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Taming surprises

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# Taming Surprises

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## ABSTRACT

A methodological trajectory has been described dealing with the ‘novelty’ or ‘surprise’ issue in time series records arising from real world complex systems. It is based on extracting regularity (or scaling) characteristics of non-differentiable time series with wavelet transform, on modelling the complex system using multi-fractal properties and on investigating novelty in the context of the possible non-stationarity of such a model.

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A full colour version of this paper can be downloaded from [www.cwi.nl/~zbyszek](http://www.cwi.nl/~zbyszek)

## 1. INTRODUCTION: NOVELTY IN COMPLEX SYSTEMS

This paper has been motivated by the recent trend in automated data analysis suggesting techniques for novelty detection and knowledge discovery [1, 2, 3]. Such techniques are often applied to real life data known to be subject to complex dynamics inaccessible for modelling by deterministic dynamical systems. The local reconstruction of the phase space trajectories (or other deterministic characteristics) of such systems may not be possible or may pose substantial difficulty. These difficulties may be linked to critical behaviour characterising such systems and may be misleading the capturing of the evolution of time series arising from such systems. This in turn may result in false novelty or surprise knowledge assessment.

Let us take an example. In the top panel of figure 1 we present a record of heartbeat from a healthy patient. To the untrained eye, this record is either plain noise or it is full of most interesting features, spikes etc. <sup>1</sup> A guess of knowledge, suggesting that stable, cyclic, regular heartbeat rate should become a straight line in this plot, would prompt novelty discoveries at almost every single point. Indeed, the heartbeat rate shown is full of such ‘surprises’, each subsequent record seems to depart from the previous one in a most wild fashion. The methods of novelty (or discovery or surprise) detection suggested to date would also most likely detect surprises in every single point of the record.

Indeed, a record of heartbeat is used as an example in the work [3]. The novelty of detection of a long pause between beats of the heart after one or a series of shorter beats is, however, very questionable, if one realises that this is the most likely behaviour of the healthy heartbeat. Indeed, it has been established in the study of complex systems that heartbeat records show anti-persistence characterised by a high probability of long intervals after short intervals and vice versa. In fact, healthy heartbeat is at the ultimatum of the range of anti-persistence measured by the Hurst exponent of anti-persistence - it reaches levels near  $H = 0.0$  (on the scale 0-1) [4, 5, 6]. By comparison, Brownian

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<sup>1</sup>This duality of ‘novelty’ interpretation can be appreciated in a record as ‘simple’ as a white noise time series. On the one hand, it contains no correlations at all, no coherent structures and thus no novelty. On the other, it represents perfectly coded information - each and every new sample carries new surprising information, independent and orthogonal.

