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Ghasser-Mobarakeh, Forouzan; Voosoghi, Behzad; Amiri-Simkooei, Alireza

DOI
10.1007/s11600-025-01577-7

Publication date
2025

Document Version
Final published version

Published in
Acta Geophysica

Acta Geophysica
https://doi.org/10.1007/s11600-025-01577-7

RESEARCH ARTICLE - SOLID EARTH SCIENCES

Stochastic model identification of GNSS time series using multivariate NNLS-VCE

Forouzan Ghasser-Mobarakeh[1] · Behzad Voosoghi[1] · Alireza Amiri-Simkooei[2]

Received: 17 May 2024 / Accepted: 16 March 2025

Abstract

Identifying the correct stochastic model in GNSS time series is essential to study geophysical parameters such as site velocities, and hence enhancing their accuracy. The rate uncertainty is a critical aspect in GNSS time series analysis. The variance component estimation (VCE) methods commonly utilize unconstrained estimation principles. Simulating 1000-time series for 4 different noise combinations with 10 years' time span, we have investigated the performance of non-negative least squares VCE (NNLS-VCE) method for identifying an appropriate noise model. Our results are provided for both univariate and multivariate analysis. As the noise model's complexity increases, the significance of employing multivariate analysis is prominent in contrast to univariate analysis. After thorough analysis, we have determined that treating the false-positive model as a stochastic model in time series yields significant insights. Specifically, if the accumulative spectral index is lower than the true value, it results in an underestimation of the rate uncertainty. Conversely, if the index is higher than the actual value, it leads to an overestimation. Additionally, we observed that as the noise model complexity increases, the number of false-positive models also increases. However, the implementation of multivariate analysis mitigates this increase, offering a more realistic and reliable approach. In case of four distinct noise models, the detection power percentages of 98.5%, 90.5%, 69.5%, 29.3% of univariate analysis increased to 99.5%, 99.8%, 88.4% and 83.7% for multivariate analysis.

Keywords NNLS-VCE · Rate uncertainty · Model identification · Multivariate analysis

Introduction

Over the last three decades, global navigation satellite system (GNSS) has provided a tremendous opportunity for researchers working on the geodynamics and geophysics fields through the analysis of daily GNSS position time series (Wang et al. 2021; Broerse et al. 2023; Roberts et al. 2020). Many researchers have implemented GNSS observations to study geophysical phenomena including Earth's surface motion due to the plate tectonics (Chousianitis et al 2021; Chen et al 2020), pre-, co- and post-seismic deformations (Montillet et al. 2015), tectonic strain and glacial isostatic balancing (Stefen and Wu 2011), volcanic deformations (Cervelli et al. 2006) and vertical land motion to study the sea level changes (Bos et al. 2013).

Appropriate analysis of GNSS time series plays a crucial role in investigating the key parameters associated with geophysical phenomena. This involves the identification of both functional and stochastic models. The former helps discern deterministic signals like trends, offsets, and seasonality, while the latter focuses on understanding the noise characteristics of GNSS time series. There is ongoing research showing the presence of time-dependent noise structure in geodetic time series in general and in GNSS position time series in particular (Williams et al. 2003; Amiri-Simkooei et al. 2007). It is therefore crucial to determine the realistic noise of model of GNSS time series (Gobron et al. 2021;

Edited by Prof. Maria Marsella (ASSOCIATE EDITOR) / Prof. Ramón Zúñiga (CO-EDITOR-IN-CHIEF).

✉ Behzad Voosoghi
vosoghi@kntu.ac.ir

Forouzan Ghasser-Mobarakeh
ghasserforouzan@gmail.com

Alireza Amiri-Simkooei
ar.amirisimkooei@gmail.com

[1] Faculty of Geodesy and Geomatics Engineering, K N Toosi University of Technology, Tehran, Iran

[2] Department of Control and Operations, Faculty of Aerospace Engineering, Delft University of Technology, Delft, 2629 HS, Netherlands

Published online: 30 April 2025

Santamaría-Gómez and Ray 2021), aiming to improve the estimation of uncertainty for the desired parameters, such as site velocities (Benoist et al. 2020).

Various researchers have identified different noise models for the aforementioned time series. For example, at medium frequencies, the noise model is often expressed as flicker noise, while at high frequencies, it is commonly described as white noise (Williams et al. 2008). Therefore, the composite characteristic can be effectively captured by the linear combination of white noise and flicker noise, denoted as "$W+F$". There are two main alternatives to the usual "$W+F$" model, each modeling power gain or stabilization at low frequencies (He et al 2019, 2021; Santamaría-Gómez and Ray 2021). The first alternative is labeled "$W+F+R$", which aims to account for the presence of random walk noise in GNSS time series, caused by small movements of the antenna due to the instability of station building (Tehranchi, et al. 2021). The second alternative considers only the combination of white and power-law noise like before comment insert references, denoted as "$W+P$". Both the "$W+F$" and "$W+P$" models describe most of the stochastic properties of geodetic time series. Ongoing research has also identified the presence of fractal power-law noise in GNSS time series analysis, which is referred to as power-law (P) noise model in this contribution (He et al. 2019). There are also other noise components in GNSS time series like Generalized Gauss–Markov (GGM) noise model introduced by Langbein (2004), which is outside the scope of the present contribution. This contribution will thus consider combinations of four variants of power-law noise models resulting in "$W+P+F+R$".

In GNSS time series analysis, the accurate identification of the noise model is important. Various methods have been employed for this purpose. One commonly used approach is the log-likelihood (LLL) criterion, where different stochastic models are estimated and compared to determine the most suitable one. Alternative criteria such as Akaike information criterion (AIC) and Schwarz's Bayesian information criterion (BIC) utilize penalty terms to account for additional parameters and to avoid overfitting in stochastic models. Smaller AIC/BIC values indicate superior stochastic model performance. The above criteria require a few noise components ("W", "P", "F", and/or "R") be estimated using variance component estimation (VCE) methods. In GNSS time series, two commonly used methods are the maximum likelihood estimation (MLE) and least squares variance component estimation (LS-VCE).

The VCE methods typically rely on unconstrained estimation principles, which can lead to the possibility of estimating negative variance components. Negative estimates of VCs result in (co)variance matrices that are not positive definite, lacking physical justification. This occurrence may be attributed to factors such as insufficient degrees of freedom in the functional model, inappropriate initial values for variance components, or inadequate stochastic modeling (Amiri-Simkooei 2007). Additionally, there can be other causes for negative variance component estimates. In GNSS time series analysis, negative variance component estimates can also arise from factors such as an over parametrized stochastic model, particularly when there is a large number of noise components included (Amiri-Simkooei 2016). The over-parameterization can lead to high correlations and less precision among estimates of different noise components, thereby increasing the likelihood of negative variance estimates. This study focuses on the utilization of non-negative LS-VCE (NNLS-VCE), developed by Amiri-Simkooei (2016), as an important tool for estimating non-negative variance components. The goal of incorporating NNLS-VCE in this research is to facilitate stochastic model identification.

The current research aims to achieve four interrelated objectives. 1) We examine the performance of the non-negative LS-VCE (NNLS-VCE) method, for identifying an appropriate stochastic model. All noise components ("$W+P+F+R$") are introduced as potential noise model, and the algorithm allows them to be estimated within a non-negative framework. If a noise component is unlikely to be present, its corresponding variance is expected to become zero. 2) We aim to investigate how the type and number of noise components, along with the length of the time series, can impact the true-positive (TP) results. This analysis identifies the factors that influence the performance of identifying true noise components. 3) We examine how the false positives (FP) can potentially lead to under- or overestimation of rate uncertainties. This is particularly of interest because it allows to investigate the effect of incorrectly identified stochastic models on rate uncertainties. 4) We explore the role of multivariate analysis in stochastic model identification. This investigation will provide insights into the impact of considering three coordinate components simultaneously on the effectiveness of the stochastic model identification.

