule aims at enabling users to compute a
 vast amount of complexity indices. The code is designed to be as fast as possible, while
 still written in pure Python (though with the help^of dependencies such as Numpy or
 Pandas, Harris et al., 2020; McKinney et al., 2010) to maximize the re-usability,
 transparency, and correctness.
- Leveraging this tool, the goal of this study is to empirically compare a large number of complexity indices, inspect how they relate to one another, and derive recommendations for indices selection. More specifically, we will quantify the complexity using 128 indices of various types of signals with varying degrees of noise, using *NeuroKit2*. We will then project the results on a latent space through factor analysis, and review the various indices that we find the most relevant and interesting in regards to their representation of the latent dimensions. This analysis will be complemented by hierarchical clustering.

74 Methods

The script to generate the data can be found at

 $_{76} \quad github.com/neuropsychology/NeuroKit/studies/complexity_benchmark.$

We started by generating 5 types of signals, one random-walk, two oscillatory signals made (with one made of harmonic frequencies that results in a self-repeating - fractal-like - signal), and two complex signals derived from Lorenz systems (with parameters $(\sigma = 10, \beta = 2.5, \rho = 28)$; and $(\sigma = 20, \beta = 2, \rho = 30)$, respectively). Each of this signal was iteratively generated at 5 different lengths. The resulting vectors were standardized and each were added 5 types of $(1/f)^{\beta}$ noise (namely violet $\beta = -2$, blue $\beta = -1$, white $\beta = 0$, pink $\beta = 1$, and brown $\beta = 2$ noise). Each noise type was added at 48 different intensities (linearly ranging from 0.1 to 4). Examples of generated signals are presented in **Figure 1**.

The combination of these parameters resulted in a total of 6000 signal iterations. For each of them, we computed 128 complexity indices, and additional basic metrics such as the standard deviation (SD), the length of the signal and its dominant frequency. We also included a random number to make sure that our our dimensionality analyses accurately discriminate this unrelated feature. The parameters used (such as the time-delay τ or the embedding dimension) are documented in the data generation script. For a complete description of the various indices included, please refer to NeuroKit's documentation at https://neuropsychology.github.io/NeuroKit.

m_{93} Results

The data analysis script, the data and the code for the figures is fully available at github.com/neuropsychology/NeuroKit/studies/complexity_benchmark. The analysis was performed in R using the easystats collection of packages (Lüdecke et al., 2021; Lüdecke et al., 2020; Makowski et al., 2020/2022, 2020).

Computation Time. Firstly, one should note that the computation times

presented in Figure 2 are relative and do not correspond to real times, as these would

highly depend on the machine used. Instead, the goal is here to convey some intuition on

the differences between different classes of indices (using the same machine and the same

language of implementation, i.e., Python). It is possible that computational advances or

improvements in the code efficiency might change some of these values, but we believe that

the "big picture" should remain fairly stable, as it is to a large extend driven by the

inherent nature of the algorithms under consideration.

Despite the relative shortness of the signals considered (a few thousand points at most), the fully-parallelized data generation script took 24h to run on a 48-cores machine.

After summarizing and sorting the indices by computation time, the most striking feature is the order of magnitude of difference between the fastest and slowest indices. Additionally, some indices are particularly sensitive to the signal length, a property which combined with

computational cost led to indices being 100,000 times slower to compute than others.

In particular, multiscale indices were among the slowest to compute due to their iterative nature (a given index is computed multiple times on coarse-grained subseries of the signal). Indices related to Recurrence Quantification Analysis (RQA) were also relatively slow and did not scale well with signal length.

For the subsequent analyses, we removed statistically redundant indices, such as

PowEn - identical to SD, CREn (100) - identical to CREn (10), and FuzzyRCMSEn
identical to RCMSEn.

Correlation. The Pearson correlation analysis revealed that complexity indices,
despite their multitude and their conceptual specificities, do indeed share similarities. They
form two major clusters that are easily observable (the blue and the red groups in Figure
2). However, these two anti-correlated groups are mostly revealing of the fact that some
indices, by design, index the "predictability", whereas others, the "randomness", and thus
are negatively related to one-another. In order to extract finer groupings, further analyses
procedures are applied below.

Factor Analysis. The agreement procedure for the optimal number of factors
suggested that the 125 indices can be mapped on a multidimensional space of 14
orthogonal latent factors, that we extracted using a *varimax* rotation. We then took
interest in the loading profile of each index, and in particular the latent dimension that it
maximally relates to (see **Figure 3**).