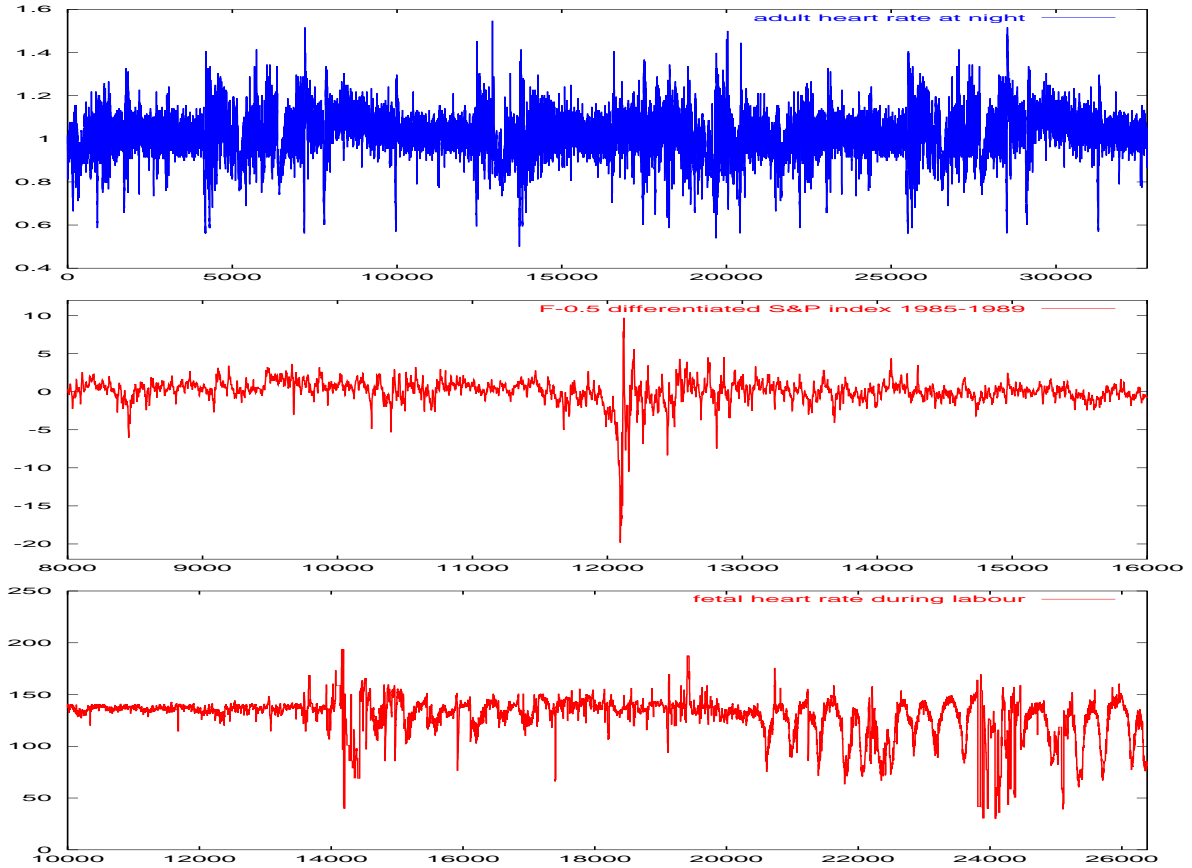


Figure 1: Top: A healthy heart rate recording, about five hours long. Center: A fractionally differentiated S&P500 record  $F(-0.5)$  about four years long centered at the '87 crash. Bottom: a fetal heartbeat record during labour, about ten hours long.

walk, in which every next jump is independent of the previous one, is characterised by  $H = 0.5$ , central on the range of  $H$ .

Such seemingly ‘anomalous’ behaviour of the healthy heartbeat is not unique in nature. In fact many complex systems show characteristics which make it impossible to use low degree oscillatory models for modelling them. Such models would, of course, be relatively easy to use for discovery and fitting, including determination of instances when they do not perform. The essence of highly developed criticality of systems like heartbeat is that making and fitting models of such a smooth oscillatory character does not seem to make sense - they would fail at every instance and point.

The degree of difficulty of novelty detection in real life complex systems can be further appreciated in the following example, shown in the second (middle) panel of figure 1. The record of *S&P* index shows the crash of '87 centrally. It perhaps appears as an ‘outlier’ or novel feature to the observer. In fact it is probably neither of these. The (multi)-fractal structure [7, 8, 9] of the financial time series guarantees that there are crashes at any scale of observation. Smaller crashes will happen at smaller scales; their magnitude follows a law which is a subject of discussion and study. Large events like the '87 crash are ‘rare’ and may appear as outliers [11, 12, 13]. They are, however, possibly just the effect of the internal complex dynamics of the system - they are determined by the history of the system to the date of the crash. [14, 15]

The last example again shows heart rate, but this time it is the heart rate of a baby being born. Fetal

heartbeat is different in characteristics from adult heartbeat. Here, additionally, the record shows the dynamic evolution of the fetal heartbeat during the final hours of the labour, ending in birth. This time it was a successful birth with positive fetal outcome. The baby born was healthy. Its heartbeat was used to make decisions about its status during labour. Such decisions are routinely taken upon observation of heartbeat, as it is the only indicator of the well-being of the fetus. The obstetrician observes the heartbeat and judges it for development of characteristics which would prompt (or better not) intervention in the case of hypoxia (lack of oxygen). The case shown did not require intervention - the heartbeat, albeit extremely complex, did not deviate from normal.

Developed around the examples given above, the structure of this paper is as follows. First a method of analysis of regularity properties of time series (wavelet transform) is introduced in section 2. It is followed, in section 3, by its use for the characterisation of the so-called multi-fractal properties of the time series, originating from real life complex systems. Analysis of the possible non-stationarity of the multi-fractal properties is suggested in section 4, together with accommodating it in both an heuristic model (section 5) and in model discovery by the use of automated Bayesian net reasoning (section 6).

