Dynamic fractal analysis on exact and empirical signals

PhD thesis

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1. INTRODUCTION

The human brain is hypercomplex, which manifests at multiple scales and dimensions. It compromises roughly 10^{11} neurons, with an estimated ten thousand synaptic connections, each. This results in a vast neural network of approximately one thousand trillion connection, the connectom. Confined within this structural or anatomical network, due to dynamic coupling and transient synchronization, neurons get in fact functionally connected. This creates a spatially complex functional network, with an emergent property, the complex neurodynamics. Furthermore, via neurovascular coupling the complex hemodynamics is brought about. The two are thus intimately interrelated. Outgoing axonal activity of any region of interest will modulate the inputs of other region of interest as their incoming neurodynamics that can be captured in summed local field potentials, typically in electroencephalography (EEG). Hemodynamics elicited by the incoming activity can be recorded for instance by blood-oxygen-level dependent contrast imaging of the functional magnetic resonance imaging (fMRI-BOLD) or near-infrared spectroscopy (NIRS), thus capturing the fluctuations in ongoing neuro-hemodynamincs. The fluctuations has been shown to follow scale-free, that is fractal structuring in time known to be a hallmark of fundamental aspects of network complexity such as criticality, small-world or modularity.

Fractal and multifractal concepts of complexity focus on characterising scale-free properties in terms of assessing scaling exponents such as the Hurst exponent (H) or spectral index (β), describing the power-law behaviour in the time or frequency domains. A fundamental classification of the fractal signals into fractional Gaussian noise (fGn) and fractional Brownian motion (fBm) signal categories is in fact based on this power-law relationship. Furthermore the homogeneity of the underlying power-law along the signal separates mono- and multifractals. In case of monofractals scaling is a global behaviour, which can be characterised by a singel scaling exponent, H. For multifractals, a range of statistical moment (q) orders are needed to obtain a family of scaling function, $S(q,s)$. This is capable of representing the local fluctuation profiles whose regression analyses yields the generalized Hurst exponent, $H(q)$, via obtaining weighted scale- and moment-wise statistics. Subsequently, $H(q)$ – carrying the essential information on multifractal scaling – is submitted to the multifractal formalism whose output yields the local roughness of the temporal process (the Hölder exponent, h) along with the multifractal spectrum, $D(h)$, which is essentially analogous to a histogram of local fractality in the signal. Accordingly, $D(h)$ captures the moment-wise distribution of the singularity strength of local roughness or multifractal scaling in the temporal process.

In addition to the scale free structuring at each and every q, the q-independent analytical constrain at signal length N, termed focus, $S(N)$, has been recently recognized as a fundamental property of the scaling function. Empirical signals may contain varying degree of heterogeneity, which by compromising the scaling function violates the $H(q)$-monotonicity, the prerequisite of obtaining $D(h)$, thus resulting in a broken singularity spectrum. A specific case of signal heterogeneity is multimodality.

Physiological processes exhibit typically scale-free temporal scaling. However, this structuring may break up due to other, physiologically relevant phenomena, such as multimodality due to concomitant processes with distinct signal generators or information transfer between subsystems of the generating process. Multimodality

penetrates the hierarchical multifractal structure along different scales; a documented but so far neglected phenomenon in the literature, which calls for revisiting the segmented line method as the gold standard in dealing with multimodality. The q-dependent assessment of breakpoints (capturing the point of deviation from power-law scaling within the multimodal scaling function) and securing valid $D(h)$ by imposing the q-independent focus on the regression scheme, is essential for a genuine multifractal handling of multimodality. The other option for treating superimposed signals is by hypothesizing the addition of the component scaling functions, whose intersect would then result in the crossover.

2. OBJECTIVES

2.1. The establishment of a framework for multifractal and multimodal analyses

The development in fractal time series methodology in the past decades opened up new areas of implementation. Nevertheless, issues in case of empirical signals, such as corrupted or inversed singularity spectra or multimodal scaling functions typically not considered in the pure mathematical and statistical physical settings of the development of the original (i.e. standard) methods. Hence the main objective of our study was to create improved algorithms capable of handling empirical signals. Specifically, we aimed to elaborate a methodology capable of reliably handling heterogeneous signals both in terms of their multimodality and multifractality.

