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

 $_{21}$ Complexity quantification, through entropy, information theory and fractal dimension

22 indices, is gaining a renewed traction in psychophsyiology, as new measures with promising

²³ qualities emerge from the computational and mathematical advances. Unfortunately, few

24 studies compare the relationship and objective performance of the plethora of existing

²⁵ metrics, in turn hindering reproducibility, replicability, consistency, and clarity in the field.

Using the NeuroKit2 Python software, we computed a list of 112 complexity indices on

27 signals varying in their characteristics (noise, length and frequency spectrum). We then

28 systematically compared the indices by their computational weight, their

²⁹ representativeness of a multidimensional space of latent dimensions, and empirical

proximity with other indices. Based on these considerations, we propose that a selection of

12 indices, together representing 85.97\% of the total variance of all indices, might offer a

parsimonious and complimentary choice in regards to the quantification of the complexity

of time series. Our selection includes CWPEn, Line Length (LL), BubbEn, MSWPEn,

34 MFDFA (Max), Hjorth Complexity, SVDEn, MFDFA (Width), MFDFA (Mean), MFDFA

35 (Peak), MFDFA (Fluctuation), AttEn. Elements of consideration for alternative subsets are

discussed, and data, analysis scripts and code for the figures are open-source.

Keywords: chaos, complexity, fractal, physiology, noise

38 Word count: 2709

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

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
(Ehlers, 1995; Goetz, 2007; Lau et al., 2021).

There has been an exponential increase in the number of complexity indices in the 48 past few decades (A. C. Yang & Tsai, 2013). Although these new procedures are usually 49 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 (Azami et al., 2017; Manis et al., 2018). As 55 such, having empirical data about the computation time of various complexity indices 56 would prove useful, for instance to objectively guide their selection, especially in contexts where time or computational resources are limited. 58

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, many 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). And complexity measures with open-source code implementations are

scattered across different packages or scripts, or embedded within a larger goal-directed
framework (e.g., *HCTSA*, a time-series comparison tool, Fulcher & Jones, 2017). To address
this lack of unified accessibility, we added a comprehensive set of complexity-related
features to *NeuroKit2*, a Python package for physiological signal processing (Makowski et
al., 2021), to provide users with a software to compute a vast amount of complexity
indices. The code is designed to be as fast as possible, while still written in pure Python
(with the help of standard 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 of various types of signals with varying degrees of noise using 112 of the predominantly used indices that are available for computation using *NeuroKit2*. Note that, even though it is one of the largest comparison to date to our knowledge (and covers the most commonly used metrics), this list is by no means exhaustive: new indices are being developed, such as for instance symmetropy (Girault & Menigot, 2022). 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.

84 Methods

The Python script to generate the data can be found at

$_{86}~~{ m github.com/DominiqueMakowski/ComplexityStructure}.$

We started by generating 6 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), two complex signals derived from Lorenz systems (with parameters $\sigma = 10, \beta = 2.5, \rho = 28$; and $\sigma = 20, \beta = 2, \rho = 30$, respectively) and one EEG-like simulated signal. Each of this signal was iteratively generated at 6 different lengths (ranging from 500 to 3000 by 500 samples). 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 128 different intensities (linearly ranging from 0.001 to 3). Examples of generated signals are presented in **Figure**

The combination of these parameters resulted in a total of 23040 signal iterations.

For each of them, we computed 112 complexity indices, and additional basic metrics such as 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, as well as to the data generation script.

106 Results

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github.com/DominiqueMakowski/ComplexityStructure. The analysis was 108 performed in R using the *easystats* collection of packages (Lüdecke et al., 2021; Lüdecke et 109 al., 2020; Makowski et al., 2020/2022, 2020). As the results are primarily presented in a 110 graphical way via the figures, the code to fully reproduce them is also included. 111 **Computation Time.** Firstly, one should note that the computation times 112 presented in Figure 2 are relative (in arbitrary units) and do not correspond to real times, 113 as these would highly depend on the system specifications. Rather, the goal here was to 114 convey some intuition on the differences between different classes of indices (using the same 115

The data analysis script and the data are fully available at

machine and the same language of implementation, i.e., Python). While it is possible that computational advances or improvements in the code efficiency might change some of these values, we believe that the "big picture" should remain fairly stable, as it is to a large extent 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 about 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 being 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 (which absolute correlation was equal to 1.0), such as *NLDFD* - identical to *LL*, *ShanEn* (15) - identical to *ShanEn* (9), and *CREn* (15) - identical to *CREn* (9). This resulting in a pool of 112 indices.