## 2. ESTIMATING REGULARITY PROPERTIES OF ROUGH TIME SERIES

Suppose we can *locally* approximate the time series (function  $f$ ) with some polynomial  $P_n$ , but the approximation fails for  $P_{n+1}$ . One can think of this kind of approximation as the Taylor series decomposition:<sup>2</sup>

$$f(x)_{x_0} = c_0 + c_1(x - x_0) + \dots + c_n(x - x_0)^n + C|x - x_0|^{h(x_0)} = P_n(x - x_0) + C|x - x_0|^{h(x_0)} .$$

It is traditionally considered to be important in data mining of time series to capture trend behaviour  $P_n$ . It is, however, widely recognised in other fields, as discussed in the previous section, that it is not necessarily the regular polynomial background but quite often the transient singular behaviour which can carry important information about the phenomena and the underlying system ‘producing’ the time series.

The exponent  $h(x_0)$  characterises such local singular behaviour by capturing what ‘remains’ after approximating with  $P_n$  and what does not yet ‘fit’ into an approximation with  $P_{n+1}$ . Thus, our function or time series  $f(x)$  is locally described by the polynomial component  $P_n$  and the so-called Hölder exponent  $h(x_0)$ .

$$|f(x) - P_n(x - x_0)| \leq C|x - x_0|^{h(x_0)} . \quad (2.1)$$

The advent of multi-scale techniques (like WT), capable of locally assessing the singular behaviour, greatly contributed to the advance of analysis of ‘strange’ signals, including (multi)fractal functions and distributions.

The wavelet transform is a convolution product of the signal with the scaled and translated kernel - the wavelet  $\psi(x)$ . [20, 21] The scaling and translation actions are performed by two parameters; the scale parameter  $s$  ‘adapts’ the width of the wavelet kernel to the resolution required and the location of the analysing wavelet is determined by the parameter  $b$ :

$$(Wf)(s, b) = \frac{1}{s} \int dx f(x) \psi\left(\frac{x - b}{s}\right) \quad (2.2)$$

where  $s, b \in \mathbf{R}$  and  $s > 0$  for the continuous version.

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<sup>2</sup>In fact the arguments to be given are true even if such a Taylor series decomposition does not exist, but it can serve as an illustration [19].

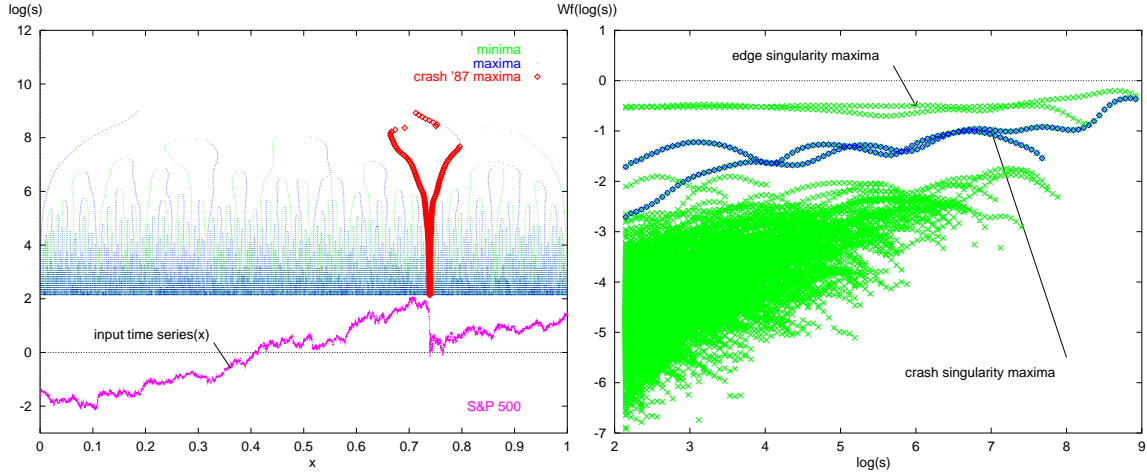


Figure 2: Left: the input time series with the WT maxima above it in the same figure. The strongest maxima correspond to the crash of '87. The input time series is de-biased and L1 normalised. Right: we show the same crash related maxima highlighted in the projection showing the logarithmic scaling of all the maxima.