This first factor is the closest to the largest amount of indices, and is positively loaded by indices that are sensitive to the deviation of consecutive differences (e.g., ShanEn - D, NLDFD, PFD - D). In line with this, this factor was negatively loaded by indices related to Detrended Fluctuation Analysis (DFA), which tends to index the presence of long-term correlations. As such, this latent factor might encapsulate the predominance of short-term vs. long-term unpredictability. The second factor was strongly loaded by signal

163

length and SD, and thus might not capture features of complexity per se. Indices with the 137 most relation to it were indices known to be sensitive to signal length, such as ApEn. The 138 third factor included multiscale indices, such as MSWPEn. The fourth factor was loaded 139 by permutation entropy indices, such as WPEn. The fifth and the sixth factors were loaded 140 by indices grouped by the signal symbolization method used (by a tolerance level r, or by 141 the number of bins for the fifth and the sixth factors, respectively). The seventh factor was 142 loaded positively by the amount of noise, and negatively by multifractal indices such as 143 MFDFA - Increment, suggesting a sensitivity to regularity. Finally, as a manipulation check for our factorization method, the random vector did not load unto any factors. 145 Hierarchical Clustering and Connectivity Network. For illustration 146 purposes, we represented the correlation matrix as a connectivity graph (see **Figure 4**). 147 We then ran a hierarchical clustering (with a Ward D2 distance) to provide additional 148 information or confirmation about the groups discussed above. This allowed us to 149 fine-grain our recommendations of complimentary complexity indices (see **Figure 5**). 150 **Indices Selection.** The selection of a subset of indices was based on the following 151 considerations: 1) high loadings on one predominant latent dimension, with additional 152 attention to the pattern of secondary loadings. For instance, an index with a positive 153 factor 1 loading and a negative factor 2 loading could complement another index with a 154 similar factor 1 loading, but a positive factor 2 loading. This was helped by 2) the 155 hierarchical clustering dendrogram, with which we attempted to indices from each 156 (meaningful) higher order clusters. Items related to clusters that we know were related to 157 noise, length or other artifacts were omitted. 3) A preference for indices with relatively 158 shorter computation times. This yielded a selection of 12 indices. Next, we computed the cumulative variance explained of this selection in respect to the entirety of indices, and derived the optimal order to maximize the variance explained (see **Figure 6**). The 12 161 included indices, representing 91.01% of the variance of the whole dataset, were: 162

• ShanEn (D): The Shannon Entropy of the symbolic times series obtained by the "D"

- method described in Petrosian (1995) used traditionally in the context of the

 Petrosian fractal dimension (Esteller et al., 2001). The successive differences of the

 time series are assigned to 1 if the difference exceeds one standard deviation or 0

 otherwise. The Entropy of the probabilities of these two events is then computed.
- MSWPEn: The Multiscale Weighted Permutation Entropy is the entropy of weighted ordinal descriptors of the time-embedded signal computed at different scales obtained by a coarsegraining procedure (Fadlallah et al., 2013).
- CWPEn: The Conditional Weighted Permutation Entropy is based on the difference of weighted entropy between that obtained at an embedding dimension m and that obtained at m + 1 (Unakafov & Keller, 2014).
- FuzzyMSEn: This index corresponds to the multiscale Fuzzy Sample Entropy

 (Ishikawa & Mieno, 1979). This algorithm is computationally expensive to run.
- AttEn: The Attention Entropy is based on the frequency distribution of the intervals between the local maxima and minima of the time series (J. Yang et al., 2020).
- NLDFD: The Fractal dimension via Normalized Length Density (NLD) corresponds
 to the average absolute consecutive differences of the standardized signal (Kalauzi et al., 2009).
- *Hjorth*: Hjorth's Complexity is defined as the ratio of the mobility of the first derivative of the signal to the mean frequency of the signal (Hjorth, 1970).
- MFDFA (Width): The width of the multifractal singularity spectrum (Kantelhardt et al., 2002) obtained via Detrended Fluctuation Analysis (DFA).
- MFDFA (Max): The value of singularity spectrum D corresponding to the maximum value of singularity exponent H.
- MFDFA (Mean): The mean of the maximum and minimum values of singularity exponent H.
- SVDEn: Singular Value Decomposition (SVD) Entropy quantifies the amount of eigenvectors needed for an adequate representation of the signal (Roberts et al.,

1999).

