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ABOUT NON-STATIONARITY IN TIME SERIES OF FIELD MEASUREMENTS

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Представлено П.П. Петровым

Abstract: The paper is aimed at analyzing the difficulties that arise when checking time series of field measurements for stationarity and identifying the main characteristics of the series. Attention is paid to the correctness of using the most popular methods of primary analysis for real data. The author's simple procedure is proposed, based on the definition of weak stationarity, which allows, in combination with other methods, to draw a conclusion about the available data. The proposed procedure is tested on synthetic data. The methods described in the paper are applied to real time series, presented in the form of measurements of the concentration of PM2.5 suspended particles in the atmospheric boundary layer of the urban city.

Keywords: primary time series analysis, stationarity tests, correlogram analysis, variance ratio test.

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1 Introduction

A time series is a collection of observations of the time evolution of some variable. Time series occur in a wide variety of fields, from economics to the physical sciences, and having prior knowledge of the causes and strength of the relationship between the dependent and independent variable (time) distinguishes a set of elements of a time series from a sample of values of a random variable, making time series analysis more labor-intensive process. Also, the behavior of a variable reflected by a time series cannot be reproduced using repeated observations, since only one implementation occurs at each point in time, and the presence of a cause-and-effect relation makes each time series unique.

The most important problem in time series analysis is their forecasting. Indeed, a large number of studies in various areas of science and technology has been devoted to the development of methods for predicting the further development of the area represented by a set of data and assessing the result of such a forecast (see review articles [1] and [2]). The popular forecasting methods here remain methods of analyzing time series of the ARIMA type [3], Holt-Winters model [4], regression and classification models [5], as well as neural networks and other machine learning type methods [2]. In the first half of 2024 alone, according to the Google Scholar service, more than 20 thousand articles appeared aimed at developing this topic. However, it is known that models based on identifying various kinds of trends give a significant error if they change [4]. This leads to the development of break-points detection methods in time series analysis [6]. On the other hand, methods based on machine learning are dependent on the choice of the training sample, which, in the case of a complex time series (for example, with implicit seasonality, imbalances, physically significant anomalies), atypical scenarios can be attributed, adding an error that cannot be assessed due to the characteristics of machine learning. Thus, prior knowledge about the properties of a series is crucial in its prediction.

At the same time, the (weak) stationarity of a series or its subsequence is actually the only guarantee that the resulting forecast will be the most accurate, regardless of the model used, since stationarity implies the preservation of the main statistical characteristics of the series over time. In a mathematically strict sense, the desire to deal with a stationary series is caused by the possibility of justifying forecast models for such a series using the Wold theorem [7] on decomposition, according to which any stationary process can be uniquely represented as the sum of two uncorrelated processes: a deterministic one, the forecast of which for any time in advance error-free, and purely random (white noise). In practice, this means a simple property: the researcher understands how the system behaves, and this behavior persists over time. This is the main reason why the test for the stationarity of a series is the first step in its forecasting. However, even such a simple test can cause a number of difficulties due to the characteristics of the available statistical criteria. This paper presents an overview of some tools for assessing the stationarity of time series of field measurements and their functional interpretations using the example of real measurements of the concentration of suspended particles with a diameter less than 2.5 microns (PM2.5) in Krasnoyarsk in 2020. Limitations on the applicability of some popular approaches are shown. It is also proposed a new procedure for testing a series, based on the analysis of histograms of the distribution of means and variances of individual subsequences of the time series.

The paper is organized as follows. Firstly, in section 2 it is described the data of field measurements under research and problems which arise in this area. After in section 3 it is proposed the overview of the most popular methods of stationarity cheking. Then the described methods is applied to available data in section 4. Section 5 has a description of the author's proposed procedure and the tests of it on synthetic and real data. And the final section is aimed to conclusions and discussions.

2 Description of the data under study

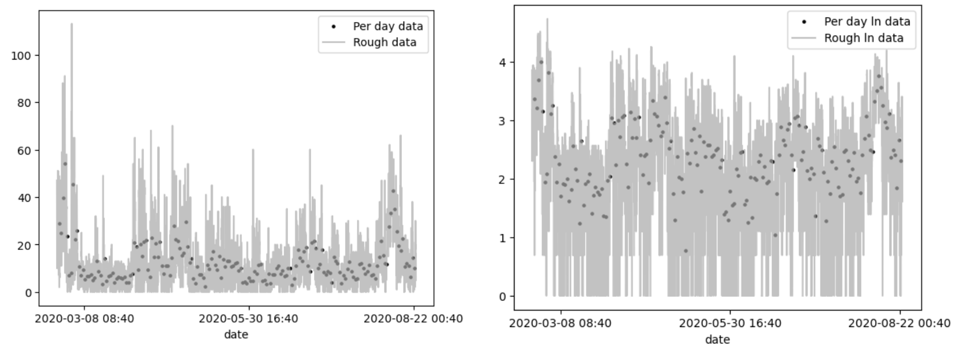
A good example of a time series encountered in practice is environmental measurements, which may include both meteorological measurements and air quality data. A generally accepted marker and, at the same time, one of the most harmful air pollutants in the ground layer of the atmosphere of modern cities are particulate matter with a diameter of 2.5 microns or less (PM2.5). The concentration of suspended particles PM2.5 is a basic indicator of pollution in a city or region, affecting the health of its residents, as well as a criterion for its attractiveness for living. This necessitates the need to identify typical scenarios for the dynamics of periods of increased PM2.5 concentrations and to develop new methods for predicting such periods. Concentrations of fine particular matters in the atmospheric boundary layer are known to be sensitive to meteorological factors (e.g., air temperature and relative humidity) [8] and human activities, and tend to show changes depending on the day of the week and season [9]. Understanding temporal trends is critical to accurately determining PM2.5 concentrations and mitigating human exposure to air pollution. Now, the methodology commonly used to estimate environmental parameters is based on classical descriptive statistics, but this is of rather limited value due to the large variability associated with air quality data and the low signal-to-noise ratio of available measurements. Time series analysis may be a good approach to avoid these difficulties by allowing the identification of underlying deterministic behavior and thus contributing to the understanding of cause-and-effect relationships in environmental problems.