2.2. The extension of the SSC method for multifractality and multimodality

The signal summation conversion (SSC) method was created by our group. Our primary aim was to enhance this method by expanding its applicability to multifractal (MF-SSC and FMF-SSC) and multimodal multifractal (qSRA-FMF and SFD-FMF) cases.

2.2.1. The establishment of the MF-SSC method

The multifractal origin of diverse physiological processes is widely recognized in the literature, thus their description on a mere monofractal level is no longer considered adequate. This may however result in abandoning monofractal algorithms, such as the SSC method altogether, despite of its outstanding performance. Thus we aimed to expand the monofractal SSC method to a reliable handling of multifractality based on the analytical design of multifractal detrended fluctuation analysis.

2.2.2. The establishment of the FMF-SSC method

We modified the MF-SSC method by imposing the focus onto the regression scheme thus assuring $H(q)$ monotonicity, a prerequisite for the Legendre-transformation incorporated in the multifractal formalism to yield enhanced output.

2.2.3. The establishment of the qSRA-FMF-SSC method

Multimodality penetrates the hierarchical multifractal structure along different scales, resulting in a scale- and moment-dependent impact on the scale-free pattern, hence analysis based at a single q is not sufficient. Accordingly, our aim here was the true multifractal enhancement of the segmented line regression method incorporating the focus and moment-wise breakpoints.

2.2.4. The establishment of the SFD-FMF-SSC method

Many physical, natural, biological systems show multimodal properties, where scale-dependent impacts are often resulted from multiple co-sampled signal generator or from transfer functions. Our aim was to separate or identify and describe such processes.

2.3. Validating the enhanced SSC methods on „in silico" and „in vivo" signals

3. METHODS

The multifractal algorithms, signal syntheses, and numerical tests were implemented in Matlab (The MathWorks, Inc., Natick, MA, USA), with code written by the authors. Furthermore, to test for empirical applicability, and to prove physiological relevance, we implemented our algorithms on previously published empirical signals (NIRS, EEG and fMRI-BOLD). Human NIRS measurements using a NIRO 500 Cerebral Oxygen Monitor at a rate of 2 Hz were carried out to record the relative change in total hemoglobin concentration with a length of N = 16,384 data points. Human EEG signals were sampled with a length of N = 16,384 data points with eyes closed during random hand movements at 500 Hz using a Neurofax EEG System. These empirical records were acquired from healthy volunteers above the pre-frontal area. Rat fMRI-BOLD data with a length of N = 4,096 data points were obtained by using a modified 11.7 T Bruker horizontal-bore spectrometer using a 1 H surface coil (1.4 cm diameter) with sequential sampling gradient echo planar imaging sequence, field of view of 2.56×2.56 cm^2; image matrix of 64×64, slice thickness of 2 mm; repetition time of 200 ms (5 Hz of sampling frequency) and echo time of 13 ms; and voxel size of 400×400×2000 μm^3.

The new multifractal and multimodal analytical framework is elaborated on modules of fractal (SWV, SSC, DFA) and multifractal (MFDFA, MFDMA, WTMM, WL) algorithm. A modified scaled windowed variance (SWV) method, termed SSC, served as foundation for our multifractal, multimodal framework. The SWV is a monofractal time domain method, where the statistical measure is the standard deviation (σ). The pretreated signal is divided into a series non-overlapping windows of size s. After detrending σ can be computed in each of these windows. Averaging σ at a selected window size for the non-overlapping windows, and repeating this computation for wide ranges of window sizes results in the input of the regression for Hurst exponent. If the pretreatment contains signal classification, then the algorithm is termed SSC.

4. RESULTS

4.1. Theoretical results

Exploiting the basic properties of the variance and also the connection between standard deviation and scaling function, one can identify and model universal characteristics pertinent to fractal crosscorrelation, multifractal phase transition and multimodal signal decomposition.

