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MATHEMATICAL MODELS FOR THE ANALYSIS AND FORECASTING OF RIVER WATER POLLUTION USING THE MULTIFRACTAL METHOD

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Abstract. This paper explores multifractal analysis for the selected time series water pollution data set and further prediction based on BOD measure with ARFIMA-based fractal model. MFDFA multifractal algorithm is applied for estimating the fractal differentiation parameter of the ARFIMA. The obtained results are compared with similar obtained with autoregressive ARIMA model and basic ARFIMA fractal model. The study reveals an enhancement in accuracy with the use of combination of multifractal analysis and fractal methods for water pollution prediction.

Keywords: Time series, autoregressive model, ARIMA, Biochemical Oxygen Demand, long memory, fractal model, ARFIMA, multifractal analysis, MFDFA, fractal differentiation parameter.

Introduction

Industrial development and human economic activity cause not only the improvement of the conditions of human life, but are accompanied by the simultaneous emergence of various environmental problems. These problems are caused by the impact of human activity on the environment and require decisions of a global scale. In 2015, the United Nations adopted the goals of sustainable development, which are known as the Global Goals [1]. Their main goal is to reduce poverty, protect the planet and ensure global peace and prosperity by 2030. Among the 17 proposed goals, goal number 6 is the availability of clean water and adequate sanitation for the global population. This goal involves increasing attention to the issue of preserving natural systems and organizing the activities of industrial facilities in compliance with the requirements of international standards in the field of environmental protection. One of the most important aspects of environmental protection is the protection of surface and river waters from technogenic pollution.

Review of Modern Information Sources on the Subject of the Paper

Among all types of pollution, organic pollution of river systems is a key indicator of river water quality. This indicator determines the safety of drinking water supply and shows the rate of spread of organic substances in the river basin [2-4]. However, organic pollution consists of a complex mixture of different chemicals. This includes the vital activity of aquatic creatures, waterlogging of riverbeds, discharge of sewage from sewage systems, livestock farms, etc. [5, 6]. Therefore, to evaluate its content, it is necessary to choose generalizing indicators. The main indicators of the level of organic pollution are chemical oxygen demand (COD) and biochemical oxygen demand (BOD). Both indicators are usually measured in mg/l. Both the first and the second indicator to a certain extent can serve as an indicator of the suitability of water for drinking water supply and a general assessment of the state of the river ecosystem [7]. If we take into account that BOD correlates with many other indicators of river water quality [7, 8], then its measurement and prediction of its temporal changes is a universal tool for ecomonitoring of the state of the river water environment.

Advances in qualitative forecasting of BOD changes can serve as a valuable method to complement global and regional efforts to monitor this parameter in river water. Such forecasting relies on time series analysis, which, in this case, examines the trends in BOD indicators over time. Such analysis involves identifying data patterns over time, with autoregressive models like ARIMA (AutoRegressive Integrated Moving Average) among the most widely used for modeling and forecasting [9]. ARIMA uses three key parameters: the autoregressive order p, which indicates significant lags; the integration order d, showing series differencing; and the moving average order q, indicating significant error lags. A generalization, the ARFIMA (AutoRegressive Fractionally Integrated Moving Average) model, extends this approach by allowing non-integer d-values, making it suitable for long-memory processes. Anderson's 1998 study shows that failing to account for long memory when present can seriously worsen forecast accuracy, underscoring ARFIMA's relevance for contemporary time series analysis [10]. Fractal mathematical models have broad applicability across numerous disciplines, especially in the analysis of natural systems that exhibit self-similarity within complex structures. These models are particularly useful in fields such as financial markets, biological signal processing, and the study of physical properties [11, 12], where they effectively capture the heterogeneous and fractal-like nature inherent in such systems.