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• MFDFA (Increment): The cumulative function of the squared increments of the generalized Hurst's exponents between consecutive moment orders (Faini et al., 2021).

Finally, we visualized the expected value of our selection of indices for different types of signals under different conditions of noise (see **Figure 7**). This revealed that two indices, namely *ShanEn (D)* and *NLDFD*, are primarily driven by the noise intensity (which is expected, as they capture the variability of successive differences). The other indices appear to be able to discriminate between the various types of signals (when the signal is not dominated by noise).

oo Discussion

215

As the span and application of complexity science grows, a systematic approach to 201 compare their "performance" becomes necessary to reinforce the clarity and structure of the 202 field. The term *performance* is here to be understood in a relative sense, as any such 203 endeavor faces the "hard problem" of complexity science: various objective properties of signals (e.g., short-term vs. long-term variability, auto-correlation, information, randomness, Namdari & Li, 2019; Xiong et al., 2017) participate in forming together 206 over-arching concepts such as "complex" and "chaotic". Indices that are sensitive to some 207 of these objective properties are thus conceptually linked through these over-arching 208 framework. However, it remains unclear how these high-level concepts transfer back, in a 209 top-down fashion, into a combination of lower-level features. As such, it is conceptually 210 complicated to benchmark complexity measures against "objectively" complex 211 vs. non-complex signals. In other words, we know that different objective signal 212 characteristics can contribute to the "complexity" of a signal, but there is not a one-to-one 213 correspondence between the latter and the former. 214

To circumvent the aforementioned consideration, we adopted a paradigm where we

generated different types of signals to which we systematically added distinct types - and
amount - of perturbations. It is to note that we did not seek at measuring how complexity
indices can discriminate between these signal types, nor did we attempt at mimicking
real-life signals or scenarios. The goal was instead to generate enough variability to reliably
map the relationships between the indices.

Our results empirical confirm the plurality of underlying components of complexity
(although it is here defined somewhat circularly as what is measured by complexity
indices), and more importantly show that complexity indices vary in their sensitivity to
various orthogonal latent dimensions. However, the limited possibilities of interpretation of
these dimensions is a limitation of the present investigation, and future studies are needed
to investigate and discuss them in greater depth (for instance, by modulating specific
properties of signals and measuring their impact on these latent dimensions).

Taking into account the increasing role of complexity science as a field and the sheer 228 number of complexity indices already published, our study aimed at empirically map the 229 relationship between various indices and provide useful information to guide future 230 researchers in their selection. Indices that were highlighted as encapsulating information 231 about different underlying dimensions at a relatively low computational cost include 232 ShanEn (D), MSWPEn, CWPEn, FuzzyMSEn, AttEn, NLDFD, Hjorth, MFDFA (Width), MFDFA (Max), MFDFA (Mean), SVDEn, MFDFA (Increment). These indices might be complimentary in offering a comprehensive profile of the complexity of a time series. Moving forward, future studies are needed to validate, analyze and interpret the nature of 236 the dominant sensitivities of indices groups, so that studies results can be more easily 237 interpreted and integrated into new research and novel theories. 238

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Grimm, 2021b).