4.1.1. Superposing scaling functions

Superposing scaling functions are based on a fundamental principle derived from the additive property of the variance ($\mathrm{Var}[X+Y]=\mathrm{Var}[X]+\mathrm{Var}[Y]+2*\mathrm{Cov}[X,Y]$), where the covariance can be expressed with the help of the Pearson correlation coefficient ($\mathrm{Cov}[X,Y]=r*\mathrm{Var}[X]*\mathrm{Var}[Y]$). Furthermore, as the measure of the SSC algorithm is standard deviation, thus the square of its multiscaling structure (scaling function) is an averaged (power mean) variance with corresponding properties. Therefore, superposing fractals (^{n} and ^{f}) leads to the following formalism:

$$S[{}^{n}X_i + {}^{f}X_i](q,s) =$$

$$\sqrt{S[{}^{n}X_i](q,s)^2 + S[{}^{f}X_i](q,s)^2 + 2 \times r[{}^{n}X_i, {}^{f}X_i](q,s) \times S[{}^{n}X_i](q,s) \times S[{}^{f}X_i](q,s)}\,.$$

Owing to the fact that the correlation coefficient appears in the equation, this formula can be simplified in cases when correlated, anticorrelated or uncorrelated signals are considered. If the two signals are uncorrelated at r=0 (an arguable hypothesis in case of fractals with different scale-invariance), then the scaling function of the superimposed uncorrelated fractal is the root sum square of the composing scaling functions:

$$S\left[\sum_{c=1}^{N_C} {}^{c}X_i\right](q,s) = \sqrt{\sum_{c=1}^{N_C} S[{}^{c}X_i](q,s)^2}\,.$$

This relationship is readily seen as a realisation of the Bienaymé formula. In addition to the optimal q-wise bias, the validity of the applied hypothesis and the applicability of the suggested equation can be proven for the focus and for the monofractal case. The validity of this expression is not limited to empirical scaling functions, it is also applicable to exact scaling functions, thus fulfilling the prerequisite for decomposing multimodal scaling functions resulted from signal superposition.

4.1.2. Multifractal phase transition

There are cases when the superposition of two fractal components yields a composite signal with a crossover falling outside the observed range of scales. The multifractal spectrum in this case is typically asymmetric. While under these conditions the crossover is not directly accessible to our SFD-based analysis, our additive model still allows for its characterisation and offers an explanation for the asymmetry in $D(h)$. This way, a composite process yielding asymmetric $D(h)$ can be modelled too. Asymmetric $D(h)$ can also be interpreted as a phase transition based on the deep analogy that exists between the multifractal formalism and equilibrium statistical thermodynamics. According to this model, the superimposed partition functions under and above a critical q only slightly perturb each other, creating a prompt dominance shift; thus, the partition function, $\tau(q)$ and $D(h)$ are always dominated by a single component. Under such condition the Bienaymé formula yields similar result, describing the superposition already at the level of the scaling function:

$$S_{superimposed} \approx \sqrt{{}^{n}S^2 + 0} = {}^{n}S \text{ , if } q < q_{critical} \text{ and}$$

$$S_{superimposed} \approx \sqrt{0 + {}^{f}S^2} = {}^{f}S \text{ , if } q > q_{critical}.$$

4.1.3. Fractal crosscorrelation

Characterizing the fractal, that is (auto)correlated dynamics in our signals, is only one aspect of extracting information on physiological complexity. When two or more signals or their modalities can be acquired simultaneously, an extended analysis should elicit the strength of their connection. Depending on the process (e.g. neuro- or hemodynamics) or its sampled representation (EEG, NIRS or fMRI), one may reveal hidden information such as functional connectivity or neuro-vascular coupling. One of the basic measures capturing the strength of connection is the Pearson correlation coefficient, r. In case of multimodality a single correlation coefficient is insufficient, due to the scale dependent and independent effects impacting different scales, hence the cross-correlation should also be assessed in a scale-wise manner. This can be achieved by rearranging the equation of fractal superposition, that inherently contains the Pearson

correlation coefficient:

$$r[{}^{n}X_i, {}^{f}X_i](2,s) = \frac{S[{}^{n}X_i + {}^{f}X_i](2,s)^2 - S[{}^{n}X_i](2,s)^2 - S[{}^{f}X_i](2,s)^2}{2 \times S[{}^{n}X_i](2,s) \times S[{}^{f}X_i](2,s)}.$$