Objectives and Problems of Research

This study presents the development of an intelligent system designed to automate data processing and improve the precision of forecasting decisions based on the BOD indicator, utilizing the ARFIMA model. The system integrates multifractal analysis to derive the fractal differentiation parameter of the ARFIMA model, supporting the early detection of environmental concerns.

The object of the study is the dynamics of water pollution, which must be assessed based on historical data.

The subject of the study is the mathematical models that that leverage the multifractal properties of time series to enhance the forecasting of water pollution levels.

The main objective of this research is to develop and implement a mathematical fractal model that incorporates multifractal characteristics to improve time series forecasting accuracy, surpassing the performance of standard autoregressive and fractal models. To achieve this goal, the following sub-tasks have been outlined:

- to identify an appropriate dataset for a specific river, analyze a limited sample from a selected monitoring station, and perform data cleaning to ensure reliability for subsequent steps;
- to decompose the time series and investigate the presence of long-term dependencies within the data;
- to perform MFDFA algorithm, examine the multifractal strength and other relevant multifractal characteristics;
- to utilize the fractal differentiation parameter derived from the MFDFA algorithm to develop an ARFIMA-based forecasting model and perform time series forecasting;
- to compare the performance of the created fractal model with the same model with automatic parameter selection, as well as with the most appropriate autoregressive model on different sizes of training and test data and evaluate the adequacy and effectiveness of the proposed approach.

The scientific innovation consists of the development of an analytical system for dynamic analysis and forecasting of river water pollution, utilizing the MFDFA multifractal algorithm for time series processing. This approach enables the estimation of the fractal differentiation parameter for analysis and forecasting based on the ARFIMA model, facilitating data analysis automation and enhancing the accuracy of forecasting decisions.

The practical significance of this research lies in the development of a software solution based on multifractal modeling approaches. This system aims to enhance forecasting accuracy, facilitating the early detection of environmental issues and contributing to more effective water quality management.

Main Material Presentation

Analysis of software tools

The time series analysis in this study was conducted using Python, with the pandas and numpy libraries for data handling and numerical computations. For multifractal analysis and time series forecasting, the R programming language was employed, utilizing the mfdfa, forecast, and arfima libraries. The use of two different programming languages was necessitated by the lack of ARFIMA and other fractal model implementations in widely used libraries for Python. In contrast, R provides more comprehensive support for fractal time series models.