Krasnoyarsk is one of the Russian cities where atmospheric air quality is monitored at stationary observation posts. The Ministry of Ecology and Rational Natural Resources Management of the Krasnoyarsk Territory maintains the regional departmental information and analytical data system on the state of the environment of the Krasnoyarsk Territory (RDIAS). Nine automated observation posts (AOP) of RDIAS are located in Krasnoyarsk. Once every 20 minutes, automatic measurements of meteorological parameters and the concentration of pollutants in the surface layer of the atmosphere are performed. To monitor PM2.5 concentrations, RDIAS uses dust analyzers model E-BAM (Met One Instruments Inc., USA, see [10]), the operating principle of which is based on measuring the absorption of β radiation by dust particles deposited on a filter tape. This method is certified by the U.S. EPA (United States Environmental Protection Agency, see [11]). Analyzers of this class are recommended for measuring the content of PM10 and PM2.5 fractions in the atmosphere, certified and accredited in many countries around the world, including Russia (No. 57884-14 in the State Register of Measuring Instruments). The available data set contains measurements from 00:20 January 1, 2019 to 23:40 December 31, 2022. Note that the data contains a very large number of gaps due to failures of dust analyzers. The longest subsequence of the time series from the "Kirovsky" post (link to the geoportal with the location https://air.krasn.ru/map.html?2=) is 181 days in the period from 2020-02-23 11:20 to 2020-08-23 07:40 ($181\times72=13032$ measurements).

Note that at present, dozens of works by researchers are devoted to the analysis of data on PM2.5 concentrations from a network of spatially distributed sensors and subsequent forecasting of the development of the environmental situation in the region, for example, see studies [3, 9, 12, 13, 14, **?**].

Figure 1 shows a graphical representation of the data under study. Here, Figure 1a shows the original data (measurements every 20 minutes) and averaged measurements per day. And Figure 1b displays logarithm of data on PM2.5 concentrations and their averages per day. To simplify the text, below it will be called the measurements obtained directly from the post as "original data"; averaged original data for a day as "daily original data"; and logarithmic original measurements (and their averaging) as "logarithmic data" ("daily logarithmic data"). Briefly describe the data and the problems associated with them.

To check the studied data for normality, the Kolmogorov-Smironov, Shapiro-Wilk, Jarque-Bera, Anderson-Darling, and D'Agostino-Pearson tests were performed on each sample. Here it is not proposed the description and comparison of the used tests with each other; it is only noted that there are many works on their comparison on various synthetic data (see, for example, the works [15, 16, 17, 18, 19]. Note that the mentioned studies don't contain an unambiguous conclusion on the optimality of one of the selected methods when used to study the normality of a sample, when the distribution of sample elements is not known for certain. When applied to the data studied in this work, all tests performed indicate the need to reject the null hypothesis of normal distributions, except for "daily logarithmic data". For the mentioned time series, all tests, except the Kolmogorov-Smirnov test, indicate a high probability of accepting the null hypothesis about the



a) b)

Рис. 1. a) "original data" (gray line), "daily original data" (black dots); b) "logarithmic data" (gray line) and "daily logarithmic data" (black dots)

normality of the sample distribution. The obtained result can be explained by the fact that the Kolmogorov-Smirnov test doesn't work well on large samples with a weakly skewed distribution. Note that visual analysis of histograms of distributions of the studied data confirms the test results. Consideration of logarithmic data separately, as is already clear, is due to the log-normality of the original data.

The main problem with this type of data is the physicality of outliers that cannot be excluded from the sample. An increase in PM2.5 concentration can develop both in short periods, associated, for example, with street traffic during rush hours, and in long-term excesses (several days, several hundred measurements), associated with emissions from manufacturing companies and lack of wind. And all the specified templates are embedded in the data. The second problem is related to numerous data gaps due to hardware failure. There can be up to a dozen such gaps per year (several hundred measurements). And for the correct use of data in the future, these missing data must be restored.

The primary assumption about the series depicted in Figure 1 is that the "original data" (and "daily original data") are most likely not stationary, since trend change points which don't fit within the standard deviation are visible. A visual analysis of the logarithmic series shows that it may turn out to be stationary, which will allow to use almost any model to predict it. One of the goals of the work is to test this thesis in different ways and identify associated difficulties.