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
3). That being said, 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
analysis procedures are applied below.

Factor Analysis. The agreement procedure for the optimal number of factors
suggested that the 112 indices can be mapped on a multidimensional space of 13
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 4**). Below are a description of factors that we found to be
interpretable.

The first extracted 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., LL, PFD (Mean)) as well as indices that capture the amplitude of fluctuations
(DispEn (fluctuation), MFDFA (Max)). 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 and repetitions. As such, this latent factor might be
related to the predominance of short-term vs. long-term unpredictability.

The second factor was strongly loaded by by indices that measure the
feature-richeness of the signal's system (as most of them operate on a state-space
decomposition). It is positively related to SVDEn and the Kozachenko-Leonenko
differential entropy (KLEn), and negatively with the RQA Recurrence Rate and Hjorth
Complexity.

The third factor was loaded predominantlys by permutation-based metrics (*PEn*, *WPEn*, *BubblEn*, etc.). The fourth factor included multiscale indices, such as *MSWPEn*.

The fifth factor was strongly loaded by signal *length*, and thus might not capture features of complexity *per se*. Indices with the most relation to it were indices known to be sensitive to signal length, such as *ApEn*. The sixth factor was loaded by indices in which the signal or the Poincaré plot was discretized via binning or gridding, respectively. The ninth factor was loaded by *EnofEn* and Kolmogorov Entropy (*K2En*). The tenth factor was loaded positively by the amount of noise, and negatively by multifractal indices such as *MFDFA*

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(Width), suggesting a sensitivity to regularity. Finally, as a manipulation check for our factorization method, the random vector did not load unto any factors.

Hierarchical Clustering and Connectivity Network. For illustration

purposes, we represented the correlation matrix as a connectivity graph (see Figure 5). 171 We then ran a hierarchical clustering (with a Ward D2 distance) to provide additional 172 information or confirmation about the groups discussed above. This allowed us to 173 fine-grain our recommendations of complimentary complexity indices (see **Figure 6**). The selection of a subset of indices was based on the following Indices Selection. 175 considerations: 1) high loadings on one predominant latent dimension, with additional 176 attention to the pattern of secondary loadings. For instance, an index with a positive 177 factor 1 loading and a negative factor 2 loading could complement another index with a 178 similar factor 1 loading, but a positive factor 2 loading. This was helped by 2) the 179 hierarchical clustering dendrogram, with which we attempted to indices from each 180 (meaningful) higher order clusters. Items related to clusters that we know were related to 181 noise, length or other artifacts were omitted. 3) A preference for indices with relatively 182 shorter computation times. This yielded a selection of 12 indices. Next, we computed the 183 cumulative variance explained of this selection in respect to the entirety of indices, and 184 derived the optimal order to maximize the variance explained (see Figure 7). The 12 185 included indices, representing 85.97% of the variance of the whole dataset, were: 186

- 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).
- *LL*: The Line Length index stems out of a simplification of Katz' fractal dimension

 (KFD) algorithm (Esteller et al., 2001) and corresponds to the average of consecutive

 absolute differences. It is equivalent *NDLFD*, the Fractal dimension via Normalized

 Length Density (Kalauzi et al., 2009). As it captures the amplitude 1-lag

 fluctuations, this index is likely sensitive to noise in the series.

• BubbEn:

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- 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).
- MFDFA (Max): The value of singularity spectrum D corresponding to the maximum value of singularity exponent H.
 - *Hjorth*: Hjorth's Complexity is defined as the ratio of the mean frequency of the first derivative of the signal to the mean frequency of the signal (Hjorth, 1970).
- SVDEn: The Singular Value Decomposition (SVD) Entropy quantifies the amount of eigenvectors needed for an adequate representation of the system (Roberts et al., 1999).
- MFDFA (Width): The width of the multifractal singularity spectrum (Kantelhardt et al., 2002) obtained via Detrended Fluctuation Analysis (DFA).
- MFDFA (Mean): The mean of the maximum and minimum values of singularity
 exponent H, which quantifies the average fluctuations of the signal.
- MFDFA (Peak): The value of the singularity exponent H corresponding to peak of singularity dimension D. It is a measure of the self-affinity of the signal, and a high value is an indicator of high degree of correlation between the data points.
 - MFDFA (Increment): The cumulative function of the squared increments of the generalized Hurst's exponents between consecutive moment orders (Faini et al., 2021).
- 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).
- Finally, we visualized the expected value of our selection of indices for different types
 of signals under different conditions of noise (see **Figure 8**). This confirmed that *LL* was
 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).