For analysis purposes, one is not so much concerned with numerical or transmission efficiency or representation compactness, but rather with accuracy and adaptive properties of the analysing tool. Therefore, in analysis tasks, continuous wavelet decomposition is mostly used. The space of scale  $s$  and position  $b$ , is then sampled semi-continuously, using the finest data resolution available.<sup>3</sup>

The only *admissibility* requirement for the wavelet  $\psi$  is that it has zero mean - it is a wave function, hence the name *wavelet*.

$$\int_{-\infty}^{\infty} x \psi(x) dx = 0 \quad (2.3)$$

However, in practice, wavelets are often constructed with orthogonality to a polynomial of some degree  $n$ .

$$\int_{-\infty}^{\infty} x^n \psi(x) dx = 0 \quad (2.4)$$

Indeed, if the number of the vanishing moments of the wavelet is at least as high as the degree of  $P_n$ , the wavelet coefficients will capture the local scaling behaviour of the time series as described by  $h(x_0)$ . Thus, what wavelets provide in a unique way is the possibility to tame and manage singularities and trends in a local fashion, through localised wavelets components [19, 20, 21, 22].

$$W^{(n)}f(s, x_0) = \frac{1}{s} \int C|x - x_0|^{h(x_0)} \psi\left(\frac{x - x_0}{s}\right) dx = C|s|^{h(x_0)} \int |x'|^{h(x_0)} \psi(x') dx' .$$

Therefore, we have the following power law proportionality for the wavelet transform (WT) of the (Hölder) singularity of  $f(x_0)$ :

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<sup>3</sup>The numerical cost of evaluating the continuous wavelet decomposition is not as high as it may seem. Algorithms have been proposed which (per scale) have complexity of order  $n$ , the number of input samples, at a relatively low constant cost factor. [16]. Additionally, computationally cheap, discretised, semi-continuous versions of the decomposition are possible [17, 18].

$$W^{(n)}f(s, x_0) \sim |s|^{h(x_0)}.$$

From the functional form of the equation, one can attempt to extract the value of the local Hölder exponent from the scaling of the wavelet transform coefficients in the vicinity of the singular point  $x_0$ . A common approach to trace such singularities and to reveal the scaling of the corresponding wavelet coefficients is to follow the so-called maxima lines of the WT, converging towards the analysed singularity. This approach was first suggested by Mallat et al [22] (it resembled edge detection in image processing) and was later used and further developed among others in Refs [19, 23, 24]. However, any line convergent to the singularity can be used (to estimate the singularity exponent). Moreover, estimating local regularity at any point is possible by following the evolution (decay/increase) of the wavelet transform. This includes the smooth polynomial-like components of the time series.<sup>4</sup>

In figure 2, we plot the input time series which is a part of the S&P index containing the crash of '87. In the same figure, we plot corresponding maxima derived from the WT decomposition with the Mexican hat wavelet. The maxima corresponding to the crash stand out both in the top view (they are the longest ones) and in the side log-log projection of all maxima (they have a value and slope different from the remaining bulk of maxima). The only maxima higher in value are the end of the sample finite size effect maxima. These observations suggest that the crash of '87 can be viewed as an isolated singularity in the analysed record of the S&P index for practically the entire wavelet range used.

The size, as reflected in maxima scale span, and the strength  $h$  of the crash related singularity, may suggest 'novelty' and 'surprise' to be associated with the event. For the strongest crashes observed, obviously due to their economical impact, there is a great interest and an ongoing debate whether they can be classified as outliers or whether they actually belong to the dynamics of the economical system [11, 12, 13, 14, 15]. In the case of the crash of '87, there are indications that it resulted from the past history of the development of the index [14], in particular as it lacked any evident external reason for occurring.

### 3. MULTIFRACTAL DESCRIPTION OF COMPLEX SYSTEMS

The time series, the examples of which have been given in the previous sections belong to a class of systems recently characterised as multifractal (MF) [25, 26, 27, 7, 8, 9]. Several models of multifractality have been suggested, starting at the early extensions of fractality and classical examples [28], to sophisticated wavelet cascade based models recently suggested [29, 30]. Let us briefly hint at the main characteristic of multifractals.