Dataset for forecasting river water pollution

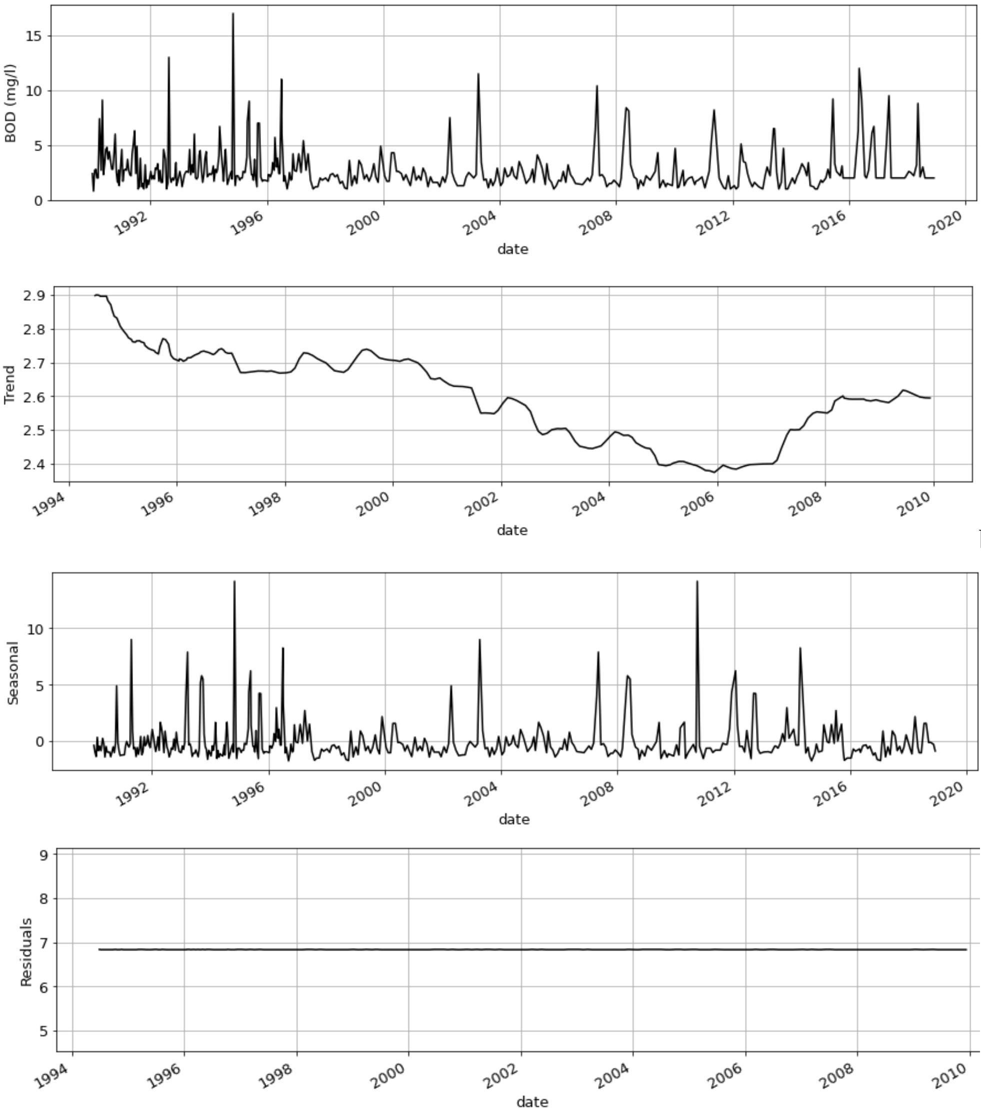
The dataset [13] includes data collected between 1990 and 2018. It comprises raw data from river monitoring sites, including Water Framework Directive sites, in a single CSV file with aggregated measurements for various UK rivers. Each entry reflects a reading from a specific monitoring station at a particular time and location, collected at intervals of few times per month.

The River Quoyle in Northern Ireland, with the highest measurement count in the dataset (458 entries), was selected for study and BOD parameter was chosen as a primary pollution indicator, widely recognized in scientific research for assessing river quality.

Investigating the presence of trend, seasonality, stationarity and long memory

Before proceeding with modeling and forecasting, it is crucial to identify the key characteristics of the time series of the BOD values of River Quoyle to determine the appropriateness of specific machine learning models. Preliminary data cleaning was performed as not all records included these values.

Fig. 1 demonstrates the decomposition the selected time series. It was performed using the statsmodels.api module in Python, revealing the presence of a trend while indicating the absence of seasonality.



a) b) c) d)

Fig. 1. Time series of BOD in the Quoyle River (a), decomposed trend (b), seasonality (c) and residuals (d)

The final graph in Fig. 1 represents the residual (noise) component of the time series, which highlights the presence of outliers. Ideally, this residual component should exhibit the characteristics of white noise, defined by a zero mean, constant variance, and the independence of variables, which is allowing machine learning models to capture all essential signals within the training sample, thereby optimizing algorithm efficiency. However, in our case, while the variance remains stable, the mean consistently exceeds zero, allowing us to reject the white noise hypothesis in the redundancy graph.

An important characteristic of time series analysis is examining evidence of long-term memory. Fig. 2 presents the Autocorrelation Function (ACF) graph, which displays the correlation between the time series and its lagged values across varying time lags. The graph reveals that certain time lags extend beyond the confidence interval (depicted by the shaded blue area), indicating persistent dependencies in the data. This observation suggests the presence of long-term memory effects within the time series, which may significantly influence forecasting accuracy and model selection.