This contribution is organized as follows. In Sect. "Functional and stochastic models of GNSS time series" the functional and stochastic models in GNSS time series are described. It is hereby shown how the cofactor matrices of different stochastic processes are formed. Sect. "Remarks on stochastic model identification" reviews previous works in stochastic model identification. Also, the NNLS-VCE method as a tool to facilitate the model identification procedure is introduced in univariate and multivariate analysis. In Sect. "Applications, results and discussion", the simulated dataset is described. We consider 4 case studies with different noise combination to evaluate the role of NNLS-VCE in detecting the existing noise structure in the simulated time series. Additionally, we assess the influence of using multivariate analysis in NNLS-VCE to identify stochastic model.

Functional and stochastic models of GNSS time series

GNSS position time series primarily consist of deterministic terms known as trajectory models and stochastic terms referred to as noise (Bevis and Brown 2014). The deterministic terms in time series analysis consist of various components that can be identified and modeled. These components include long-term variations, such as linear trends that show gradual changes over time. Additionally, offsets account for sudden shifts or changes in the time series. Seasonal variations represent patterns that repeat annually or semiannually. In addition to these deterministic terms, time series also incorporate noise models. These models account for random fluctuations or variability in the data. The noise component can have varying spectral indices, indicating the frequency characteristics of the fluctuations. In the following sections, we will delve into these two parts of time series analysis, discussing how deterministic terms and noise models are utilized in understanding and modeling time series data.

Functional model

The functional model, which is known as the trajectory model in the coordinate time series, describes the mathematical expectation E(.) of the $m \times 1$ observation vector y. In the linear observation equations, the functional model can be expressed as:

$$\mathrm{E}(y) = Ax, \tag{1}$$

where A represents the $m \times n$ design matrix and x is the unknown $n \times 1$ vector in the functional model. The design matrix A of functional model generally includes the linear trend, annual and semi-annual signals and offset. Hereafter, in order to study the stochastic model, the functional part is assumed to be given and identical for all-time series.

Stochastic model

The stochastic model describes the mathematical dispersion D(.) of the $m \times 1$ observation vector expressed as the covariance matrix Q_y. It is usually written as a linear combination of p stochastic processes with unknown amplitudes.

$$\mathrm{D}(y) = Q_y = \sum_{k=1}^{p} \sigma_k Q_k, \tag{2}$$

where Q_k is the cofactor matrix for the kth stochastic process and σ_k is the corresponding variance component. The cofactor matrices, functions of the spectral index, can be formed using the following power-law process:

$$Q_k = \Delta T^{\kappa/2} U^T U, \tag{3}$$

where $\Delta T = \frac{1}{365.25}$ year is the sampling rate of the daily time series, κ denotes the spectral index and U is an $m \times m$ transformation matrix defined as:

$$U = \begin{bmatrix} h_0 & 0 & \dots & 0 \\ h_1 & h_0 & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ h_{m-1} & \dots & h_1 & h_0 \end{bmatrix}, \tag{4}$$

where h_i is obtained using the following recurrence expression (Bos et al. 2020):

$$h_i = \left(\frac{\kappa}{2} + i - 1\right)\frac{h_{i-1}}{i}, \quad h_0 = 1, \tag{5}$$

and κ is the spectral index. In this contribution, we take $\kappa = 0$, $\kappa = 0.5$,$\kappa = 1$ and κ =2, respectively referring to white (W), fractal power-law (P), flicker (F) and random walk (R) noise. The covariance matrix is then:

$$Q_y = \sigma_w^2 I + \sigma_p^2 Q_p + \sigma_f^2 Q_f + \sigma_r^2 Q_r, \tag{6}$$

where I, Q_p, Q_f and Q_r are the given cofactor matrices of white noise (identity matrix), power-law noise, flicker noise and random walk noise, respectively, and σ_w^2, σ_p^2, σ_f^2 and σ_r^2 are their corresponding variance components to be estimated.

Remarks on stochastic model identification

Previous works

One of the primary goals of time series analysis is to create an optimal stochastic model. The optimal model takes into account all the inherent noises present in the observations and realistically models them. Despite the advances in utilizing statistical concepts and models across various fields of engineering and science, the challenge lies in developing an appropriate and optimal model when only limited information is available based on finite observations.

Various methods can be employed to determine the most accurate representation of noise model through noise model combination selection. Statistical tests, such as the w-test, can be utilized to evaluate the null hypothesis and its opposite hypothesis. Amiri-Simkooei et al. (2007) applied the w-test to identify the optimal noise model for observations from permanent GNSS stations. They determined the optimal noise model separately for three coordinate components. In practice, null hypotheses are often approximations that differ from reality. Consequently, selecting a model based purely on statistical tests of these assumptions can lead to a contradiction between the chosen model and the actual reality. Recognizing that statistical hypothesis tests alone are not accurate representations of real-world conditions, there has been a growth in the development of practical methods for model identification. Nowadays, the criteria based on MLE method is vastly applied to detect the existing noise in the GNSS time series including log-likelihood (LLL) criterion and some information criteria (IC). One can use the log-likelihood (LLL) criterion to estimate and compare different stochastic models to determine the most suitable one. For different noise combinations, one computes log-likelihood based on its corresponding Q_y matrix, estimated by MLE method, and the optimal noise model is the one for which LLL is maximized. This method has been used by Amiri-Simkooei (2016) to identify the best noise model. Langbein (2012) conducted research to examine the performance of the likelihood function with simulated data. Their findings indicate that the log-likelihood function, represented as LLL, incorrectly selects the $W+P$ noise model instead of the $W+F+R$ noise model in 50–70% of cases. This suggests that the LLL criterion lacks the capability to distinguish between these types of noise models. In the case where the spectral index is the same, the criterion described does not differentiate between flicker noise and power-law noise due to its inability to penalize the additional parameters in the noise model. Another disadvantage of the LLL criterion is its limited power to detect random walk noise.

Alternative criteria such as the Akaike Information Criterion (AIC) and Schwarz's Bayesian Information Criterion (BIC) are commonly used in stochastic models (Mazerolle 2020). They incorporate penalty terms to take into account the number of parameters in the model and aim to prevent overfitting. These criteria are valuable tools in statistical modeling as they help in selecting the most appropriate model by striking a balance between model complexity and goodness of fit. Smaller AIC/BIC values indicate better performance of a stochastic model. However, as ICs penalizes different combinations of noise with parallel noise parameters (e.g., "$W+P+R$" and "$W+F+R$" with 3 unknown components) equivalently, it may not effectively distinguish between these different noise models. He et al. (2019) used the BIC-TP criterion to distinguish between flicker noise, power-law noise and generalized Gauss–Markov (GGM) noise. BIC-TP demonstrates similar detection power to BIC when considering the mentioned noises. It has shown the capability to enhance the detection power of random walk by almost 50% (He et al. 2019).

Negative variance components

As already mentioned, to select the optimal stochastic model for several existing noise models, AIC/BIC or LLL criteria are calculated. These criteria require a few noise components ("W", "P", "F", and/or "R") to be estimated using variance component estimation (VCE) methods. The maximum likelihood estimation (MLE) method is the most commonly employed VCE technique in geodetic time series analysis. It is utilized in various statistical modeling software programs like CATS and Hector (Bos et al. 2013).