4.2. Methodological results

We developed a genuinely multifractal and multimodal framework (see Figure "The comprehensive strategy of the multifractal analysis", page 9). Based on this approach the SSC methodology – introduced previously by our group – was extended and validated for multifractal (MF-SSC and FMF-SSC) and multimodal multifractal (qSRA-FMF and SFD-FMF) cases.

4.2.1 The MF-SSC method

In case of the monofractal SSC method, after pre-treatment, the signal is divided into non-overlapping windows, in which the standard deviation or in other word the measure (μ) at a given scale is calculated. Utilising the congruity (as stated in the MF-DFA methodology) found between squared fluctuation and variance (i.e. squared standard deviation), one can identify the conversion rule in between standard deviation and scaling function:

$$S[X_i](q,s) = \left(\frac{1}{N_v}\sum_{v=1}^{N_v}\sigma(v,s)^q\right)^{1/q},$$

where v refers to the position of the s sized window; and N_v refers to the number of non-overlapping windows of a given size. This equation can also be generalised, thus a method independent formula can be created:

$$S[X_i](q,s) = \left(\frac{1}{N_v}\sum_{v=1}^{N_v}\mu(v,s)^q\right)^{1/q}.$$

From the scaling function, we can derive the singularity spectrum through deterministic steps identical to that of the MF-DFA method, which includes both regression and singularity analysis.

Our method was tested "in silico" and validated against the MF-DFA method. Based on the two-way non-parametric Friedman test, we found no significant difference. Nevertheless, a clear advantage of the MF-SSC method is with its embedded signal classification step, which becomes a critical aspect in applications to real-world signals.

4.2.2 The FMF-SSC method

Incorporating the moment-independent focus into the regression scheme of the MF-DFA method yields a new method termed (focus-based multifractal) FMF-SSC. Instead of a moment-wise regressing for H, thus essentially performing repetitive monofractal analyses through a set of empirical scaling functions, an exact multifractal is fitted to this family of moment-wise scaling functions all at once:

$$SSE = \sum_{q=q_{\min}}^{q_{\max}}\sum_{s=s_{\min}}^{s_{\max}}\left((\log s - \log N)\times\hat{H}[X_i](q) + \log\hat{S}[X_i](N) - \log S[X_i](q,s)\right)^2.$$

Through iterative minimisation the residual sum of squared errors, SSE, one can determine the focus as a scale-dependent iterated parameter and the generalised Hurst exponent as a set of scale-independent iterated parameters. The resulted $H(q)$ is the input parameter for both signal classification and singularity analysis.

It is generally known that Legendre transformation suffers from numerical errors making this indirect, moment-based approach to obtain $D(h)$ less appealing than those of the direct methods. However enforcing an expected value at signal length found in the value of focus as a reference in the regressive fitting process, one can assure the monotonicity of $H(q)$ and thus the concavity of $\tau(q)$ as the pre-requisite for a proper coupling of the Legendre transformation to $D(h)$. Based on this approach the FMF-SSC method effectively enforces monotonicity. Furthermore, with the two-way non-parametric Friedman test, we found no significant difference in the performance of MF-SSC and FMF-SSC on exact fGn and fBm signal.

4.2.3 The qSRA-FMF-SSC method

Multimodality penetrates the hierarchically organised multifractal structure at different scales. This – otherwise well-known principle – has not been taken into account in methods commonly used in the literature. The qSRA-FMF-SSC method was introduced and validated to avoid the pitfall represented by the moment-dependent breakpoints and crossovers. Accordingly, multifractal handling of multimodality was shown to require the i) the q-wise identification of breakpoints, ii) a focus-based regression method on q-dependent scaling ranges associated with the same scale-independent process, and iii) the classification of modalities, respectively. Taking these requirements into account, we have created the qSRA-FMF methodology, e.g. the qSRA-FMF-SSC method. This method captures the breakpoints based on the moment-wise repeatedly employed segmented line method. Finally the FMF-SSC method can be applied on q-dependent scaling ranges separated by breakpoints.