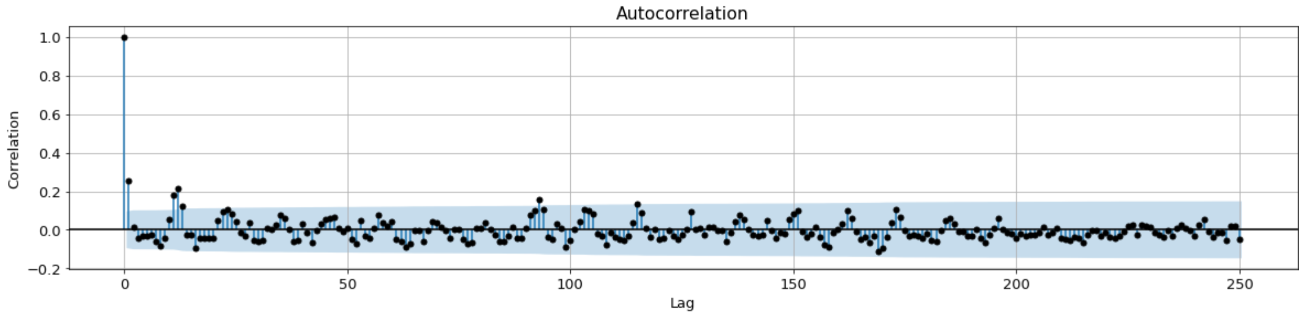


Fig. 2. ACF function for the time series of BOD in the Quoyle River

The subsequent step in the analysis involves assessing the stationarity of the time series, a fundamental property that enhances predictability and facilitates the application of various forecasting techniques. Two widely used statistical tests for evaluating stationarity are the Augmented Dickey-Fuller (ADF) test and the Kwiatkowski-Phillips-Schmidt-Shin (KPSS) test [14]. These tests provide complementary results by assessing opposing hypotheses. Specifically, if the ADF test fails to reject the null hypothesis of non-stationarity, while the KPSS test rejects the null hypothesis of stationarity, this indicates the presence of a unit root, classifying the series as an I(1) process, thus confirming its non-stationarity.

In this study, stationarity was examined using Python's `statsmodels.tsa.stattools` module. The ADF test returned a p-value below the 0.05 significance threshold, leading to the rejection of the null hypothesis and suggesting stationarity. Conversely, the KPSS test produced a p-value exceeding the threshold, thereby failing to reject the null hypothesis of stationarity for this series.

Mathematical description of the fractal model ARFIMA

Autoregressive (AR) model of order p:

$$X_t = c + \sum_{i=1}^{p} \phi_i X_{t-i} + \varepsilon_t \,, \tag{1}$$

$\phi_1, \dots, \phi_p$ are autoregressive parameters, ε_t is white noise, c is a constant.

Moving Average (MA) model of order q:

$$X_t = \mu + \sum_{i=1}^{q} \theta_i \varepsilon_{t-i} + \varepsilon_t \,, \tag{2}$$

$\theta_1, \dots, \theta_p$ are parameters of the moving average, ε_t, $\varepsilon_{t-1}, \dots$ is white noise, μ is constant.

Generalisation of the above models is:

$$\left(1 - \sum_{i=1}^{p} \phi_i B^i\right)(1 - B)^d (X_t - \mu) = \left(1 + \sum_{i=1}^{q} \theta_i B^i\right)\varepsilon_t \,, \tag{3}$$

$(1 - B)^d$ is the differentiation operator. The ARMA and ARIMA models are designed to capture short-memory processes, as the differencing parameter d in ARIMA is restricted to integer values. Consequently, these models are not well-suited for time series exhibiting long-memory properties. To address this limitation, the ARFIMA (p, d, q) model extends ARIMA by allowing d to take on fractional values, enabling it to effectively model time series with long-range dependencies and self-similar structures.