Assume that$\Phi = \ln\det(A) = \ln u$, where A represents the design matrix. The first-order derivative of $\Phi,\frac{d\Phi}{dx} = \frac{u\prime}{u}$, is defined as the change of Φ with respect to variable x:

$$\frac{d\Phi}{dx} = \frac{d\det A}{\det A} = \frac{\det A}{\det A}.tr\left(A^{-1}\frac{\mathrm{d}A}{dt}\right). \tag{7}$$

In the MLE method, the objective function is the quadratic form of residuals that result the derivative is calculated as follows:

$$\Phi = \hat{e}^T Q_y^{-1}\hat{e} \Rightarrow \frac{d\Phi}{dx} = -\hat{e}^T Q_y^{-1}\frac{\partial Q_y}{\partial x}Q_y^{-1}\hat{e}. \tag{8}$$

Now, the goal is to estimate unknown parameters by maximizing the maximum likelihood function. Therefore, the objective function is considered to be the argument that would maximize the likelihood function:

$$\Phi = \arg\max_{\sigma} \frac{-m}{2}\ln 2\pi - \frac{1}{2}\ln\det\left(Q_y\right) - \frac{1}{2}\hat{e}^T Q_y^{-1}\hat{e}. \tag{9}$$

Therefore, by deriving the objective function and setting it to zero, the following equation is obtained:

$$\frac{\partial\Phi}{\partial\sigma_k} = -\frac{1}{2}\,\mathrm{tr}\left(Q_y^{-1}Q_k\right) + \frac{1}{2}\hat{e}^T Q_y^{-1}Q_k Q_y^{-1}\hat{e} = 0, \tag{10}$$

and,

$$\frac{1}{2}\mathrm{tr}\left(Q_y^{-1}Q_k\right) = \frac{1}{2}\hat{e}^T Q_y^{-1}Q_k Q_y^{-1}\hat{e}. \tag{11}$$

As tr $(AA) = \mathrm{tr}(A)$,and Q_y can be written as the sum of covariance matrices, $Q_y = \sum_{i=1}^{P}\sigma_i Q_i$:

$$\frac{1}{2}\mathrm{tr}\left(Q_y^{-1}Q_k Q_y^{-1}Q_y\right) = \frac{1}{2}\mathrm{tr}\left(Q_y^{-1}Q_k Q_y^{-1}\sum_{i=1}^{P}\sigma_i Q_i\right) = \frac{1}{2}\hat{e}^T Q_y^{-1}Q_k Q_y^{-1}\hat{e}, \tag{12}$$

$$\frac{1}{2}\sum_{i=1}^{P}(Q_y^{-1}Q_k Q_y^{-1}Q_i)\sigma_i = l_k. \tag{13}$$

The observation equations for estimating variance components (σ) using the maximum likelihood estimation (MLE) method are structured as follows:

$$\sum_{i=1}^{P} N_{\mathrm{k}i}\sigma_i = l_k, \tag{14}$$

where N and l are:

$$l_k = \frac{1}{2}\hat{e}^T Q_y^{-1} Q_k Q_y^{-1} \hat{e}, \tag{15}$$

$$N_{\mathrm{ki}} = \frac{1}{2}\mathrm{tr}\left(Q_y^{-1} Q_k Q_y^{-1} Q_i\right). \tag{16}$$

Also, one can uses LS-VCE method to estimate variance components. In contrast to MLE, which gives biased estimators, LS-VCE provides unbiased and minimum variance estimators. Also, LS-VCE is much faster than MLE, implemented in the downhill simplex method (Amiri-Simkooei 2009). The above MLE formulation (Eqs. 14–16) can however have comparable complexity as LS-VCE and hence a replacement for downhill simplex method.

One limitation of variance component estimation (VCE) methods is the possibility of estimating negative values for variance components (VCs). Negative estimates of VCs lead to (co)variance matrices that are not positive definite, which is not acceptable from a statistical standpoint. Negative VCs can arise in a model due to various factors. These may include insufficient degrees of freedom in the functional model, inappropriate initial values assigned to the variance components, or inadequate stochastic modeling. It is important to address these issues to ensure accurate and meaningful. In addition, with an over-parameterized stochastic model, which includes many noise models, variance components tend to be estimated negative. To avoid negative variance occurrence, one can use non-negative LS-VCE in which the non-negativity of VCs is guaranteed. This also provides a useful tool for stochastic model identification in GNSS time series analysis.

Stochastic model identification using NNLS-VCE

Theory of NNLS-VCE

The least squares variance component estimation method (LS-VCE) is based on the principle of least squares. This method was proposed by Teunissen in 1988 and then developed by Amiri-Simkooei and Teunissen (2008). One drawback of LS-VCE is that the estimated variance components may become negative, which is not acceptable. Amiri-Simkooei (2016) presented the NNLS-VCE method to estimate non-negative variance components. This approach solves a convex minimization problem by imposing non-negativeness constraints. The Karush–Kuhn–Tucker (KKT) conditions are employed to ensure the non-negative variances. Since the objective function in this method is convex, it exhibits low computational complexity compared to general optimization techniques. We briefly review this theory.

To evaluate non-negative variance components in GNSS time series, one can add the inequality constraint $\sigma \geq 0$ to the objective function $\mathrm{F}(\sigma)$ (Amiri-Simkooei 2016).

$$\hat{\sigma} = \arg\min_{\sigma\geq 0} \mathrm{F}(\sigma) = \arg\min_{\sigma\geq 0}\left(\frac{1}{2}\sigma^T N \sigma - l^T\sigma\right), \tag{17}$$

where N and l are defined as follows:

$$n_{kl} = \frac{1}{2}\mathrm{tr}\left(Q_y^{-1} P_A^{\perp} Q_k Q_y^{-1} P_A^{\perp} Q_l\right), \tag{18}$$

and

$$l_k = \frac{1}{2}\hat{e}^T Q_y^{-1} Q_k Q_y^{-1} \hat{e}, \tag{19}$$

and $P_A^{\perp} = I - A(A^T Q_y^{-1} A)^{-1} A^T Q_y^{-1}$ is an orthogonal projector (Teunissen 2000).

NNLS-VCE in multivariate model

To implement the method in multivariate analysis, we consider the three east, north and up components of a station together, consequently having an $m \times 3$ observation matrix as $Y = [ENU]$. We will use multivariate analysis that leads to following observation equation:

$$\mathrm{vec}(Y) = \left(I_s \otimes A\right)\mathrm{vec}(X), \tag{20}$$

with the covariance matrix of:

$$\mathrm{D}(\mathrm{vec}(Y)) = \Sigma \otimes Q = \Sigma \otimes \left(\sigma_w^2 I + \sigma_p^2 Q_p + \sigma_f^2 Q_f + \sigma_r^2 Q_r\right), \tag{21}$$

where I_s is an identity matrix of size s and Σ represents the correlation of noise. For the properties of the vec-operator and the Kronecker product $\otimes$, we refer to Magnus (1988). For the multivariate linear model, we have (Amiri-Simkooei 2009):

$$n_{\mathrm{kl}} = \frac{s}{2}\,\mathrm{tr}\left(Q^{-1} P_A^{\perp} Q_k Q^{-1} P_A^{\perp} Q_l\right). \tag{22}$$

If Σ matrix is unknown, we have to execute a two-step procedure estimate the variance components. Firstly, we should estimate Σ and then applies the preceding formulation. This will then give the $l_k, k = 1, \ldots, s$ vector as:

$$l_k = \frac{m-n}{2}\mathrm{tr}\left(\hat{E}^T Q^{-1} Q_k Q^{-1} \hat{E}\left(\hat{E}^T Q^{-1} \hat{E}\right)^{-1}\right), \tag{23}$$

with

$$\hat{E} = P_A^{\perp} = \left[\hat{e}_1, \hat{e}_2, \cdots, \hat{e}_s\right], \tag{24}$$

where m-vectors $\hat{e}_i i = 1, \cdots, s$ are the least squares residual estimators for s time series.