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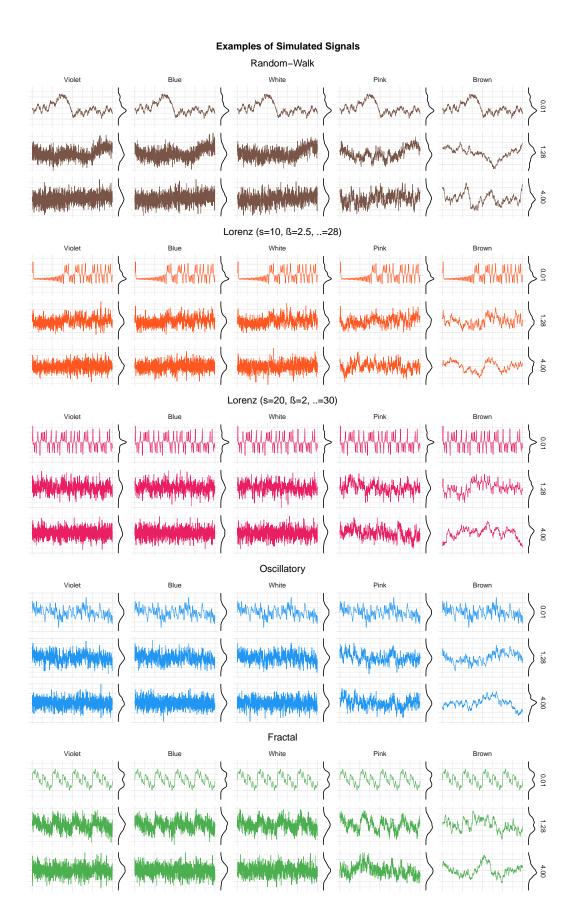
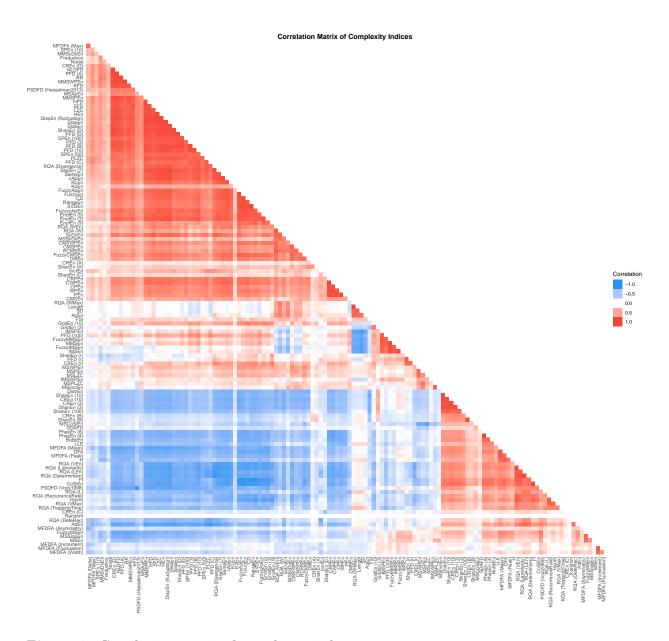


Figure 1. Different types of simulated signals, to which was added 5 types of noise (violet, blue, white, pink, and brown) with different intensities. For each signal type, the first row shows the signal with a minimal amount of noise, and the last with a maximal amount of noise. We can see



 ${\it Figure~2.}$ Correlation matrix of complexity indices.

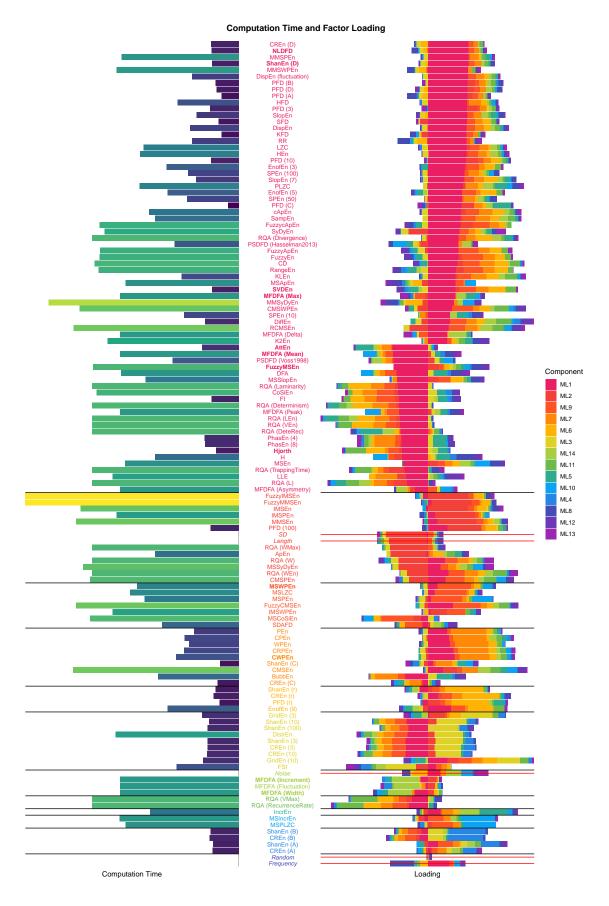


Figure 3. Factor loadings and computation times of the complexity indices, colored by the factor they represent the most.