3 The "stationarity" concept

A time series is called stationary if its main statistical characteristics do not depend on time. In mathematical statistics, there are two types of stationarity: strong and weak one. They are defined as follows [20]: a random process $X_t = \{x_t\}$ with $t \in \{t_1, t_2, ..., t_N\}$ is said to be strongly stationary if for any set of times $t_1, t_2, ..., t_n$ and any integer k joint probability distributions $x_{t_1}, x_{t_2}, ..., x_{t_n}$ and $x_{t_1+k}, x_{t_2+k}, ..., x_{t_n+k}$ are the same. In the language of dynamical systems, this means that in every conceivable embedding space, the statistical properties of the phase flows relating to different parts of the time series are the same. A less stringent requirement is weak stationarity, in which the theoretical expectation and variance of the time series do not depend on time. In what follows, by "stationarity" of a time series, as in most cases described in the literature, we will understand weak stationarity.

Regarding non-stationary time sequences in the analysis of time series, it is customary to distinguish between TS-series (trend stationary), which are stationary or stationary with respect to a deterministic trend, and DS-series (difference stationary), which are not related to TS series and are reduced to stationary only as a result of their single or multiple differentiation. The fundamental difference between these two classes of series is that in the case of a TS series, subtracting the corresponding deterministic trend from the series leads to a stationary series, whereas in the case of a DS series, subtracting the deterministic component of the series leaves the series non-stationary due to the presence of a stochastic trend.

3.1. Review of methods for primary testing of time series. Mostly, methods for checking time series for stationarity can be divided into three groups:

- graphic;
- statistical tests;
- procedures for estimating the statistical characteristics of a series.

3.1.1. Graphic methods. As methods of *graphical analysis*, it can be distinguished both the simplest ones as analysis of the graph of a time series and the graph of moving statistics; and the analysis of (partial) autocorrelation functions. It is clear that the first two "naive" methods are practically not applicable to real data series, since for them it is not clearly determined whether there is noise in the data or a trend change has occurred (as for example for the series shown in Figure 1).

Autocorrelation Function Analysis

The more mathematically correct graphical method is analysis of time series correlograms. The degree of closeness of linear relationship between sequences of observations $\bar{X}_t = \{x_{t_1}, x_{t_2}, ..., x_{t_n}\}$ and $\bar{X}_{t+k} = \{x_{t_1+k}, x_{t_2+k}, ..., x_{t_n+k}\}$ of a stationary series (with lag k) can be determined using the correlation coefficient

$$\rho(k) = \frac{E[(\bar{X}_t - a)(\bar{X}_{t+k} - a)]}{\sigma^2}, \tag{1}$$

where $E[X_t] = E[\bar{X}_t] = E[\bar{X}_{t+k}] = a$ is the expectation of the time series X_t, σ is the standard deviation of the series X_t, $\bar{X}_t$, $\bar{X}_{t+k}$. Since the coefficient $\rho(k)$ measures the correlation between members of the same series, it is called the autocorrelation coefficient, and the dependence of $\rho(k)$ on the lag value k is called the autocorrelation function (ACF). In time series analysis, the autocorrelation function shows the degree of linear statistical relationship between the values of a time series. If any long-term external factors act on a series, this leads to the appearance of trends (tendencies) and a cyclical component in the series, which the ACF allows to detect. Based on the appearance of the correlogram, one can, for example, draw the following conclusions. If the expressed maximum of the correlogram turns out to be for lag $l = k$, then the time series contains a cyclic component with period k. If the correlogram has a maximum at $l = 1$, then the series contains only a linear trend. If the correlogram does not have pronounced maxima, then the series does not contain a trend or a cyclic component, and the random component dominates in it. This may also indicate that the series contains a strong nonlinear trend that cannot be expressed by a linear correlation coefficient. Also, if the correlogram represents small changes around zero, then the series is random.

Also, together with the autocorrelation function, the autocorrelation function (PACF) is considered. For a time series X_t, partial autocorrelation with lag k is the autocorrelation between X_t and X_{t+k} obtained after removing the influence of any correlation with shorter lags $1, 2, ..., k-1$. Note that the autocorrelation of observation x_i and the observation at the previous time step x_{i-1} includes direct correlation and indirect correlation. These indirect correlations are correlations of observations of linear functions. The partial autocorrelation function attempts to remove these indirect correlations. Partial autocorrelation of time series is used to find periodicities in time series and find the order of the autoregressive model of the series. Partial autocorrelation with lag k can be found according to the Durbin-Levinson algorithm [21]

$$\phi(k,k) = \frac{\rho(k) - \sum_{i=1}^{k-1} \phi(k-1,i)\rho(k-i)}{1 - \sum_{i=1}^{k-1} \phi(k-1,i)\rho(i)}, \tag{2}$$

where $\phi(k,i) = \phi(k,i) = \phi(k-1,i) - \phi(k,k)\phi(k-1,k-i)$ $1 \le i \le k-1$ and $\rho(k)$ is the value of the autocorrelation function with lag k.

It should be noted that ACF and PACF analysis is most often used in time series forecasting using ARIMA model, where the lag at which the regression coefficients become insignificant determines the order of the model, see, for example, the results of modeling in Hydrological Processes [22]. But it is necessary to understand that such an analysis is based on the assumption of linear autocorrelation of the series terms, and in other cases, it may be clocked incorrectly.