For the stationary fractional Brownian noise, we would expect that any local estimate of the Hölder exponent  $h$  would conform to the mean or global Hurst exponent  $H$ . Of course, for finite length samples and single realisations, we will have fluctuations in the local  $h$  exponent, but they should prove to be marginal and diminish with increasing statistics. This will not be the case with a multifractal. The local  $h$  will show a wide range of exponents regardless of the resolution and sample size [27, 31]. What we would expect to remain unchanged (or stationary) for the multifractal (cascade) is the multifractal spectrum of  $h$ , i.e.  $D(h)$ .

In figure 3, an example time series with the local Hurst exponent indicated in colour are shown. We have chosen the record of healthy (adult) heartbeat intervals and white noise for comparison. The background colour indicates the Hölder exponent  $h$  - the local counterpart to the Hurst exponent  $H$ . It is centred at the mean value corresponding with the Hurst exponent at green. The colour goes towards blue for higher  $h$  and towards red for lower  $h$ . In the same figure 3, we show corresponding

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<sup>4</sup>Note that the interestingness of the time series is relative to application. The maxima of the WT can often be very well used since they converge to singular structures which they help in detecting and estimating. However, if one is interested in smooth components, this may not necessarily be the best alternative. Similarly, for localisation of oscillatory components, phase detection using complex wavelets may prove a more appropriate alternative than the maxima of real valued WT.

log-histograms of the local Hölder exponent <sup>5</sup>. Each  $h$  measures a so-called singularity strength, and thus a histogram provides a way to evaluate the ‘singularity spectrum’. In other words, the local  $h$  measures the local contribution to the multifractal spectra [31].

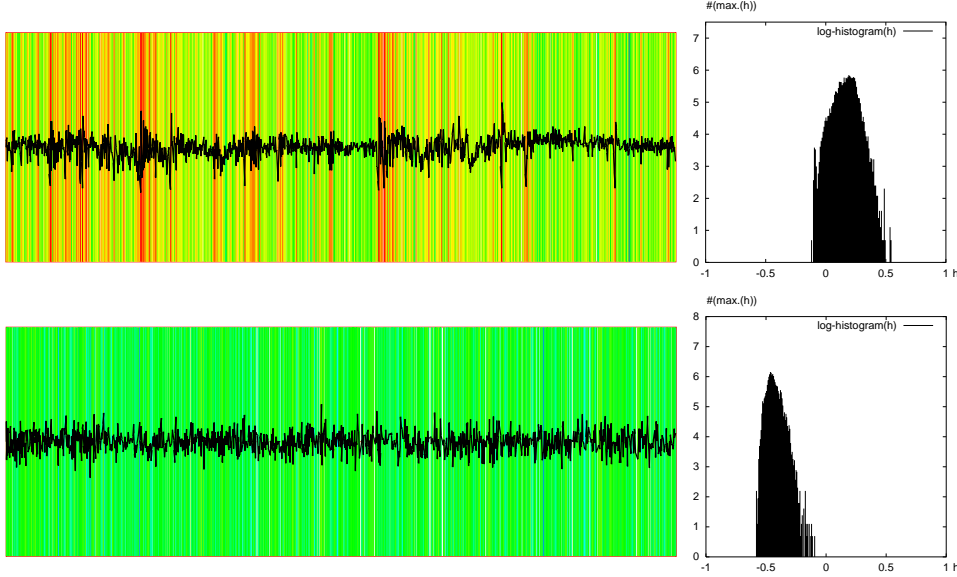


Figure 3: Left: example time series with local Hurst exponent indicated in colour: the record of healthy heartbeat intervals and white noise. The background colour indicates the Hölder exponent locally, centred at the Hurst exponent at green; the colour goes towards blue for higher  $h$  and towards red for lower  $h$ . Right: the corresponding log-histograms of the local Hölder exponent.