The NNLS-VCE method offers several advantages over the MLE method, which can be highlighted as follows. The NNLS-VCE method is relatively easy to comprehend and interpret compared to the MLE method. Estimates of negative variance components can result in a covariance matrix that is not positive definite. This means that the matrix does not have physically meaningful interpretations. Large negative variance components generally indicate potential flaws or issues in the stochastic model. NNLS-VCE is a straightforward method to implement it, which is also suitable for both univariate and multivariate analysis. It stands out for its practical efficiency, primarily due to its low computational burden. One advantage of NNLS-VCE is that it utilizes the Newton–Raphson method, which contrasts with the simplex procedure employed in MLE.

In our study, we applied the NNLS-VCE method to analyze two comparable VCE methods, where the noise components and amplitudes were kept constant. We performed this analysis on a total of 10 time series. Interestingly, we found that the time required for estimating the variance components using the NNLS-VCE method was approximately 11 times shorter than that with the MLE method. Hence, based on our findings, it is evident that the NNLS-VCE method offers a significantly faster alternative to the MLE.

One advantage of NNLS-VCE is that it utilizes smaller matrices, specifically $N_{p\times p}$ and $l_{p\times 1}$, instead of involving larger matrices like A and Q_y. Simultaneous estimation of different noise components can be challenging with MLE method as it may result in some estimated amplitudes being negative. To overcome this issue, NNLS-VCE incorporates a large penalty to the objective function during the minimization problem. This penalty helps prevent negative estimates of the variance components.

Applications, results and discussion

Simulated GNSS time series

We simulated 1000-time series to check the existing stochastic models in GNSS time series. In these time series, average value and linear trend are denoted as y_0 and r, respectively. Also, the annual and semi-annual periods have been used as follows:

$$y(t) = y_0 + rt + \sum_{i=1}^{q} a_i \cos\omega_i t + b_i \sin\omega_i t + e(t), \tag{25}$$

where $q = 2, \omega_1 = 2\pi$ and $\omega_2 = 4\pi$. As periodic signals contain mostly the annual and semi-annual signals, we merely consider them (Amiri-Simkooei et al. 2017). The pairs (a_i, b_i) can be used to obtain the phase and amplitude of the signals. Equation (18) will then yield the final time series, considering $e(t)$ to be the various generated noise including "$W+P$", "$W+F$", "$W+P+F$" and also "$W+P+F+R$" noise models. The noise vector will be generated using Cholesky decomposition. The simulating parameters are listed in Table 1.

Table 1 Parameters used to simulate time series contaminated by colored noise

	East	North	Up
WN amplitude (mm)	5	6	10
FN amplitude (mm/year$^{1/4}$)	16	18	30
PL amplitude (mm/year$^{1/8}$)	10	12	20
RW amplitude (mm/year$^{1/2}$)	8	9.6	16
Phase of annual signal (mm)	−2	−2	−2
Amplitude of annual signal (mm)	−3	−3	−3
Phase of semi-annual signal (mm)	−1	−1	−1
Amplitude of semi-annual signal (mm)	−2	−2	−2
Linear trend (r) (mm/	1	1	1
Initial position (y_0)(m)	1.35	1.35	1.35

The values in Table 1 were obtained through pre-analysis of the time series of the 347 permanent GPS stations provided by JPL's second reprocessing campaign (Khazraei and Amiri-Simkooei 2019). Figure 1 depicts a 10-year time series generated using the values from Table 1. It showcases a randomly displayed time series within the figure. The red line represents the result obtained by fitting the least squares method to the East component of the three noise models analyzed in the figure, namely, "$W+F$", "$W+P+F$", and"$W+P+F+R$".

To conduct a more detailed analysis, we consider three separate spectral indices in our stochastic model: 0.5, 1 and 2, representing fractional power-law noise, flicker noise and random walk noise, respectively. For brevity, we denote this stochastic model as "$W+P+F+R$" where "W" refers to white noise, and "P," "F" and "R" represent fractional power-law, flicker noise, and random walk noise, respectively.

We examine four cases: case I ("$W+P$"), case II ("$W+F$"), case III ("$W+P+F$"), and case IV ("$W+P+F+R$"). These cases represent progressively more complex noise models, with case IV being the most complex (refer to Table 2). However, it is noted that our algorithm is not limited to any specific noise structure. The same analysis can be applied to other noise combinations such as "$W+F+R$" or any other combination of noise types.

Infeasibility of correct noise model detection using MLE

In the field of GNSS time series analysis, accurately identifying the noise model is crucial. To achieve this, multiple methods have been utilized. Nowadays, the criteria based on the maximum likelihood estimation (MLE) method are widely used to detect existing noise in GNSS time series. These criteria include the log-likelihood (LLL) criterion, as well as various information criteria (IC). In this

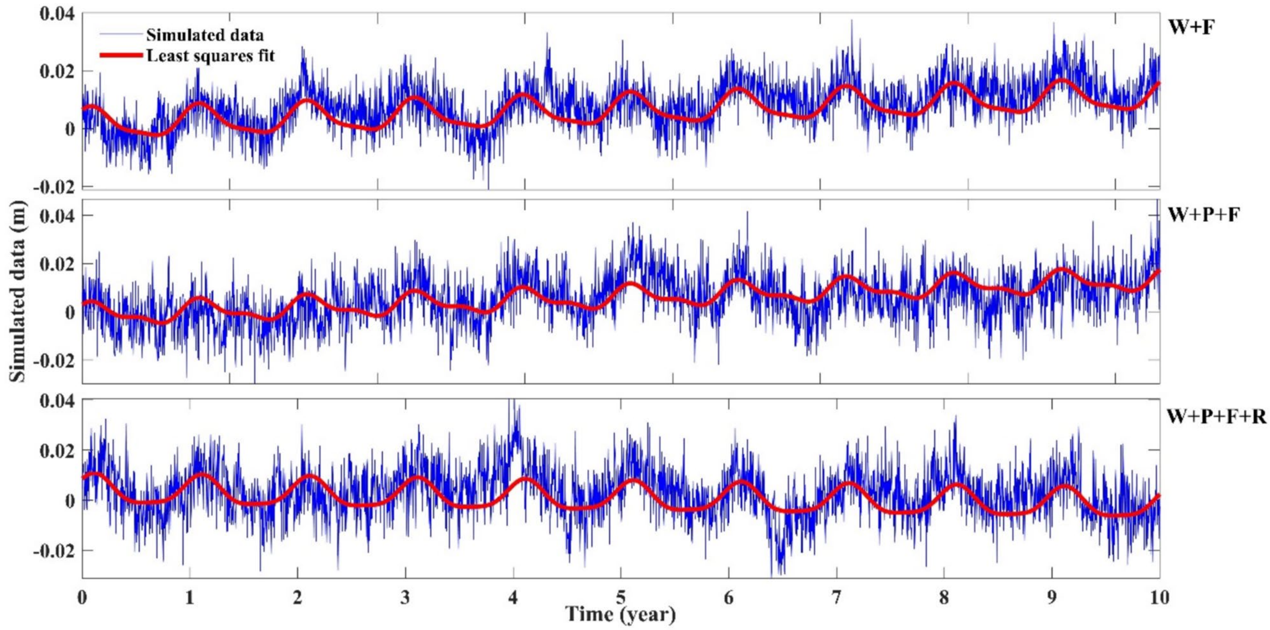

Fig. 1 Simulated time series generated by a linear trend, an annual and semi-annual periodic signal contaminated by "W + F" noise (top), "W + P + F" noise (middle) and "W + P + F + R" noise (bottom)