222 Discussion

As the span and application of complexity science grows, a systematic approach to 223 compare their "performance" becomes necessary to reinforce the clarity and structure of 224 the field. The term *performance* is here to be understood in a relative sense, as any such 225 endeavor faces the "hard problem" of complexity science: various objective properties of 226 signals (e.g., short-term vs. long-term variability, auto-correlation, information, 227 randomness, Namdari & Li, 2019; Xiong et al., 2017) participate in forming together 228 over-arching concepts such as "complex" and "chaotic". Indices that are sensitive to some 229 of these objective properties are thus conceptually linked through these over-arching 230 framework. However, it remains unclear how these high-level concepts transfer back, in a 231 top-down fashion, into a combination of lower-level features. As such, it is conceptually 232 complicated to benchmark complexity measures against "objectively" complex vs. non-complex signals. In other words, we know that different objective signal characteristics can contribute to the "complexity" of a signal, but there is not a one-to-one 235 correspondence between the latter and the former. 236

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 empirically 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 250 number of complexity indices already published, our study aimed at empirically map the 251 relationship between various indices and provide useful information to guide future researchers in their selection. Indices that were highlighted as encapsulating information 253 about different underlying dimensions at a relatively low computational cost include 254 CWPEn, Line Length (LL), BubbEn, MSWPEn, MFDFA (Max), Hjorth Complexity, 255 SVDEn, MFDFA (Width), MFDFA (Mean), MFDFA (Peak), MFDFA (Fluctuation), 256 AttEn. These indices might be complimentary in offering a comprehensive profile of the 257 complexity of a time series. Moving forward, future studies are needed to validate, analyze 258 and interpret the nature of the dominant sensitivities of indices groups, so that studies 259 results can be more easily interpreted and integrated into new research and novel theories. 260

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Grimm, 2021b).

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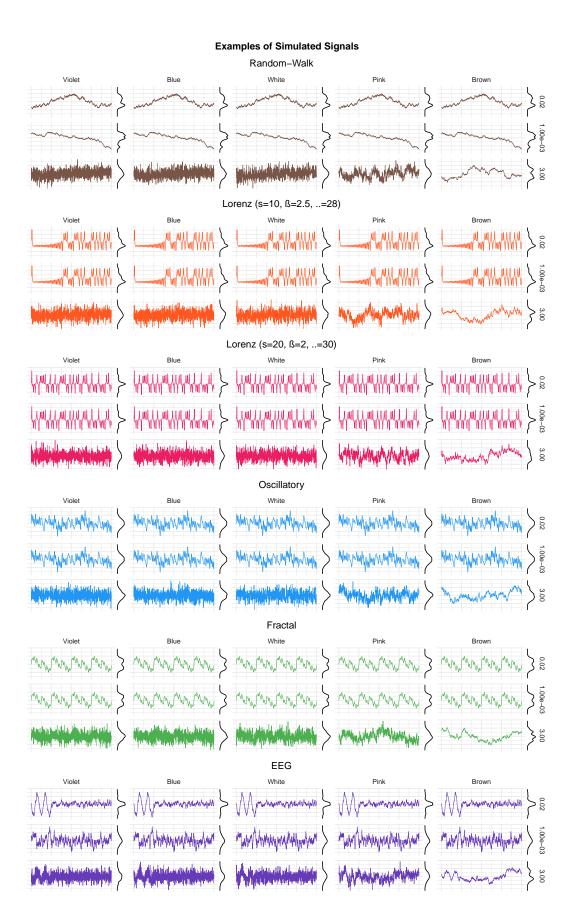
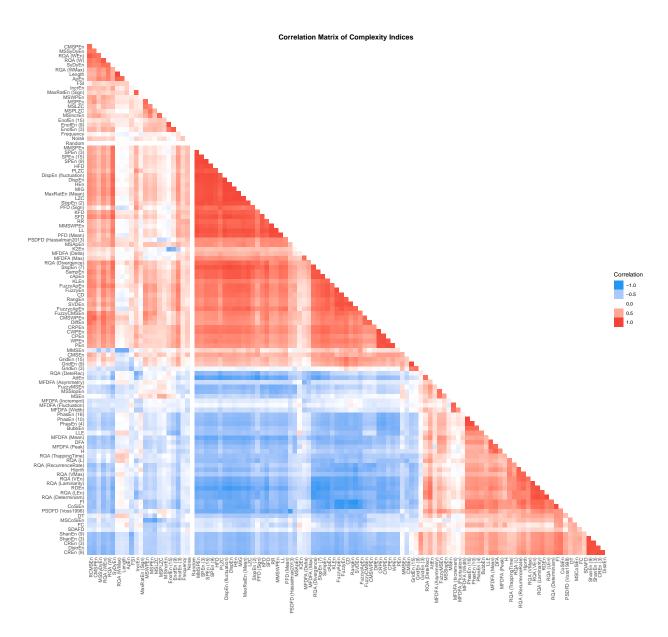