The method performs best, on synthesised test signals near the ideal breakpoint, owing to the fact that all the components are equally well represented, when the breakpoint is located near the middle of the available SR. This method is applicable independent of the scale-dependent effect with the only precondition being the scale-free structuring within the identified scaling ranges. This later criterion may not be present as the actual multimodal scaling function may well deviates in its genesis from that of the segmented line model. See for instance the case of the additive model and the exclusion range. Hence, while this method may offer practical advantages in estimating the multifractal parameters or perhaps crossover scales without formulating any a priori concept on signal genesis, it would not allow for the application of the theory associated with the segmented line method given the lack of scale-free scaling ranges.

4.2.4 The SFD-FMF-SSC method

Based on the superposition of the SF, with the use of the Bienaymé formula we can fit the calculated scaling function with an exact multimodal SF by the addition of the componential scaling functions iterated with $S(N)$ and $H(q)$:

$$\hat{S}[{}^{n}X_i](q,s) = \exp\left((\log s - \log N) \times \hat{H}[{}^{n}X_i](q) + \log \hat{S}[{}^{n}X_i](N)\right)^2,$$

$$\hat{S}[{}^{f}X_i](q,s) = \exp\left((\log s - \log N) \times \hat{H}[{}^{f}X_i](q) + \log \hat{S}[{}^{f}X_i](N)\right)^2,$$

$$SSE = \sum_{q=q_{\min}}^{q_{\max}} \sum_{s=s_{\min}}^{s_{\max}} \left(\log \sqrt{\hat{S}[{}^{n}X_i](q,s)^2 + \hat{S}[{}^{f}X_i](q,s)^2} - \log S[X_i](q,s)\right)^2.$$

Based on this approach we developed and validated the so-called scaling function decomposition, SFD (-FMF) methodology, where the SFD-FMF-SSC method is of particular importance due to the fact that both SSC and Bienaymé formula are standard deviation-based approaches.