Table 2 Four cases of noise inputs ranging from simple stochastic model (I) to complex stochastic model (IV)

Input noise	Stochastic model			
	W	P	F	R
Case I	■	■		
Case II	■		■	
Case III	■	■	■	
Case IV	■	■	■	■

method, variance components can be estimated negative. Negative estimates of variance components (VCs) lead to covariance matrices that are not positive definite, which lacks physical justification. This issue could potentially be caused by various factors, including limitations in the functional model's degrees of freedom, incorrect initial values for variance components, inadequate stochastic modeling as well as over parametrized stochastic model (Amiri-Simkooei 2016). Over parameterization refers to the inclusion of a large number of noise components in a stochastic model, when not all of these noise components are present in the data. It can result in heightened correlations and reduced precision among estimates of noise components. Consequently, this increases the probability of encountering negative variance estimates.

To address this issue, we will thoroughly examine all possible combinations of " *W*", "*P*", "*F*" and "*R*" (15 combinations in total). By doing so, we then determine the variance components associated with each combination. We intend to answer the following question: "What percentage of the variance components, estimated using MLE, exhibits negative values across various noise combinations?".

To calculate the variance components using MLE, we use Eq. (14). In this study, we simulated 100-time series for each cases according to the values provided in Table 1. We then calculated the number of negative amplitudes for the 15 combinations of existing noise in all cases. If the variance components become negative, the next step is to examine whether or not the eigenvalues of the variance–covariance matrix also become negative. If the eigenvalues of the covariance matrix become negative, the matrix is no longer positive definite. As a result, Q_y cannot be considered a valid covariance matrix, and its feasibility in the problem is not justified.

Figure 2 presents the estimated negative noise components (blue bars) plotted next to the negative eigenvalues (red bars) of the covariance matrix for study cases 1–4. When considering a single noise component, any of "*W*", "*P*", "*F*", or "*R*", it was determined that no negative noise amplitude values were mathematically obtained. Also, the combinations of "$W+F$" and "$P+F$" exhibited no negative noise amplitude in all cases. As a result, we exclude these six combinations and proceed to assess the percentage of negative variance components in the remaining noise combinations.

Figure 2 provides insights into the presence and distribution of negative components and negative eigenvalues in different models. In all four cases, it demonstrates that to detect noise in time series using indicators based on MLE, it is

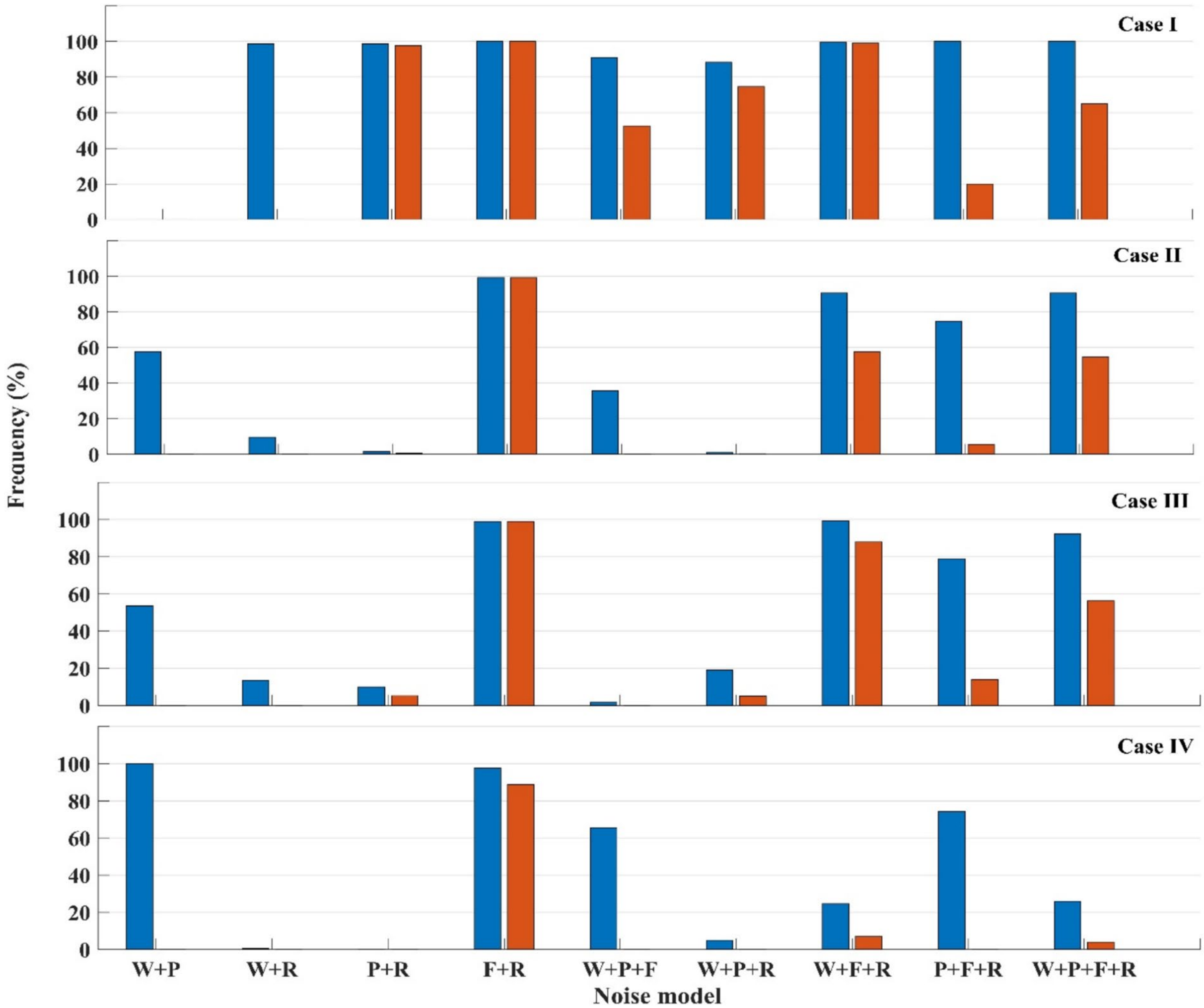

Fig. 2 The frequency of negative noise amplitudes estimated by the MLE method (represented by blue bars) is compared to the frequency of negative eigenvalues in the covariance matrix of the observables (represented by red bars), expressed as a percentage. This comparison is done for Case I, Case II, Case III and Case IV

essential to estimate the amplitude of the noise components in every scenario. If the stochastic model is selected correctly, the occurrence of negative values is lowest compared to the other cases. Specifically, the percentages of negative values are 0%, 0%, 1.6% and 26% in cases I, II, III and IV, respectively. In case IV, however, the "$W+R$" stochastic model exhibits the smallest estimated negative amplitude at 0.6%. This indicates that when there are more than three noise components in the stochastic model, this approach fails to identify the correct model. It can be inferred that an increase in the number of noise variables leads to the emergence of negative components in the estimation. In the MLE, if the model is identified as true positive (TP), the negative components cannot be estimated with the increase in noise variables. Consequently, the positive definite condition of the covariance matrix is not satisfied in this scenario, where 4% of the eigenvalues in case IV have a negative value among the estimated negative values, accounting for 20%.