#### 4. ‘NOVELTY HINTS’ FROM THE ‘FAILURE’ OF THE (MF) MODEL

A true multifractal process would share the same parameters (like MF spectrum) for any sub-part of the record. Thus, for an ideal multifractal system, each new data recorded would not affect the spectrum already estimated. Testing for this *stationarity* property can be done for our example records. In particular, new sample information can be simulated by running a simple moving average (MA) filter, which may capture collective behaviour of the local  $h$  characteristic. A  $n$ -MA filtering of  $n$  base is defined as follows:

$$h_{MA_n}(i) = \frac{1}{n} \sum_{i=1}^{i=n} h_i(f(x)) , \quad (4.1)$$

where  $h_i(f)$  are the subsequent values of the effective Hölder exponent of the time series  $f$ . Standard deviation from the  $h_{MA_n}(i)$  mean exponent can also be calculated and is closely linked to the instantaneous MF spectrum width:

$$SDh_{MA_n}(i) = \frac{1}{n} \sqrt{\sum_{i=1}^{i=n} (h_i(f(x)) - h_{MA_n}(i))^2} . \quad (4.2)$$

<sup>5</sup>They are made by taking the logarithm of the measure in each histogram bin. This conserves the monotonicity of the original histogram, but allows us to compare the log-histograms with the spectrum of singularities  $D(h)$ . By following the evolution of the log-histograms along scale, one can extract the spectrum of the singularities  $D(h)$  (multifractal spectrum).



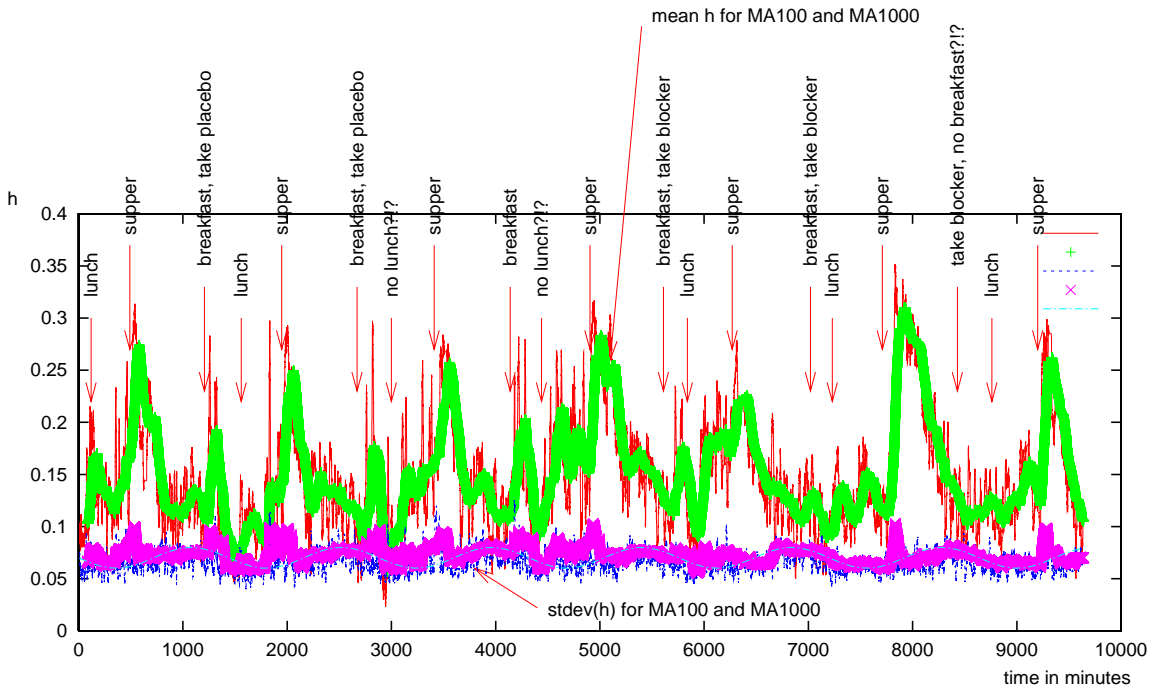


Figure 4: The variability plot from a long run of experiments where the test persons were given placebo or beta-blocker. Two runs of  $MA$  filter were performed with 100 and 1000 maxima long window. An interesting pattern of response to food is evident.

An interesting pattern of ‘surprising’ features can be identified in the example (7 days long) record of the heartbeat. Upon verification, it confirms a pattern of response to activity, suggesting novel links to external information. Without going into much detail of the record given, there is a particularly strong response of the person in question to food. The observed shift towards higher values as the result of eating (it is almost possible to estimate the volume of the meal!) may indicate some nearly pathologic response in this individual case [32].