3.1.2. Statistical Tests. Note that the main method of checking a time series for stationarity remains statistical tests. The tests are based on the assumption that the modeled process is represented as an autoregressive process, for which the characteristic equation can be easily written (for details, see [23]). If a given characteristic equation has a unit root, then this indicates a strong correlation between neighboring terms of the series, that is, nonstationarity. There are several unit root tests and most of them have common implementations in Python, R and other statistical packages.Let's highlight some of them. *Augmented Dickey-Fuller* test checks the stationarity around a trend under the assumption that time series is presented as p-order autocorrelation process [24]. The modern implementation of *Phillip-Perron test (PP)* [25] makes the same under the assumption that the residuals cannot be distributed normally. In the *KPSS test*, the time series under study is written as the sum of a trend, a random walk process [26]. There are also tests that evaluate a series for stationarity under the assumption that it has one or more break points (trend changes). These include the *Zivot-Andrews test (ZA)* (for a single structural break point, see in [27]) and the *CUSUM test* (for multiple ones, see original works [28] and its improvements [29]). Note, that CUSUM (CUmulative SUM) is, first of all, a procedure for searching for points of characteristic change. The original procedure, proposed in 1975 [30], was focused on checking whether changes occur in the statistical mean of the series. The first work that took into account the joint change in the mean and variance of a series (that is, dividing the series into stationary subsequences) was [31]. Now, there are many modifications (see [32, 33, 34] and other) of the method, including for series with a long memory [35]; real-time detection [36] and with the combination with other methods [37]. Today, CUSUM is able to detect transitions between a stationary and non-stationary segment, but it cannot guarantee the accuracy of this identification.

The popularity of the designated tests in the Google Scholar system for the partial year 2024 is distributed as follows: almost 5000 works using the Dickey-Fuller test, just over 3000 works mentioning the CUSUM test, about 2000, 1500 and 300 for the PP, KPSS and ZA tests respectively. At the same time, in most cases, works related to the CUSUM test are research related to the study of the procedure and its modifications. The remaining tests have been developed and researched for more than 20 years and works related to them mention them as a tool used in making predictions in real-world areas. Thus, when solving real problems, the Dickey-Fuller test remains the most used, and its usefully is confirmed by works comparing classical tests with each other, where the ADF test shows good results [38]. Here, the ZA and CUZUM methods will not be used to analyze the data under study, since it was previously assumed that the data does not have structural changes. Describe the remain tests in more detail and show what their difference is.

Augmented Dickey-Fuller (ADF) Test

In statistics, ADF procedure [24] tests the null hypothesis that a sample of time series has an unit root. The alternative hypothesis differs depending on which version of the test is used, but it is usually stationarity or stationarity of trend. In fact, the null hypothesis of the Dickey-Fuller test is that the series belongs to the DS class, and the alternative – to the TS class. The process of constructing the extended Dickey–Fuller test begins by considering an autoregressive process of order p:

$$\Delta x_t = f(t) + \alpha x_{t-1} + \theta_1 \Delta x_{t-2} + ...\theta_p \Delta x_{t-p} + \varepsilon_t, \quad (3)$$

where $f(t)$ is the expected trend (usually, constant or linear); p is the number of lags; ε_t are random variables having a normal distribution with zero mean; and $\Delta x_{t-i} = x_{t_i} - x_{t-i-1}, \ \forall i = 0, ..., p$. The equation (3) is estimated using the least squares method, after which the statistical significance of the coefficient α is checked. The null hypothesis $H_0 : \ \alpha = 0$ corresponds to the situation of a non-stationary time series. Alternative hypothesis H_1: the coefficient α is significant and negative. Calculated statistics

$$\tau = \frac{\bar{b}}{SE_{\bar{b}}} \quad (4)$$

has a distribution provided by the Dickey-Fuller table (see [39]). A formalized procedure for using the Dickey–Fuller criteria with a sequential check of the possibility of reducing a statistical model is given in the work [40]. As mentioned above, the Dickey-Fuller test is most often used by researchers.

Phillips-Perron (PP) test

This criterion, proposed by [25], reduces testing the hypothesis that the series X_t belongs to stationary (DS class) to testing the hypothesis $H_0 : \alpha = 0$ within the framework of a statistical model

$$\Delta x_t = f(t) + \alpha x_{t-1} + \varepsilon_t, \quad (5)$$

where, as in the Dickey–Fuller criterion, $f(t)$ can be taken equal to zero. However, in contrast to the Dickey–Fuller criterion, random components ε_t with zero mathematical expectations can be autocorrelated (with a fairly rapid decrease in the autocorrelation function), have different variances (heteroscedasticity) and are not necessarily selected from the normal distribution. Thus, in contrast to the criterion Dickey–Fuller, a wider class of time series is allowed for consideration. A more detailed description of the Phillips-Perron test is presented in [41].

Kwiatkowski–Phillips–Schmidt–Sheen (KPSS) test

The main difference between the KPSS test [26] and those discussed above is the permutation of hypotheses. In the KPSS test, the null hypothesis states that the time series is stationary, against the alternative that there is non-stationarity (belonging to the DS class). It is also necessary to note significant methodological differences. The KPSS test approach assumes that the time series X_t tested for stationarity with respect to trend can be decomposed into the sum of deterministic trend βt, random walk r_t and stationary error ε_t:

$$x_t = \beta t + r_t + \varepsilon_t, \ r_t = r_{t-1} + u_t, \quad (6)$$

where u_t is a normally distributed process with zero mean and variance σ^2 ($u_t \sim N(0, \sigma^2)$).