As depicted in Fig. 2, in case I, when the correct model is not determined, the estimation of variance components shows percentages close to 100 as negative, and the eigenvalues of the covariance matrix are observed to be highly negative. This poses a contradiction considering the positive definiteness requirement for the covariance matrix. For case I, the "$W+P+F$", "$W+P+R$", "$P+F+R$" and "$W+P+F+R$" models identified negative variance components with percentages of 91%, 88.3%, 100% and 100%, respectively. Similarly, it was found that 52.6%, 74.6%, 20% and 65% of the eigenvalues of the covariance matrix was estimated to be negative. Remarkably, this occurred when the spectral indices of the noises in case I were closely aligned and both close to zero.

Based on the results obtained in case II, if the number of noise components is the same as in case I and there is a noticeable difference in their spectral index, the percentage of negative components in the estimated variances will decrease. Additionally, the percentage of values with negative eigenvalues in the covariance matrix will also be lower compared to case I. In case II, specifically for the models "$W+F+R$", "$P+F+R$" and "$W+P+F+R$", the estimated negative variance components are 90.6%, 74.6%, and 90.6% respectively. Among them, 57.6%, 5.6% and 54.6% have negative eigenvalues in the covariance ma.

Application of NNLS-VCE to stochastic model identification

In this section, we aim to demonstrate the effectiveness of the NNLS-VCE method in identifying noise models in two modes: univariate analysis and multivariate analysis. Unlike methods that penalize the objective function, NNLS-VCE utilizes an inequality constraint on the objective function. This constraint inherently guarantees that the variance components remain non-negative.

One crucial component in GNSS time series analysis is the uncertainty of trend (σ_r)). It plays a significant role in determining the confidence level in the obtained results. Consequently, we have also examined the sensitivity of the noise model identified through NNLS-VCE by assessing the level of estimated rate uncertainties.

To comprehensively study the noise structure of GNSS time series, we simulate the coordinate components (east, north and up), separately. Each time series has its own noise structure with variable amplitudes, as shown in Table 1. Our results are provided for both univariate and multivariate analysis. In the univariate analysis, we analyze each time series separately. Using the NNLS-VCE method, we obtain the optimal noise model for each individual series. In the multivariate analysis, we process the east, north, and up coordinate components together. This approach also allows to account for the potential correlations between the time series and provides a more realistic estimation of the noise structure.

The noise amplitudes in the stochastic model (Eq. 6) are computed for the desired noise inputs. In univariate analysis, we employ Eqs. (18) and (19) through an iterative process. In multivariate estimation, we consider coordinate time series simultaneously, and the noise amplitudes are estimated using Eqs. (22) and (23). If a particular noise is not present in the time series, its amplitude should be estimated zero using NNLS-VCE. To investigate this matter, 1000-time series are generated for each noise input, and their amplitudes are estimated using NNLS-VCE.

Effective parameters on TP results

When identifying the stochastic model of a time series, there are key factors to consider, which includes the number of noise components, their spectral indices, univariate versus multivariate analysis and the length of the time series. These factors play a significant role to effectively analyze the stochastic noises within the time series. In this section, each of these factors will be examined. The spectral index is a crucial parameter in identifying stochastic noises effectively. When the spectral index is higher, the noise detection power becomes lower. Additionally, if the time series contains a larger number of noises, their identification ability will be diminished. Utilizing time series with a high data count is one of the effective approaches for accurately identifying stochastic noises in time series. The significance of having a large number of data points in a time series is that it allows for a more comprehensive analysis and accurate predictions. Ideally, the time series should be relatively uninterrupted or gap-free, ensuring continuity and consistency in the data. Additionally, a time series length of more than 10 years provides a broader historical context, enabling better trend identification and capturing long-term patterns. In the following, we explore the aforementioned factors to demonstrate the effectiveness of NNLS-VCE for stochastic model identification.

Type of noise is a critical factor that influences the ability of NNLS-VCE to accurately identify the appropriate stochastic model. We generated a time series simulation that consisted of white noise. Through the utilization of NNLS-VCE in both univariate and multivariate analysis, we successfully detected and characterized the underlying noise components. Considering case I and case II, we investigated the effect of spectral index in noise identification. Table 3 displays the noise detection power utilizing the NNLS-VCE method in both univariate and multivariate analysis, showcasing results for four distinct case studies. According to Table 3, the univariate analysis shows that case I has an average noise identification power of 98.5% for all three coordinate components. On the other hand, case II has an average noise identification power of 90.5% for the same components. Additionally, the average spectral index for case I is 0.25, while for case II, it

Table 3 Mean detection power of NNLS-VCE in univariate analysis and multivariate analysis for different case studies

Case study	Univariate	Multivariate
case I	98.5	99.5
case II	90.5	99.8
case III	69.5	88.4
case IV	29.3	83.7

is 0.5. Generally, as the spectral index increases, identification power tends to decrease.

To study the impact of number of noise components on the detection power of the proposed method, we focus on case III as the input for our simulations. Table 3 indicates that the average detection power for the three coordinate components decreases to 69.5%. In a study conducted by He et al. (2019), it was found that the LLL index incorrectly identifies fractal power-law noise as flicker noise in approximately 66% of cases.

After incorporating random walk ("case IV"), the identification power even decreases to 29.3%. This indicates that, as the number of noises in the GNSS time series increases, the detection power of NNLS-VCE to identify and separate colored noise with different spectral indices diminishes. Although the multivariate analysis outperforms the univariate analysis, we also observe a decrease in the multivariate identification power when using complex noise models (e.g., case IV) compared to the simpler models (cases I and II).

Using longer time series is expected to result in a higher likelihood of detecting the correct noise model of the series. In their study, He et al. (2019) explored the effectiveness of information criteria derived from MLE in time series data spanning 10, 15 and 25 years. Their results indicated that the identification of random walk noise becomes easier as the time span increases. To assess the impact of time series length on the NNLS-VCE performance, we generated data for a duration of 20 years for case II. The NNLS-VCE method was then used to identify and estimate the noise components. Figure 3 displays the results for three coordinate components in both univariate and multivariate