Expand the differentiation operator using the binomial expansion for any real number d:

$$(1-B)^d=\sum_{k=0}^{\infty}\binom{d}{k}(-B)^k = 1 - dB + \frac{d(d-1)}{2!}B^2 - \frac{d(d-1)(d-2)}{3!}B^3 + \dots \quad (4)$$

When d=0, X_t it is simply white noise, and its autocorrelation function is 0. When d=1, X_t is a random walk that is a stochastic process in which the autocorrelation function (ACF) at lag 1 is equal to 1, indicating a strong dependence between consecutive values. After applying first-order differencing, which involves computing the difference between consecutive values in the time series, the process can be transformed into white noise.

When d is already a real number, $X_t = -\sum_{k=1}^{\infty}\left(\frac{\Gamma(k-d)}{\Gamma(k+1)\,\Gamma(-d)}\right)X_{t-k} + \varepsilon_t$, and, therefore, X_t is affected by all historical data ($X_{t-1}, X_{t-2}, \dots$).

Mathematical description of the multifractal analysis method MFDFA

The Multifractal Detrended Fluctuation Analysis (MFDFA) [15] method follows a similar approach to Detrended Fluctuation Analysis (DFA) but incorporates additional steps to capture multifractal properties by examining a spectrum of fluctuations. This technique is widely regarded as an effective tool for detecting and quantifying the presence of multifractal characteristics in time series data.

For time series $X = \{x_\tau\}_{\tau=1}^{n}$, n is time series data length, and the computational procedure can be described as follows:

1. calculate the profile time series $Y = \{y_\tau\}_{\tau=1}^{n}$

$$y_\tau=\sum_{k=1}^{\tau}(x_k - \bar{x}),\ (\tau = 1,2,\dots,n), \quad (5)$$

where $\bar{x}$ is the mean value of $X = \{x_\tau\}_{\tau=1}^{n}$.

2. divide the profile time series Y into $I_s = int(n/s)$ non-overlapping segments of equal length s. In segmentation, the total length n of the time series data is often not an integer multiple of the segmentation length s, which results in the truncation of the tail of the profile time series data. To address this, the segmentation process was repeated in reverse order of the profile data, resulting in a total of $2I_s$ segments.

3. Calculate the trend of each $2I_s$ segment, and the detrended time series $z_t(i)$ can be obtained by the following equation:

$$z_t(i) = v_t(i) - p_t(i),\ (1 < i < s), \quad (6)$$

where $v_t(i)$ and $p_t(i)$ represent the segment time series and trend time series at each segment t, respectively.

4. Determine the variance $F^2(s,t)$ by the following equation:

$$F^2(s,t) = \frac{1}{s}\sum_{i=1}^{s} {z_t}^2(i), \quad (7)$$

and then the *q*th-order fluctuation function of all $2I_s$ segments are obtained by the following equation:

$$\begin{cases} F_q(s) = \sqrt[q]{\frac{1}{2I_s}\sum_{t=1}^{2I_s}\left(F^2(s,t)\right)^{\frac{q}{2}}},\ if\ q \neq 0 \\ F_q(s) = \exp\left\{\frac{1}{4I_s}\ \sum_{t=1}^{2I_s}\ln\left(F^2(s,t)\right)\right\},\ if\ q = 0 \end{cases} \quad (8)$$

5. There is a power-law relationship between the fluctuation function Fq(s) and scale s.

$$\mathrm{Fq}(s) \propto s^{H(q)}. \quad (9)$$

The scaling behavior of the fluctuation function could be determined by analyzing log–log plots of $F_q(s)$ versus scale s for each value of q. The least squares method is then applied to fit the ln $F_q(s)$ against ln s, with the resulting slope representing the generalized Hurst exponent H(q). If H(q) remains constant and independent of q, it indicates the absence of multifractal characteristics in the time series data.. On the contrary, if H (q) exhibits significant dependence on q, this suggests the presence of multifractal properties in the original time series.