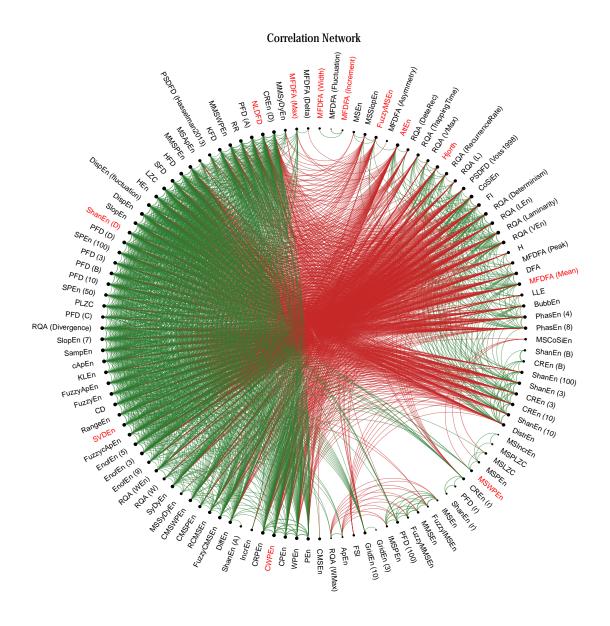


Figure 4. Correlation network of the complexity indices. Only the links where $|\mathbf{r}| > 0.6$ are displayed.

Hierarchical Clustering

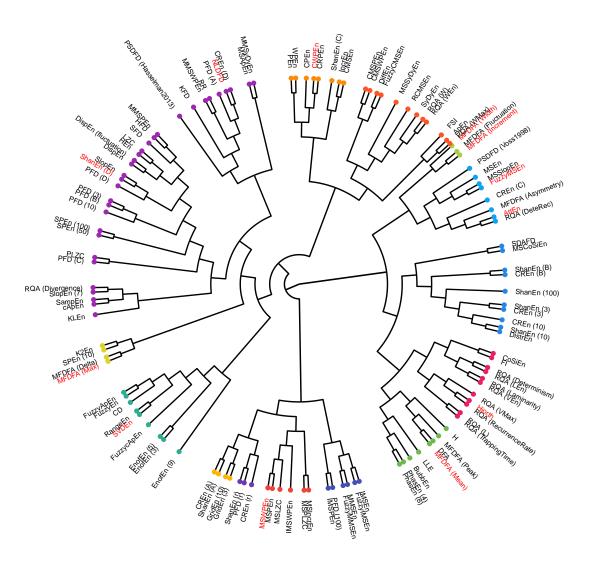


Figure 5. Dendrogram representing the hierarchical clustering of the complexity indices.

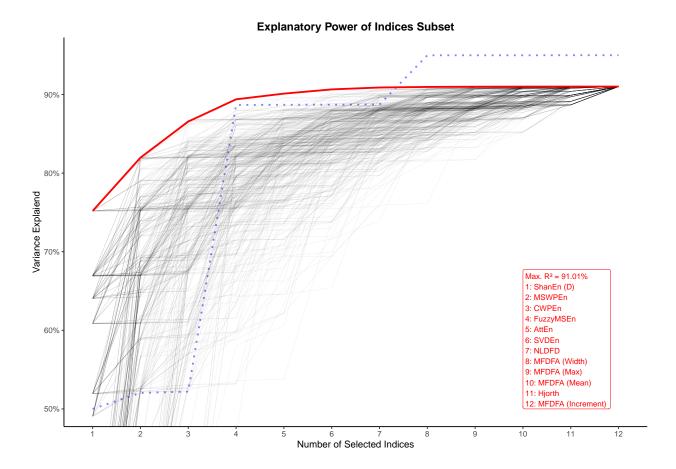


Figure 6. Variance of the whole dataset of indices explained by the subselection. Each line represents a random number of selected variables. The red line represents the optimal order (i.e., the relative importance) that maximizes the variance explained. The dotted blue line represents the cumulative relative average computation time of the selected indices, and shows that FuzzyMSEn and MFDFA indices are the most costly algorithms.

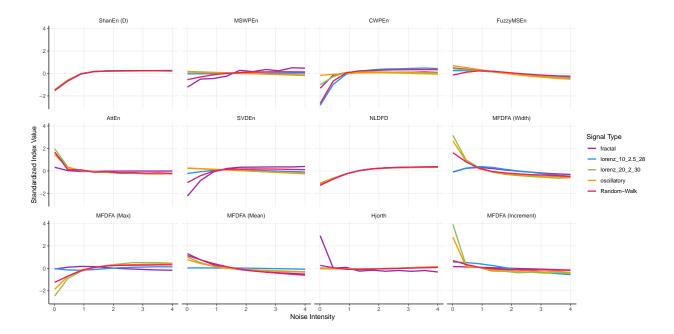


Figure 7. Visualization of the expected value of a selection of indices depending on the signal type and of the amount of noise.