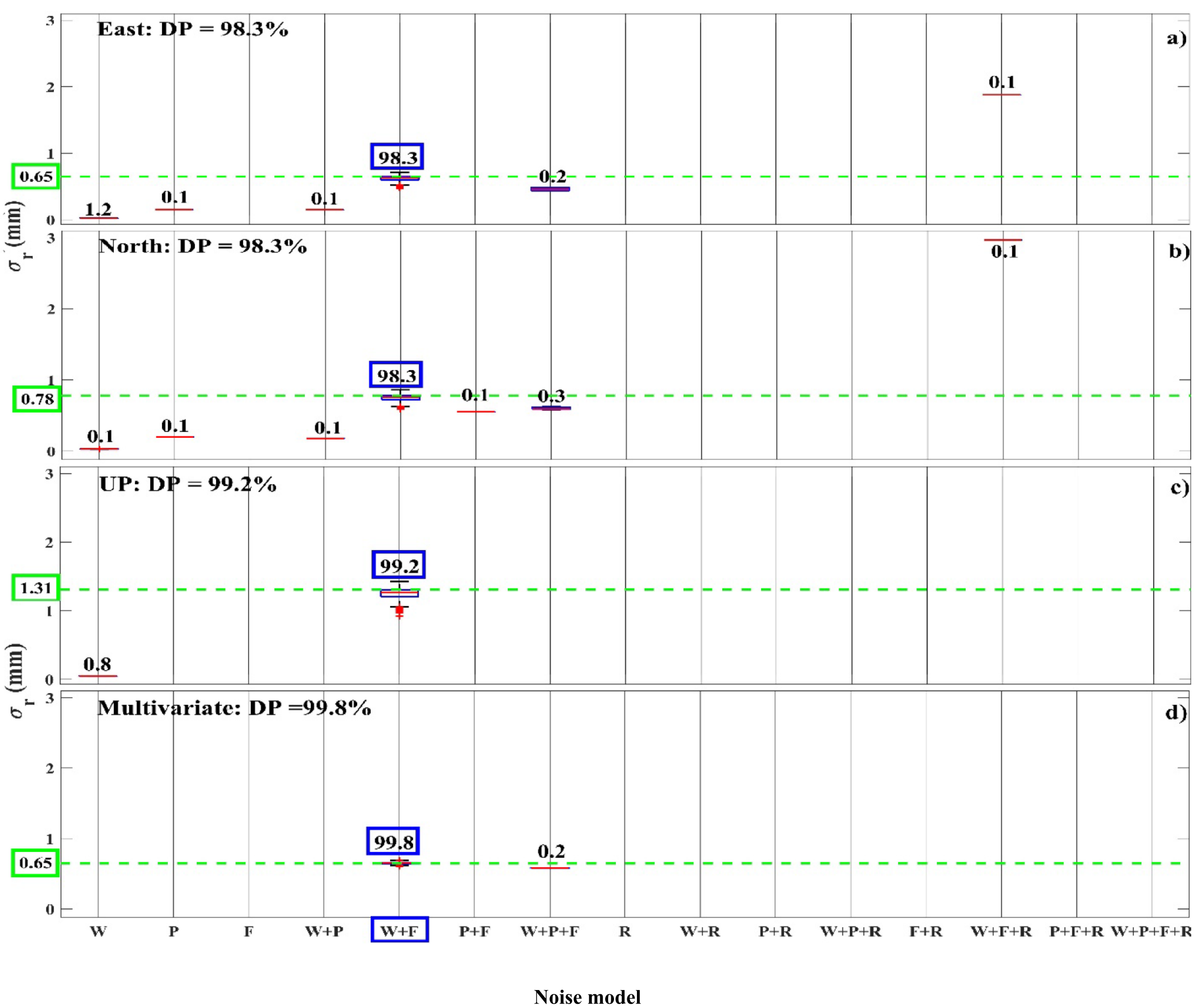

Fig. 3 The 20-year time series boxplot of East, North, UP and Multivariate components of case II are shown in (**a**), (**b**), (**c**) and (**d**), respectively. The green dashed line indicates the uncertainty of the rate

analysis. When the length of the time series is doubled, there is on average 8% increase in the identification power across three coordinate components in univariate analysis, though the detection power (99.8%) did not change in multivariate analysis. Time series length is therefore a crucial factor impacting result accuracy. Longer time series can facilitate the identification of colored noise in GNSS time series.

To examine the implications of using the false noise model (FP) in the context of time series analysis, we assess the estimated rate uncertainty for the specific cases using a box plot. Additionally, we evaluate the impact of FP noise model on the rate uncertainty values. The box plots shown in Figs. 3, 4 and 5 represent the uncertainty rate for cases I, II, III and IV, respectively. In a noise model, if the red line is positioned above the index line in the box diagram, the trend uncertainty has been overestimated. Conversely, if the red line is below the index line, underestimation has occurred. Neither scenario provides a realistic estimate of trend uncertainty. However, in both scenarios, the trend estimates will remain unbiased even for FP noise models. Nevertheless, the uncertainty values assigned to the estimates are expected to be either higher or lower than the actual value.

To assess the performance of NNLS-VCE in identifying random walk noise, an investigation was conducted on a 10-year time series (referred to as "case IV"). In this case, the identification percentage of true chosen noise model (TP) in univariate mode averaged around 30% for both the horizontal and vertical components, while He et al. (2019) identified 11% of random walk noise by analyzing a 15-year time series.

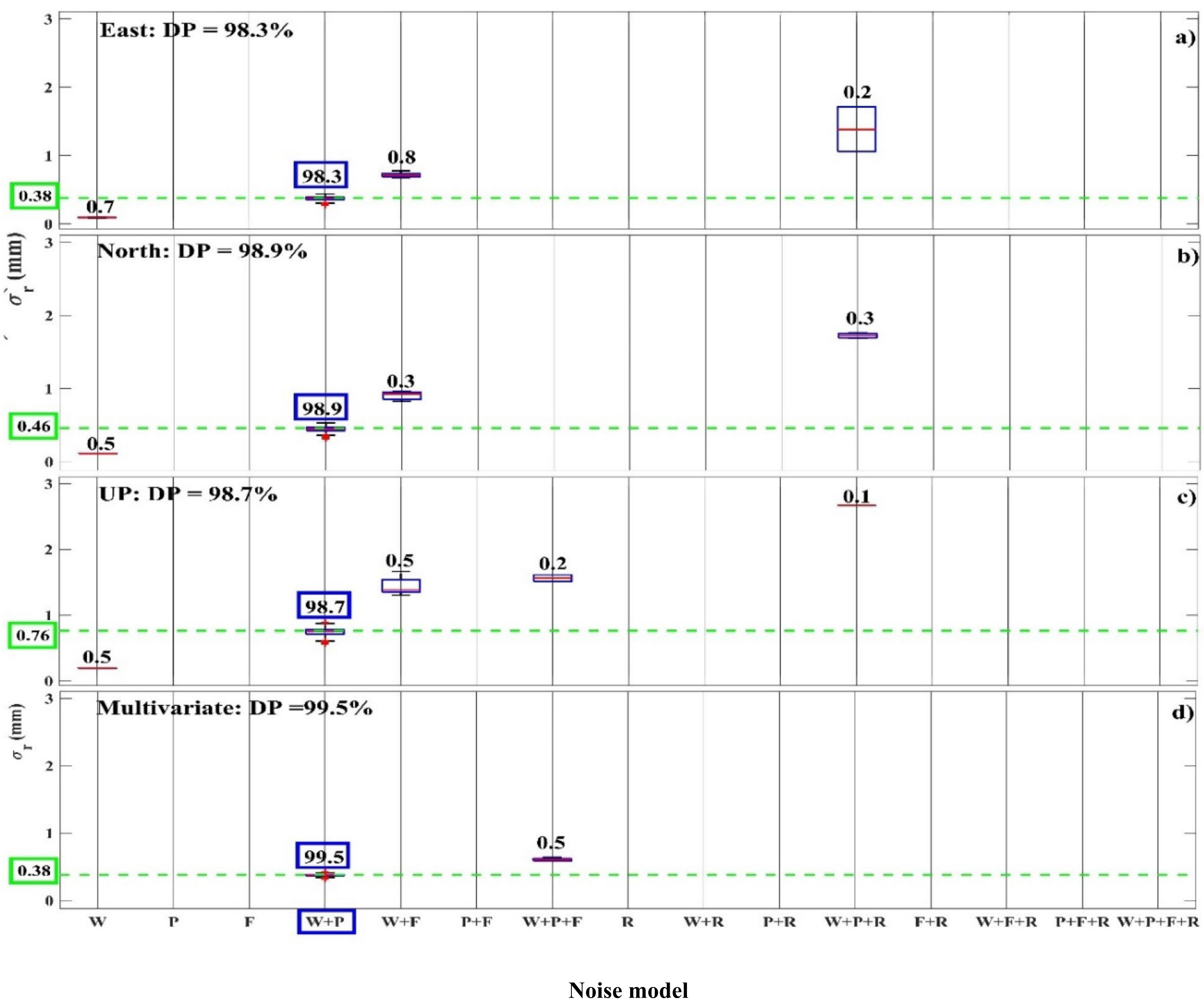

Fig. 4 Effect of identified noise models on rate uncertainties for case I in univariate analysis for East (**a**), North (**b**) and Up (**c**) components and multivariate analysis (**d**); multivariate plot is presented for east component