From the equation above, it follows that the null hypothesis H_0 that X_t is stationary is equivalent to the hypothesis $\sigma^2 = 0$, which implies that

$r_t = r_0$ for all t (r_0 is a constant). Similarly, the alternative hypothesis H_1 about nonstationarity is equivalent to the hypothesis $\sigma^2 \neq 0$. To test the hypothesis H_0 against the alternative H_1 the authors of the KPSS test obtained one-sided Lagrange multiplier test statistics [42]. They also calculate its asymptotic distribution and model the asymptotic critical values.

3.2. Procedures for estimating the statistical characteristics of a series. The last group of methods is based on determining stationarity and direct assessment of the statistical characteristics of the series. This may include *Cochrane procedure (variance ratio test)* [41, 43], which tests the random walk hypothesis against stationary alternatives, by exploiting the fact that the variance of random walk increments is linear in all sampling intervals. For real data, the representation of variance ratio is performed:

$$VR_k = \frac{V_k}{V_1}, \text{ where } V_k = \frac{N}{N-k+1}\frac{1}{k}D\left(X_t - X_{t-k}\right). \quad (7)$$

Here $D(X_t)$ is the sample variance of X_t time series and N is number of series X_t elements. If X_t is random walk, then $VR_k = 1,\ \forall k$ and if X_t is stationary process over constant or linear trend, then $VR_k \to 0$ for $k \to \infty$.

Some of the other methods for testing time series for (non)stationarity involve its spectral decomposition. These methods have been developed since the seventies of the last century and new ideas and modifications are still being proposed. Pioneering work in this area [44] proposed a method for comparing a set of evolutionary spectra of a series assessed at different points in time. This approach was further developed, for example, in the works of [45, 46]. Methods for comparatively time-varying spectral density estimation with its stationary approximation are also being developed [47]; and approaches based on Fourier transform and wavelets [48, 49, 50, 51].

Methods for assessing the stationarity of time series based on frequency analysis and spectrum analysis are now being widely developed and make it possible to isolate changes in the series through periodicity analysis. Such methods work best if it is known that the analyzed time series remains invariant for a sufficiently long number of measurements [23].

4 Discussion of problems associated with applying some well-known methods to real data

Using the example of the data presented in Section 2, it will be shown that using a single tool to understand the behavior of a system can lead to serious errors. In the table 1 $p-$values of stationarity tests performed on the studied data are presented (probability of a type I error). Values that indicate nonstationarity of the selected series are highlighted in bold. As can be seen from the table, the set of tests does not allow us to draw an unambiguous conclusion about the part of the data that is most interesting for research. This is original data from field measurements of PM2.5 concentrations and their logarithmic representation.

Таблица 1. Probability of rejecting the correct null hypothesis for statistical ADF, PP, KPSS tests in comparison with a significance level equaled 0.05

time series	tests taking into account possible constant or linear trends					
	ADF (const)	ADF (linear)	PP (const)	PP (linear)	KPSS (const)	KPSS (linear)
original data	0.00	0.00	0.00	0.00	**0.025**	**0.000**
daily original data	0.00	0.00	0.00	0.00	0.434	0.086
logariphmic data	0.00	0.00	0.00	0.00	**0.039**	**0.000**
daily logariphmic data	0.00	0.00	0.00	0.00	0.556	0.140

Note that, it would seem, the most popular tests for stationarity (ADF and PP) counted the series as stationary; but really they only indicate that the series does not have *one* unit root. At the same time, the KPSS test regarding daily data also indicates that it is impossible to confidently draw a conclusion about their stationarity. Thus, in this case, statistical testing is not a comprehensive tool in analyzing the stationarity of time series.

Now turn to the analysis of autocorrelation functions. Figure 3 shows correlograms (ACF) of the data used for analysis. Here, the x axis is the lag

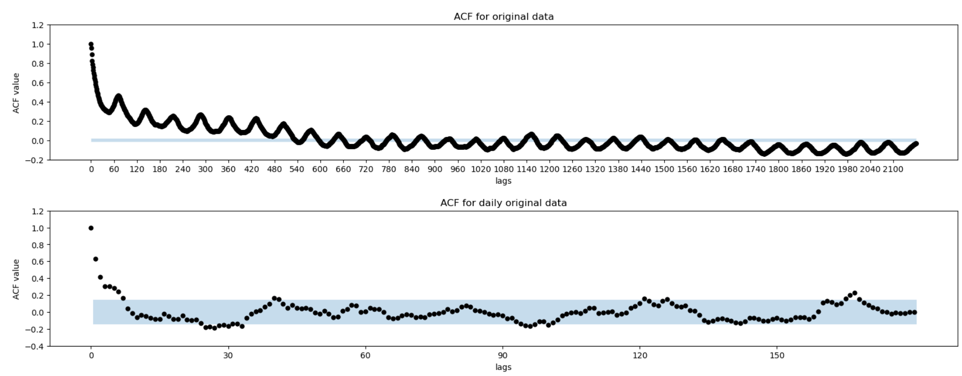


Рис. 2. ACF graphics for "original data" (top) and "daily original data" (bottom)