4.2.5 The identification of additive signal genesis

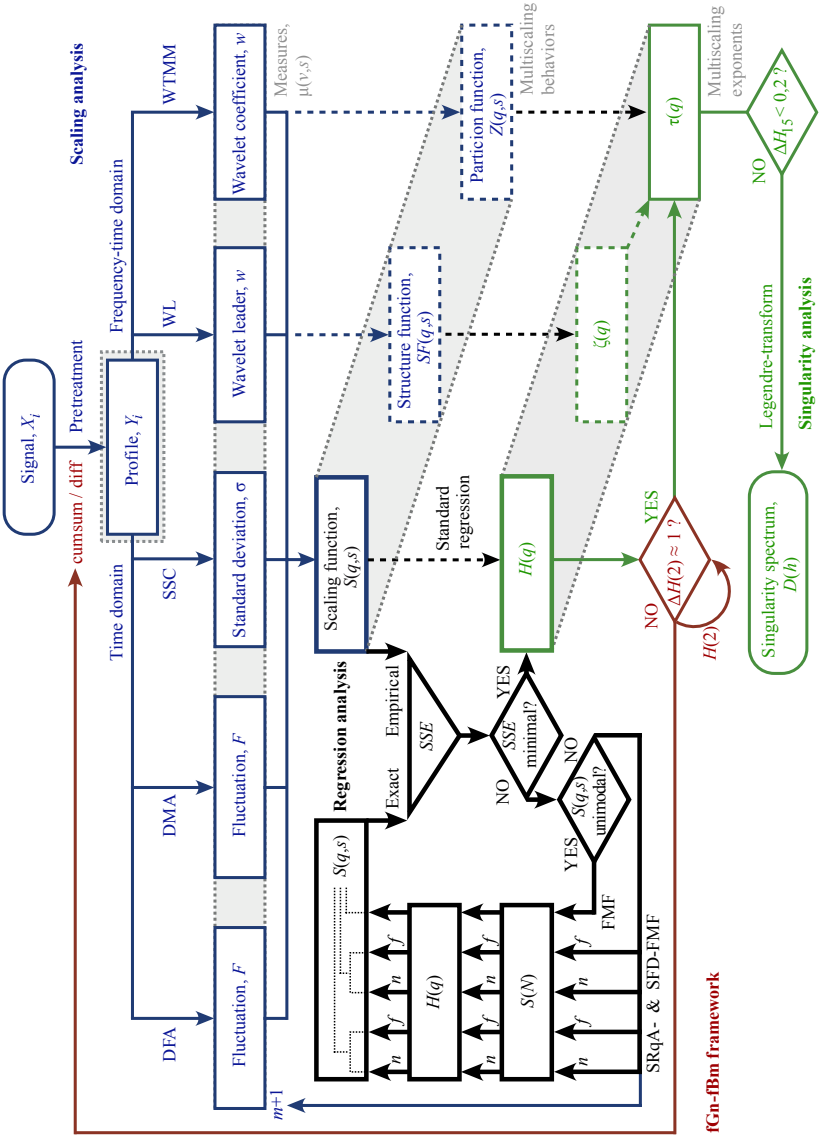
We have shown that parallel application of qSRA and SFD can be used to identify signal genesis, specifically to distinguish superposition from convolution. Goodness-of-fit statistics (for given bimodal characteristics) were used as a guide in accepting estimates obtained by the SFD-FMF or qSRA-FMF methods, as respectively valid. Specifically, based on low MSE values, when analysing bimodal EEG, NIRS, and fMRI-BOLD data we demonstrated that these signals resulted from superposition.

Since the iterated parameters are the same for both qSRA- and SFD-based regression $2\times H(q)$ and $2\times S(N)$, therefore MSE values are comparable without involving a penalty term. Lower MSE in the SFD method, when compared to that in the qSRA method, implies an additive origin of scale-dependent multimodality. Our method tested on artificially generated superimposed signals presented a high, 73%, sensitivity.

4.3. Physiological results

EEG, NIRS and fMRI-BOLD signals evaluated in our studies are shown to have resulted from the superposition of a multifractal noise dominating the high frequencies, and a more correlated multifractal dominating the low frequencies of the dynamics. We demonstrated that the multimodal pattern of the hemodynamic signal emerges from superposition and not from the low-pass filtering effect of the hemodynamic response function. As the crossover scale of the hemodynamic signals (NIRS and fMRI-BOLD) and the border of the low frequency fluctuation (LFF) commonly applied in the standard functional connectivity analysis overlap, this suggests that the multifractal correlated component is of neural origin. Furthermore, we found a wide distribution in the crossover scales of voxel-wise bimodal fMRI-BOLD data across the full range of the studied scales resulting in a particular spatial pattern. The inference of these findings are that due to the lack of a neural unimodal dynamics within the LFF range, the very precondition underlying the resting-state fMRI-BOLD-based connectivity field cannot possibly be met. Thus the demonstrated wide-spread presence of crossover scales within the LFF range should by no means introduce errors in unknown degree in the connectivity analyses of resting-state fMRI-BOLD data. Because the crossover scale of the studied hemodynamic signals (NIRS and fMRI-BOLD) were found coinciding with the border frequency of the LFF applied in connectivity analysis, we suggest that instead of using data contaminated by apparent bimodality, scale-wise crosscorrelation (i.e. fractal crosscorrelation) to be computed to yield a more reliable estimate of connectivity

The crossover between the EEG signal components was found at the boundary between the δ and θ bands. An independent δ and θ rhythm has already been proposed in the literature based on the significant interregional gap in synchrony. Our current finding is another evidence in support of the presence of an independent multifractal δ rhythm.