## 5. EXPLOITING SUSPECT ‘NOVELTY’ IN A HEURISTIC MODEL

In the case of fetal heartbeat during labour, there is no reason why the local Hölder exponent  $h(V_i)$  of the variability  $V_i$  component of fetal heartbeat intervals should be stationary. It reflects dynamic changes in the condition of the fetus and the degree of stress to which it is subjected. Despite the fact that stress has a rapid effect on heartbeat, the effects on the state of the fetus are not always immediate. This is why short dynamic changes in heartbeat characteristics (which determine the multifractal picture) may not be relevant and not representative of the state of the fetus. Rather than expanding the observation window, we have suggested [33] using a cumulative indicator, designed to capture the non-stationarity of the local  $h$  of the variability component of fetal heartbeat  $V_i$  [33].<sup>6</sup> The cumulative  $h$  is defined from the beginning of the observation and with respect to some normal reference level  $h_{ref}$ :

$$h_{cum}(V_i) = - \sum_{l=1}^i (h_{eff}(V_l) - h_{ref}) . \quad (5.1)$$

<sup>6</sup>To use the linear integral of the non-stationarity component of the variability of fetal heartbeat is simply a heuristic. Of course, other functional dependence than linear integral is possible. The discovery of a more suitable model of such possible functional dependence is the subject of our future research, involving the techniques described in section 6.

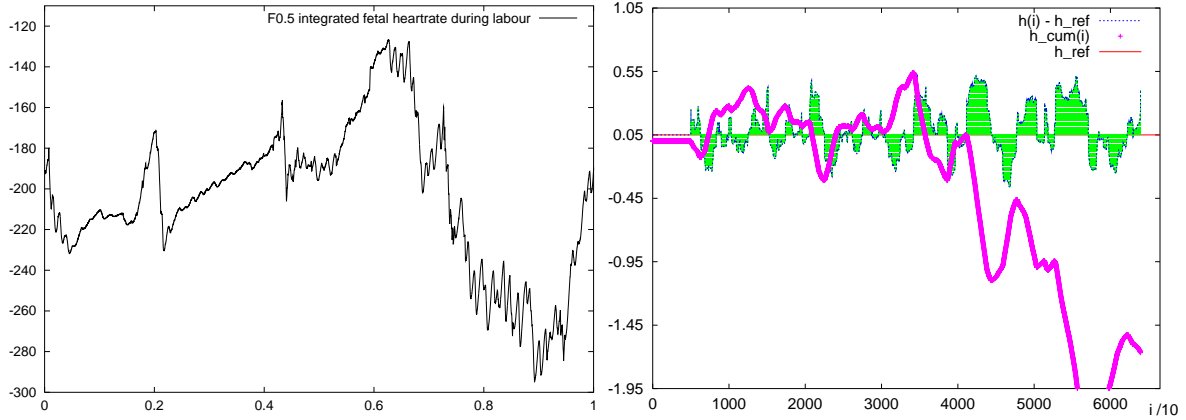


Figure 5: Left: a fractionally  $F0.5$  integrated ‘normal’ record contains no diagnostic surprises. Right: the cumulative indicator  $h_{cum}$  extracted from a bad fetal outcome record plunges after a period of homeostasis, suggesting diagnostic ‘novelty’. Both the cumulative Hölder exponent  $h_{cum}(V_i)$  (red line) and the deviation of the Hölder from the reference value  $h_{ref} = 0.05$  (blue filled curve) are plotted in the right plot.

The minus sign is introduced to give the  $h_{cum}$  indicator increasing direction when the level of local correlations is lower than  $h_{ref}$ . This corresponds with a healthy condition. The case of higher correlations is associated with problems and, therefore, the accumulation of a positive difference ( $h_{eff}(V_i) - h_{ref}$ ) will lead to decreasing cumulative  $h$ . The cumulative indicator steadily increasing or remaining within some margin of fluctuations indicates no problems and a good prediction. When the indicator plunges down, it calls for intervention. This can, of course, happen at any moment during labour. The nature of this process is dramatically non-stationary, and a period of positive evaluation can be interrupted at any stage (for example by the occlusion of the umbilical cord due to movement). One of the examples shown (figure 5 right) shows the cumulative indicator plunging after a prolonged homeostasis.