value k, and the y axis is the value of the correlation coefficient, calculated using the formula (1). The area highlighted in blue indicates that the coefficients falling within this area are not significant with a probability of 95%. Thus, the corelogram of the original data shows their obvious non-stationarity and complex seasonality. Note that the period over which the oscillations occur is approximately about 70 measurements, that is, about a day in the format of the available data. This is confirmed by the fact that the use of daily averaging makes it possible to eliminate such frequent fluctuations. The ACF of "daily original data" decreases rapidly, which may indicate both stationarity and the presence of a nonlinear trend, since the first few ACF values are significant, while the decrease in ACF also occurs non-linearity. Note that the figure does not show corelograms of the "logarithmic data", since they do not differ from the corresponding graph for the "original data".

Figure 3 shows the PACF for the data set under study. Analysis of partial

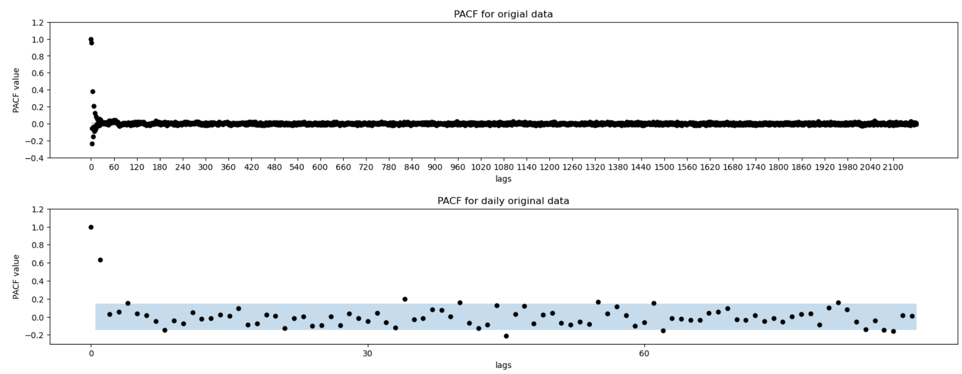
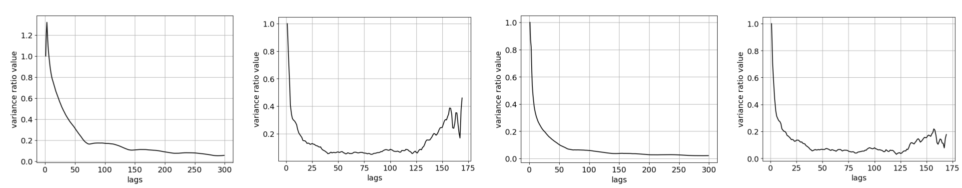


Рис. 3. PACF graphics for "original data" (top) and "daily original data" (bottom)

autocorrelation functions generally confirms the conclusions drawn from the ACF analysis.

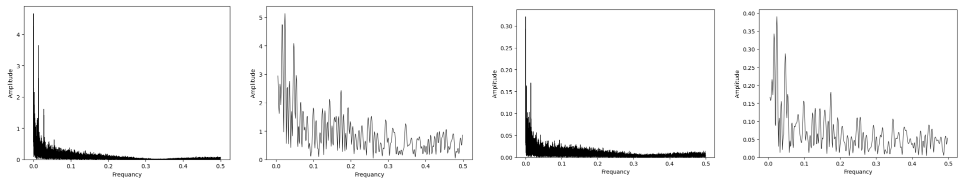
Figure 4 shows the values of VR_k as a function of lag k for the Cochrane procedure described in section 3.2. Figure 5 shows the periodograms of the analyzed data.



a) b) c) d)

Рис. 4. Variance ratio VR_k values depending on lag k for a) "original data", b)"daily original data"; c) "logarithmic data" and d)"daily logarithmic data"

Note an interesting feature. The ratio of variances for the "original data" and the "logarithmic original data" behaves like white noise or the sum of white noise and linear trend, which is no different from the procedure under consideration. At the same time, their daily averaging, on the contrary, shows the non-stationarity of the process to a greater (for "daily original data") and lesser (for "daily logarithmic data") degree. Most likely, this behavior is due to the measurement characteristics of the sensors from which the data is collected. Thus, optical sensors at low concentrations of PM2.5 can make



a) b) c) d)

Рис. 5. Periodograms for a) "original data", b)"daily original data"; c) "logarithmic data" and d)"daily logarithmic data"

significant errors (see [10]). Daily smoothing solves this problem and then the method can capture the non-stationary nature of the process itself.

Periodogram analysis is one of the representatives of the methods of spectral analysis of a series. A periodogram is a function of frequency that shows an assessment of the spectral density of a time series. High amplitudes in the low frequency region indicate the presence of red (i.e., correlated) noise in the data, which indirectly confirms the hypothesis of erroneous sensor measurements at low pollutant concentrations. More details about the analysis of periodograms and the spectrum of time series can be found in the work [52].