Figure 1. Different types of simulated signals, to which was added 5 types of noise (violet, blue, white, pink, and brown) with different intensities. For each signal type, the first row shows the signal with a minimal amount of noise, and the last with a maximal amount of noise.



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

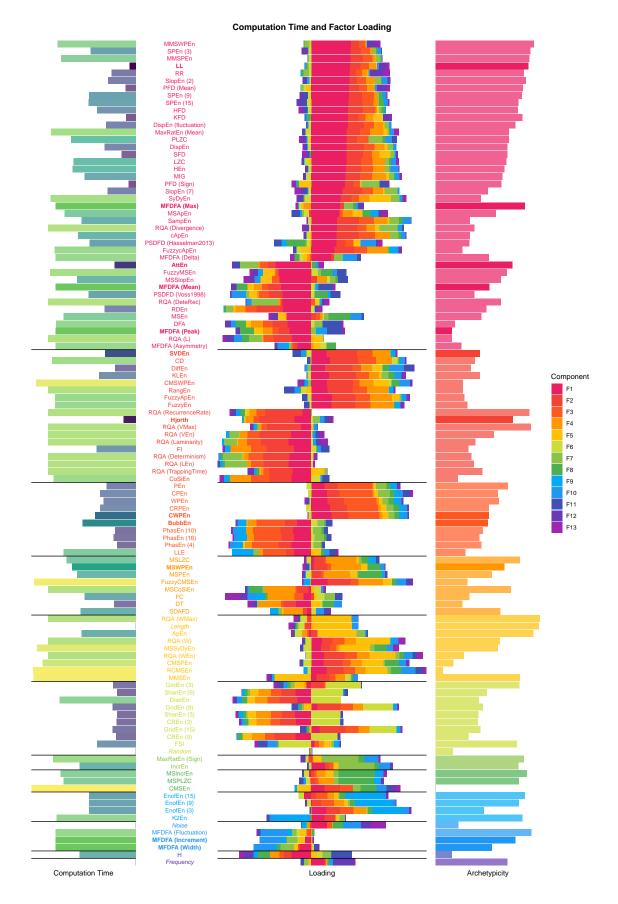


Figure 3. Factor loadings of the complexity indices, colored by the factor they represent the most (center). On the left, the median computation times and on the right, the archetypicity - the inverse of factor profile complexity, i.e., the extent to which each index is a pure representative of its dominant factor. This measure is low for indices that equally load on different factors).