The comprehensive strategy of the multifraktal analysis

5. CONCLUSIONS

5.1. Theoretical theses

(1) Based on the Bienaymé formula the scaling function of superimposed fractals (uncorrelated fractals with different origin or scale-free structuring) is the root sum square of the composing scaling functions:

$$S\left[\sum_{c=1}^{N_c} {}^{c}X_i\right](q,s) = \sqrt{\sum_{c=1}^{N_c} S[{}^{c}X_i](q,s)^2}\,.$$

(2) The multifractal phase transition can be modelled with the Bienaymé formula based on the superposition of the scaling functions.

(3) A scale-wise description of the cross-correlation coefficient can be calculated in a scale-wise manner based on fractal methodology, utilising the additive property of the scaling function:

$$r[{}^{n}X_i, {}^{f}X_i](2,s) = \frac{S[{}^{n}X_i + {}^{f}X_i](2,s)^2 - S[{}^{n}X_i](2,s)^2 - S[{}^{f}X_i](2,s)^2}{2 \times S[{}^{n}X_i](2,s) \times S[{}^{f}X_i](2,s)}\,.$$

5.2. Methodological theses

(4) The MF-SSC method was created and validated. Based on the conversion of standard deviation to scaling function (see equation), the monofractal SSC method was developed into a multifractal algorithm, with signal classification preserved, and a precision identical to that of the MF-DFA in wide-spread use.

$$S[X_i](q,s) = \left(\frac{1}{N_v}\sum_{v=1}^{N_v} \mu(v,s)^q\right)^{1/q} = \left(\frac{1}{N_v}\sum_{v=1}^{N_v} \sigma(v,s)^q\right)^{1/q}.$$

(5) The FMF-SSC method was created and validated. By applying a momentum-independent limit value at signal length (focus) within the regression scheme (see equation) one can secure $H(q)$-monotonicity, thereby avoide eventualities with corrupted and inversed singularity spectrum.

$$SSE = \sum_{q=q_{\min}}^{q_{\max}} \sum_{s=s_{\min}}^{s_{\max}} \left((\log s - \log N) \times \hat{H}[X_i](q) + \log \hat{S}[X_i](N) - \log S[X_i](q,s)\right)^2.$$

(6) The qSRA-FMF-SSC method was created and validated. With the moment-wise implementation of the segmented line method, and through the application of the FMF-SSC method within the predetermined scaling range separated by breakpoints, and dominated by the same multifractal, one can phenomenologically capture the scale dependent and independent parameters of a multifractal signal.

(7) The SFD-FMF-SSC method was created and validated as a genuinely multifractal approach. In case of multimodal superimposed signals the calculated empirical scaling function can be iteratively fitted with an exact multimodal scaling function attained with the help of the Bienaymé formula, capturing the scale-dependent and independent parameters at the best fit.

(8) One may discern additive from non-additive forms of signal genesis based on the parallel application of the qSRA and SFD methods, where goodness-of-fit statistics (MSE) can be used as a guiding principle in choosing between estimates obtained by the respective methods to be regarded as valid.

5.3. Physiological theses

(9) When analysing bimodal EEG, NIRS, and fMRI-BOLD data we could demonstrate that these records are the results of signal superposition, where a multifractal component dominates the low-frequencies and an underlying biologically relevant random noise determines the high-frequencies. This particular pattern in temporal structuring however cannot be interpreted resulting from the effect of transfer functions (filters).

(10) In case of the EEG signal a crossover scale was found at the boundary between the δ and θ bands, suggesting an independent generator for the multifractal δ rhythm.

(11) Functional connectivity utilizing hemodynamic signals such as NIRS and fMRI-BOLD has been established on cross-correlating the low frequency fluctuations (LFF) in these signals. The fact that the correlated multifractal component dominant above the crossover scale coincides with the LFF is in support of the neuronal origin of this component.

(12) In case of fMRI signals the voxel-wise distribution of crossover scales results in a genuine pattern. This suggests that applying fixed border frequencies in the field of functional connectivity should be considered as a potential pitfall, due to the possible impact of another fractal with different genesis on the LFF.

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