5 Procedure for analyzing the mean and variance of time series

5.1. Procedure description. Thus, there are no simple and accurate algorithms for classifying time series as stationary. Available visual analysis is limited by sample size and researcher choice and is not mathematically rigorous. Statistical tests do not respond well to complex series. At the same time, the concept of weak stationarity of a series is a very simple asymptotic concept to understand. In the current section, it is proposed a simple procedure for visually assessing the behavior of the main statistical characteristics of a series, based on sample duplication.

The idea of the proposed method is quite simple and is based on the fact that if a series is stationary and has a constant mean and variance, then the distribution of the specified statistical indicators of subsequences of any! sizes have a symmetrical distribution. The procedure is as follows:

1. Choose the subsecuenses of constants $\Omega = \{\omega_1, \omega_2, ..., \omega_M\}$ such that $\max \Omega \leq N/2$;

2. $\forall \omega_i$ get the set subsecuenses of time series of length ω_i:$\{x_{k\omega_i}, ..., x_{k\omega_i+\omega_i}\}$ $k = 0, ..., [N/\omega_i] - 1$;

3. Generate samples $Means = \{\bar{X}_{ik}\}$, $Stds = \{\sqrt{\sigma(X_{ik})}\}$, where $\bar{X}_{ik}$ is sample mean for subsecuense $\{x_{k\omega_i}, ..., x_{k\omega_i+\omega_i}\}$, and $\sigma(X_{ik})$ is sample variance for the same subsecuense;

4. Then shuffle samples $Means$ and $Vars$ and divide them into two samples $Means_1$, $Means_2$ and $Stds_1$, $Stds_2$ of similar sizes (or not differing by more than one);

5. Build scatterplots for $Means_1$, $Means_2$, $Stds_1$, $Stds_2$ and histograms for $Means$ and $Stds$ and draw conclusions about the time series in comparison with the reference behavior of white noise.

Now demonstrate how the procedure works on synthetically generated data.

5.2. Result of procedure application on the synthetic data. First, generate a time series that is white noise. Put

$$X_t = \varepsilon, \tag{8}$$

where $\varepsilon \sim N(0,1)$ is a normally distributed quantity with zero mean and unit standard deviation. Figure 6 shows the result of the algorithm for the time series represented by (8) (the data were previously normalized on the $[0,1]$ scale). Here and further in the figures, instead of dispersion, for convenience, the standard deviation will be displayed.

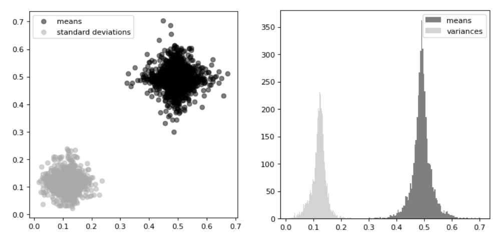


Рис. 6. Result of procedure application on white noise data represented by (8)

Now consider a time series represented by an additive model: the sum of white noise and trend.

$$X_t = at + \varepsilon, \tag{9}$$

$$X_t = at^2 + \varepsilon, \tag{10}$$

$$X_t = \exp(t^2) + \varepsilon. \tag{11}$$

Figure 7 shows the result of the proposed algorithm for the time series represented by (9)–(11) i.e. data with trends. As can be seen from the figure 7, the presence of a trend significantly changes the average values obtained using the procedure, while the standard deviation determined by white noise obviously does not change its behavior. The presence of seasonal (periodic) changes, such as, for example, for a series given by the following dependence

$$X_t = 2\sin(\pi t) + \varepsilon, \tag{12}$$

changes the scatterplot and histogram as it is shown in figure 8. As a final example, consider heteroscedastic data, i.e. heterogeneous observations, expressed in the variable variance of the random error of the regression

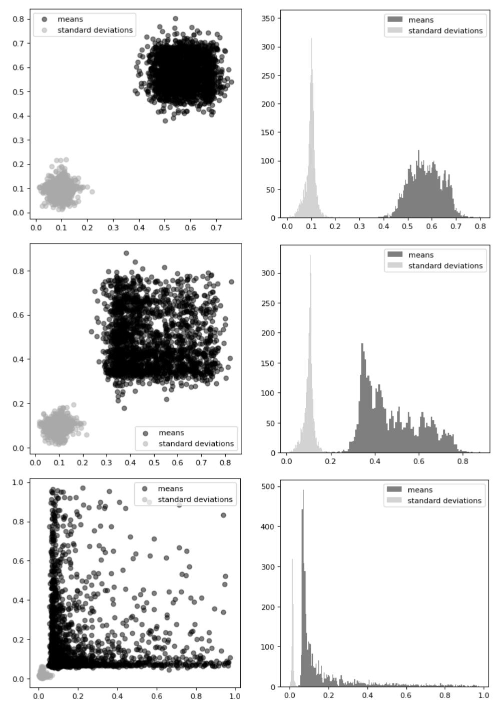


Рис. 7. Result of procedure application on white noise with trend data presented by equations (9) (first line),(10) (second line),(11) (third line)

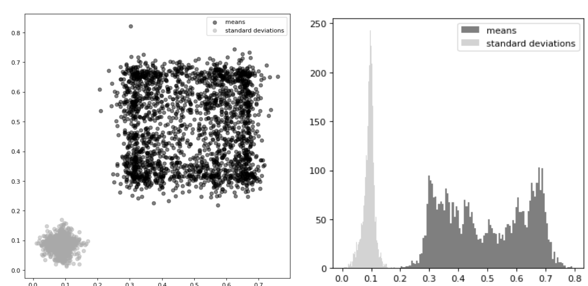


Рис. 8. Result of procedure application on white noise and seasonality data presented by (12)

model. The results of the procedure for such data are presented in Figure 9. Such data can be determined according to the law (8), where ε is a random variable distributed according to the normal law $N(0, \sigma(t))$, where $\sigma(t) = t + \theta$, θ is a uniformly distributed random variable. As can be seen from the results obtained, here the non-stationarity of the series is observed precisely in the dispersion, while the distribution of means remains symmetric.