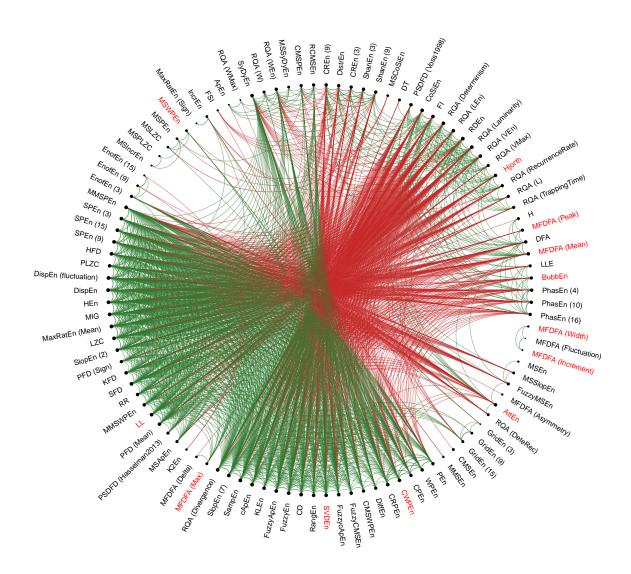
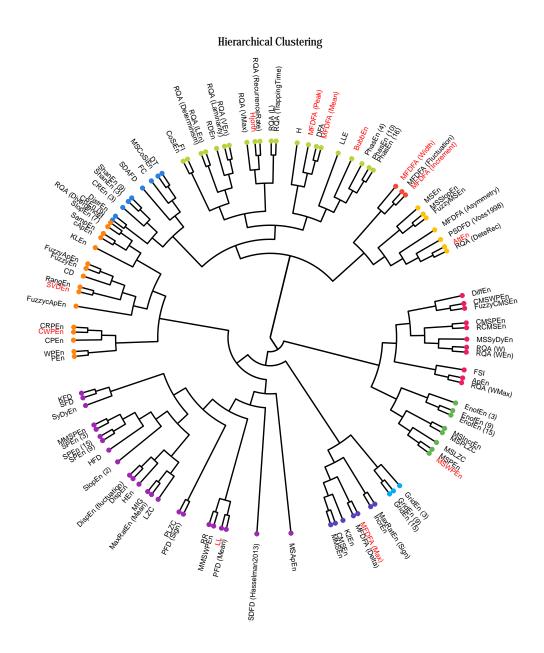


Figure 4. Correlation network of the complexity indices. Only the links where $|\mathbf{r}| > 0.6$ are displayed.



 ${\it Figure~5.}~{\rm Dendrogram~representing~the~hierarchical~clustering~of~the~complexity~indices.}$

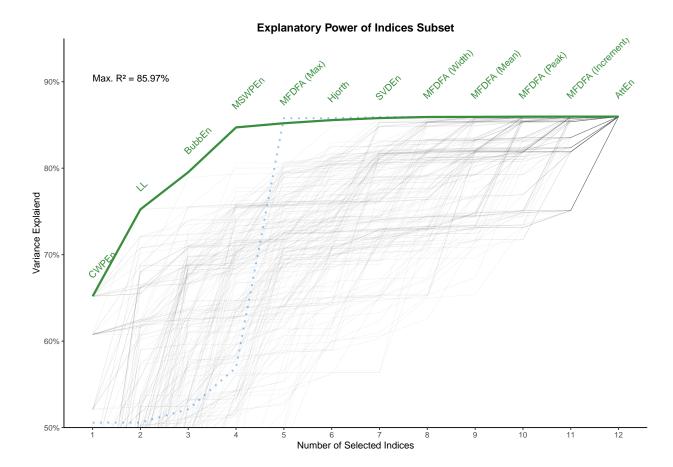


Figure 6. Variance of the whole dataset of indices explained by the subselection. Each line represents a random number of selected variables. The green line represents the optimal order (i.e., the relative importance) that maximizes the variance explained. The dotted blue line represents the cumulative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

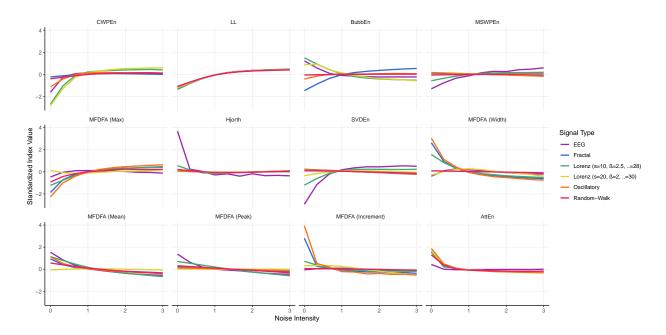


Figure 7. Visualization of the expected value of a selection of indices depending on the signal type and of the amount of noise.