This record thus shows a ‘novelty’ or ‘surprise’ in the dynamic evolution of its multifractal properties as judged by the results of the related (bad) fetal outcome. For comparison, we show in the same figure 5 in the left panel a record of the raw, fractionally integrated fetal heartbeat time series which corresponds to a good fetal outcome. This time there is no diagnostic novelty or surprise in the time series - the corresponding fetal outcome has been pronounced OK. The apparent similarity of the record evolution would however likely prompt a different opinion, that in both cases a novelty occurred! The difference is that the panel to the right (in Fig. 5) has been drawn from a diagnostic carrying information derived from the time series using a heuristic model. The panel on the left has been prepared using the raw time series transformed linearly by (fractional  $F0.5$ ) integration.

## 6. REASONING FROM NON-STATIONARITY - DATA MINING OR LOOKING FOR THE UNKNOWN MODEL

Universal descriptions of complex phenomena, like that using multifractal cascades, may prove to be inadequate for a complete description, even if valid on a restricted temporal range or in isolated or free-running conditions. The inadequacy of such models is often demonstrated by the non-stationarity of their characteristics. This aspect is usually neglected (through the selection of examples supporting the theory) or filtered out.

However, failure of the model to explain the phenomenon fully may well provide significant insight into the dependence of the system on the external conditions. Structures emerging from the non-stationarity of the (most) sophisticated description available very likely indicate that more dimensional embedding may be needed for a proper description of the system under study. Such embedding and

the right parameter choice for the more adequate model may not be easy to identify. In science, this search trajectory for better models has been routinely carried out at the cost of repeated experiments under varied input or environmental conditions (or modes of interaction with the environment).

Such a search for a better model may be shortened by automatically investigating the additional 'environmental' information often available, as has been done 'by hand' in the previous sections. Due to the modern technology of 'intelligent' data analysis and reasoning, in particular using Bayesian techniques, such 'automated research' may be possible. By incorporating the most advanced models available with explicitly identified instances where they fail to describe the model (as is manifested in non-stationarity), new theories can be generated and (dis-)proven by the system. It is important to realise that in such an approach we are looking for an unknown model, therefore not just model-fitting.

A preliminary experiment comprising building a Bayesian net based model using parameters external to the time series records of fetal heartbeat has been described in [34]. In this experiment, about a thousand cases have been investigated, continuous variables have been discretised and time series characteristics have been derived from the heartbeat for three 1/2 hour intervals just before birth. External characteristics have been treated on an equal footing to the ones derived from the time series in building Bayesian Nets best fitting the data. The best models obtained were, of course, evaluated by human experts. Among the recovered facts, primary agreement of the best networks with the expert's knowledge, the primary condition of a valid model. In addition, novel relationships were suggested, subject to further investigation.

## 7. CONCLUSIONS

We have elaborated on the difficulties which may arise in the (novelty oriented) analysis of time series arising from real life complex systems. We have also presented a number of example approaches aiming at 1) tempering the singular behaviour by means of wavelet transforming, and 2) capturing complex multifractal model characteristics. Additionally, we have suggested evaluating novelty by monitoring the instances of failure of such a model, as is pronounced in non-stationarities of its characteristics. Such novelty can be linked to external variables, can be further incorporated in a heuristic model or investigated by probabilistic methods (Bayesian net) for evidence of a higher dimensional model. The methodology, however strongly it opposes attempting to model time series by the reconstruction of the dynamic properties of the system (e.g. phase space reconstruction, feature (based) linguistic), does not preclude it. In fact some aspects of tempering (taming) the singular time series involved and reasoning using multifractal (or other appropriate stochastic model) characteristics may prove to be practical in such an alternative approach. As an additional concluding observation, it is possibly the lack of multiresolution capabilities which limits the possibilities of the techniques for novelty discovery [1, 2, 3]. They operate with one fixed resolution which makes it difficult to derive scaling laws. The wavelet transform makes multiresolution analysis possible and, in the context of novelty discovery, it has been shown to make possible the derivation of 'rules and laws from data' [10, 35, 36].

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