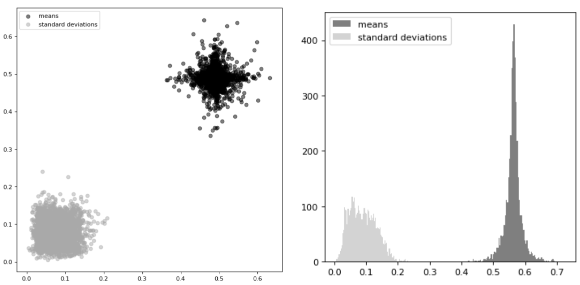


Рис. 9. Result of procedure application on heteroscedastic data

Thus, the proposed procedure allows to draw some conclusions about the behavior of the time series through the analysis of scatterplots and histograms of means and variances.

5.3. Result of procedure application on the studied data. Now the proposed procedure will be applied to the studied data on PM2.5 concentration (Figure 10). The data was previously normalized within $[0; 1]$. From the

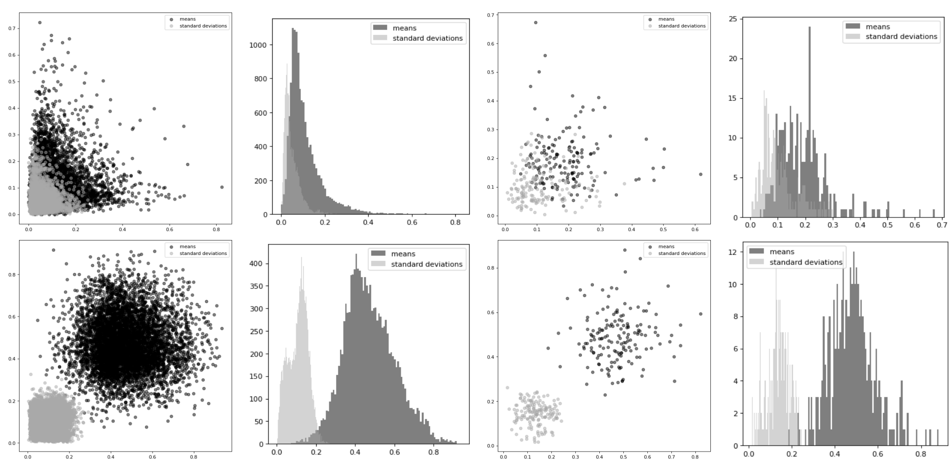


Рис. 10. Result of procedure application on studied data. From up to bottom: First line: results for "original data" and "daily original data". Second line: results for "logarithmic data" and "daily logarithmic data"

analysis of the obtained results, the following conclusion can be drawn. Histograms of means and standard deviations for the "original data" are asymmetric and have a long tail to the right. This indicates the obvious non-stationarity of the source data. At the same time, the trend present in the data is not expressed polynomially, which indicates the multiple presence of imbalances in the time series. The same can be said about the "daily original data". Note that the "logarithmic data" are stationary with respect to the mean, but the histogram of the distribution of the standard deviation is bimodal, which indicates the presence of a disorder in the dispersion of the time series. For "daily logarithmic data", the distributions of means and standard deviations are symmetrical and, taken together with the results from other methods, this series can be considered stationary.

6 Conclusions and discussion

The paper is devoted primarily to a review of methods that can be used to assess the stationarity of a time series. It is shown that there is no single criterion suitable for complex series of real data, and even such a primary analysis procedure can cause difficulties. Here attention was drown to the correctness of using the most popular tools in solving such problems. It was shown that for time series of real measurements, different statistical tests, which are most used in practice, due to the peculiarities of constructing hypotheses, can give different results. Another equally frequently used tool, ACF and PACF analysis, shows good results for autocorrelated series that do not exhibit heteroscedasticity. And spectral analysis methods give the best results only if the series remains invariant for a sufficiently long time.

At the same time, stationarity has a fairly simple criterion in its definition – constancy of the mean and variance over time. There are also tests based on this definition, such as the Cochrane procedure. But this method does not allow detecting and distinguishing poorly defined trends and trends more complex than linear. Here we propose a procedure for testing a series for stationarity, based on the analysis of scatterplots and histograms of the distribution of means and standard deviations of individual subsequences of a time series. Synthetic data shows the operation of the procedure. Thus, the presence of a trend in the data violates the symmetry of the distribution for a sample of means values; seasonality leads to multimodality. And the heteroscedasticity of the source data violates the variance histogram. The proposed procedure was applied to measurement data of PM2.5 concentrations in Krasnoyarsk, that allows to supplement knowledge about the data being studied.

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