Results and Discussion

To carry out the modeling and forecasting task, it is essential to have a dataset that includes both the measurement date and the corresponding BOD (biochemical oxygen demand) value. Thus, the time series is structured accordingly to enable the analysis.

To determine the optimal fractional differencing order for the ARFIMA model, the MFDFA method was employed to identify underlying patterns, structures, and correlations at various time scales [15]. The analysis used the MFDFA function from the MFDFA package in R, applying it to actual time series data along with a specified scale parameter (scale) that defines the range of segment sizes for detrending, and a set of Q-values (q) that affect the fluctuation function's sensitivity to different fluctuation magnitudes. The scale parameter was chosen according to the time series data length, and q values were set in the popular range from -10 to 10, where negative values of q highlight smaller fluctuations and positive values emphasize larger ones.

The MFDFA method results provided the whole list of parameters: Hurst exponent, scaling exponent, singularity spectrum, fluctuation function. Key multifractal characteristics are visually presented in Fig.3, illustrating that the time series exhibits distinct multifractal characteristics and highlighting the intensity of multifractal effects.

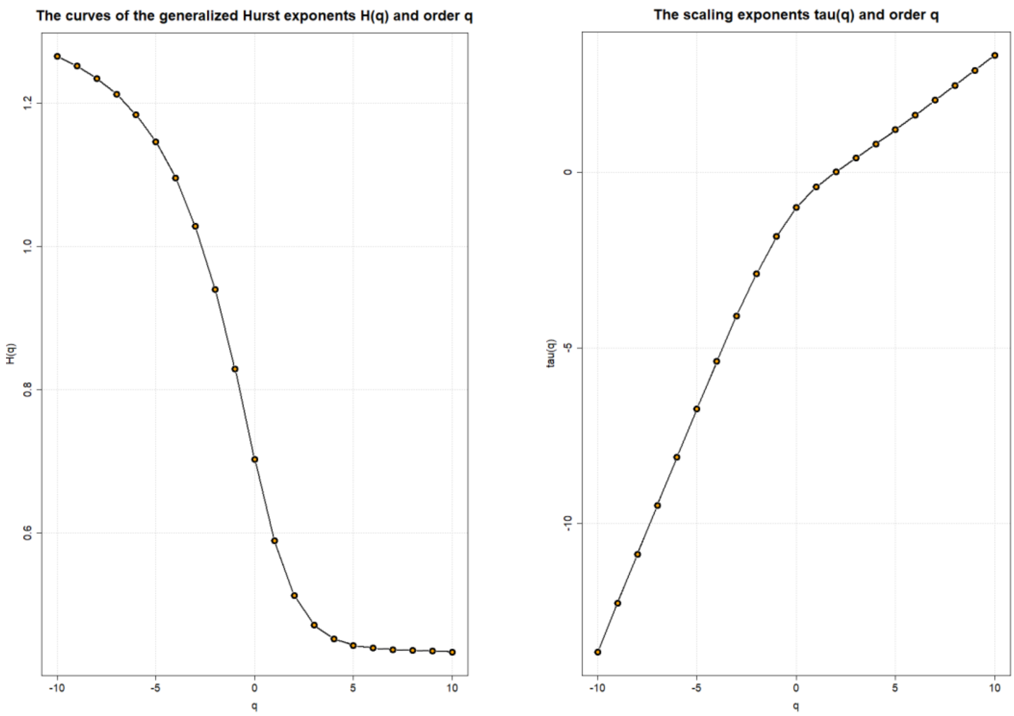
The generalized Hurst exponent h(q), a function that describes the scaling behavior of fluctuations across various q values. When q=2, h(q) corresponds to the classical Hurst exponent, which is then used to inform the optimal fractional differencing order.

It has been established that our time series behaves as a near-Gaussian stationary process with moderate to long memory [16], without extreme tail behavior and from that we can assume that

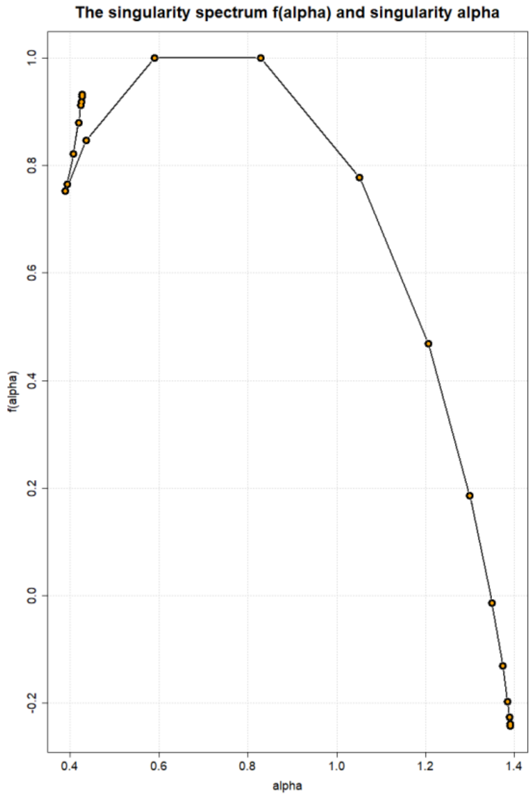
$$d = H - 1/2. \tag{10}$$

Following step is to identify AR and MA parameters of ARFIMA. In order to totally remove trend in our time series differentiation was perfomed using fractal differentiation parameter from expression (11). It has been accomplished using diffseries function of the fracdiff library of the R programming language, which uses an approximate binomial expression of the long memory filter. The values of the ACF and PACF functions of the determined differentiated series are shown in Fig. 4.

From the values of the ACF and PACF functions, we can distinguish the number of significant delays, i.e. those that are greater than the range of the confidence interval (blue dashed line in Fig. 4), which will allow us to determine the maximum number for our parameters AR(p) from the ACF graph and MA(q) from the PACF graph, respectively. The choice of the optimal model was determined by the RMSE (Root Mean Square Error) estimate, taking into account the difference between the test data. RMSE measures the root mean square deviation between predicted and actual values.



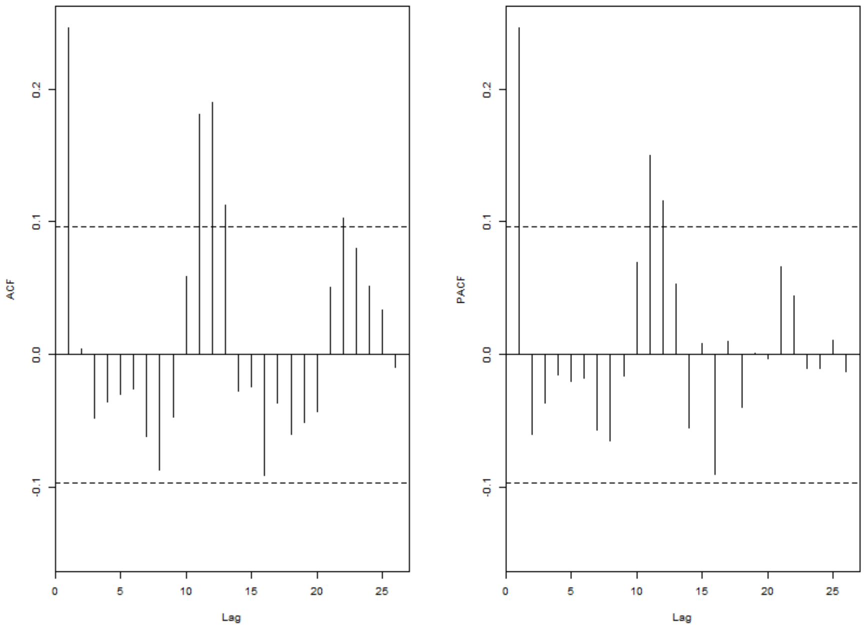
a) b)



c)

Fig. 3. Multifractal characteristics: Hurst exponent (a), scaling exponent (b) and singularity spectrum (c)

To assess how effectively the trained network predicts the BOD index for the River Quoyle (Northern Ireland), it has been utilized test datasets containing 10 and 50 units that were not included in the training process. To further evaluate the efficiency of the ARFIMA-based fractal model, forecasting was also conducted using both the ARFIMA and ARIMA models, employing automatic parameter selection from the forecast library in R. The performance of these models was compared using RMSE evaluation metric for the test set.



a) b)

Fig. 4. ACF function (a), PACF function (b) applied to differentiated time series

The results of this analysis is presented in Tables 1.

Table 1

Evaluation of the prediction accuracy using RMSE metric

Model	10 test data	50 test data
(auto) ARFIMA	2.009118	2.545665
(auto) ARIMA	2.009179	2.606649
manually fitted ARFIMA	1.687774	2.522736

Based on the aforementioned results for the key metric RMSE, we can confidently conclude that the ARFIMA-based model, utilizing parameter estimation through MFDFA, demonstrates the highest forecasting efficiency among the models analyzed. Additionally, it is noteworthy that, despite the relatively weak expression of long memory in our time series, a comparison of the models with automatic parameter selection—specifically, the fractal ARFIMA and the autoregressive ARIMA models—indicates that when forecasting larger datasets, the fractal model yields superior results.

Conclusions

This study explores data modelling and development of a software solution based on multifractal modeling approaches.

Key analyses include the assessment of Hurst exponents with the use of multifractal analysis, time series stationarity, and long memory characteristics. ARFIMA-based fractal model was developed by incorporating the fractal differentiation parameter derived from the MFDFA algorithm to enhance time series forecasting.

Using observational data from the River Quoyle in Northern Ireland, this study compares the forecasting accuracy of the proposed fractal model with its automatically parameterized version as well as with conventional autoregressive models.

Numerical experiments conducted on varying training and test dataset sizes demonstrate that the proposed architecture improves forecasting accuracy compared to traditional autoregressive and fractal models. These findings highlight that even in stationary time series with weak long-memory properties, fractal models leveraging multifractal characteristics exhibit high efficiency, facilitating the early detection of environmental issues.

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МАТЕМАТИЧНІ МОДЕЛІ ДЛЯ АНАЛІЗУ ТА ПРОГНОЗУВАННЯ ЗАБРУДНЕННЯ РІЧКОВОЇ ВОДИ З ВИКОРИСТАННЯМ МУЛЬТИФРАКТАЛЬНОГО МЕТОДУ

Отримано: Березень 20, 2025 / Переглянуто: Березень 25, 2025 / Прийнято: Березень 31, 2025

Анотація. Стаття досліджує застосування мультифрактального аналізу до вибраних часових рядів даних про забруднення води та подальше прогнозування за показником біохімічного споживання кисню (БСК) на основі фрактальної моделі ARFIMA. Для оцінки параметра фрактальної диференціації в моделі ARFIMA використано мультифрактальний алгоритм MFDFA. Отримані результати порівнюються з аналогічними, отриманими за допомогою авторегресійної моделі ARIMA та базової фрактальної моделі ARFIMA. Дослідження показує підвищення точності прогнозування при використанні комбінації мультифрактального аналізу та фрактальних методів для оцінки рівня забруднення води.

Ключові слова: часові ряди, авторегресійна модель, ARIMA, біохімічне споживання кисню, довга пам’ять, фрактальна модель, ARFIMA, мультифрактальний аналіз, MFDFA, параметр фрактальної диференціації.