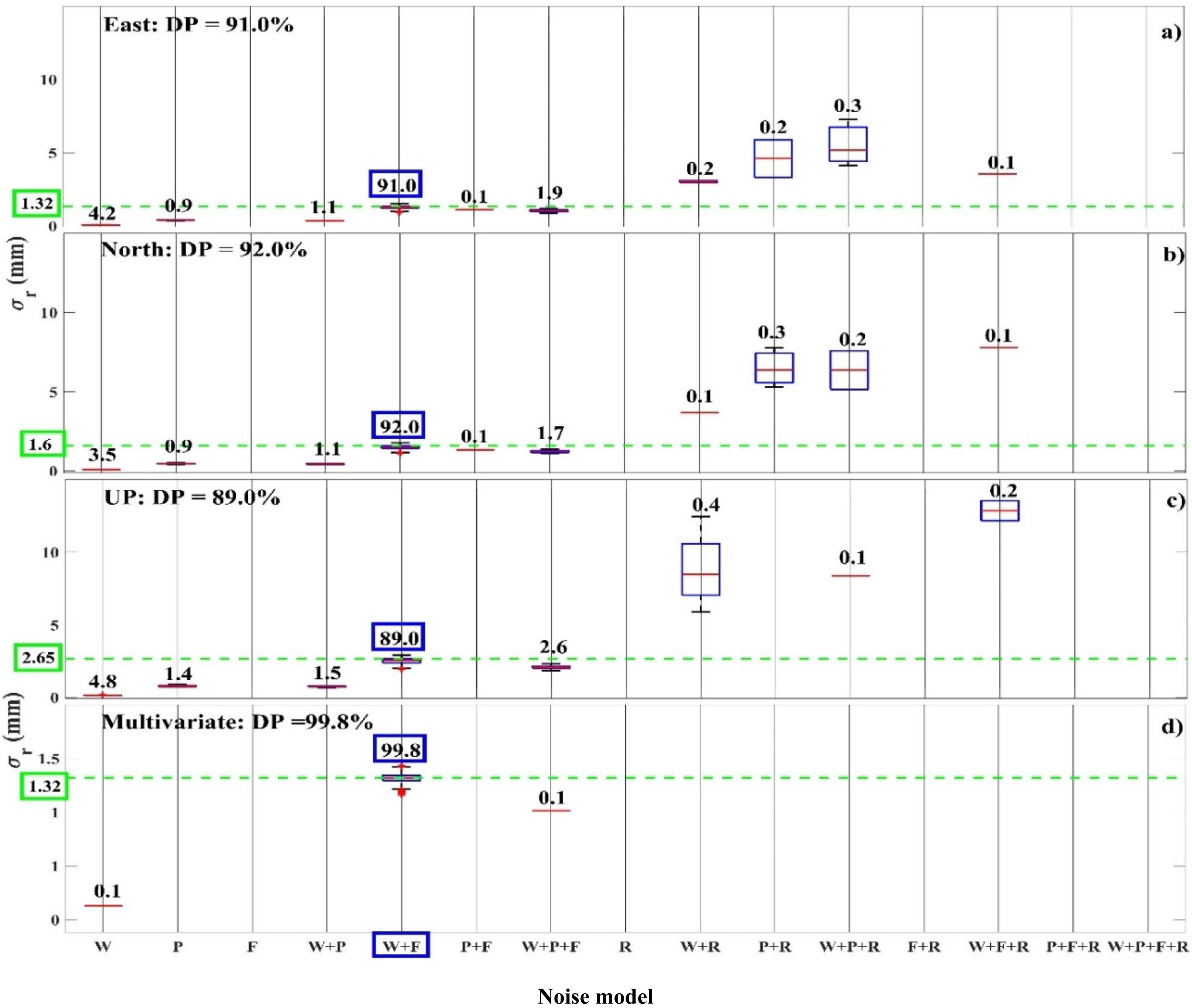

Fig. 5 Rate uncertainty value for case II in univariate analysis for East, North and Up directions for the identified noise models vs. multivariate analysis: East (**a**), North (**b**), Up (**c**) and Multivariate for East component is (**d**)

Influence of false positive (FP) on rate uncertainty

The rate uncertainty is influenced by the accuracy of the stochastic model used for detecting noise in the data. The closer the stochastic model resembles the actual noise of the data, the more reliable the rate uncertainty estimation becomes. If the stochastic model closely resembles reality, the estimated rate uncertainty is likely to be very close to the actual value. To calculate the standard deviation of the estimated unknown vector $\hat{x}$, we can obtain the covariance matrix $Q_{\hat{x}}$ of unknown parameters as:

$$Q_{\hat{x}} = \left(A^T Q_y^{-1} A\right)^{-1}, \tag{26}$$

where Q_y refers to the identified stochastic model. The rate uncertainty estimate is then obtained from $Q_{\hat{x}}$. We use box-plot diagrams to display both the central tendency and dispersion of a data set simultaneously. Boxplots are useful tools for comparing the range and distribution of average data to identify the level of dispersion in different noise models and detect outliers. In this diagram, the boxes representing each noise model can be compared based on their proximity and distance from the real value of the trend's standard deviation. This provides an easy way to assess the variability and identify any unusual data points. In a boxplot, 50% of the data is contained within the box. Additionally, 25% of the data is scattered below the box, while another 25% lies above the box. The entire length of the graph represents a probability distribution of 99.3% for the results of the analysis. Any data points outside the box plot that are marked with a red mark are considered outliers.

The spectral index is a factor that plays a significant role on the rate uncertainty to be estimated biased. Figures 4 and 5 represent the box plots for case I and II, respectively. In case I, the accumulative spectral index is reported to be 0. 5, obtained from white noise ($\kappa = 0$) and a partial power-law noise ($\kappa = 0.5$). In case II, the accumulative index is 1 (from "$W+F$" model), is positioned above the green line in all three coordinate components. When the accumulative spectral index increases, the rate uncertainty value rises.

The purpose was to estimate the noise characteristics and determine if the NNLS-VCE method could accurately identify it as a stochastic model. Both univariate and multivariate estimation techniques were employed in the NNLS-VCE method to accomplish this task. The results display if we do not consider white noise, it can lead to an underestimation of the rate uncertainty. To assess the effectiveness of the NNLS-VCE method in detecting white noise, for example, in Fig. 6, the "$P+F$" noise model with average spectral index of 0.75, which is higher than the reference spectral index of 0.5 for case III. However, despite this higher value, the σ_r value estimated using this $F+P$ noise model falls below the index line. Both the "$P+F+R$" and "$P+R$" noise models also lack white noise, but the presence of random walk noise affects the estimated σ_r.

If a stochastic process is not present in a time series but is still considered, it can lead to under/overestimation of the rate uncertainty value. For example, in case II where random walk noise is not present, the rate uncertainty estimated using the (identified) "$W+F+R$" model may be higher than the actual value. According to Fig. 6, it is observed that case III does not have random walk noise. On the other hand, the estimated rate uncertainty is affected when including random walk noise in certain FP models, such as "$W+P+F+R$", "$W+F+R$", "$W+P+R$", "$P+R$" and "$P+F+R$". In the

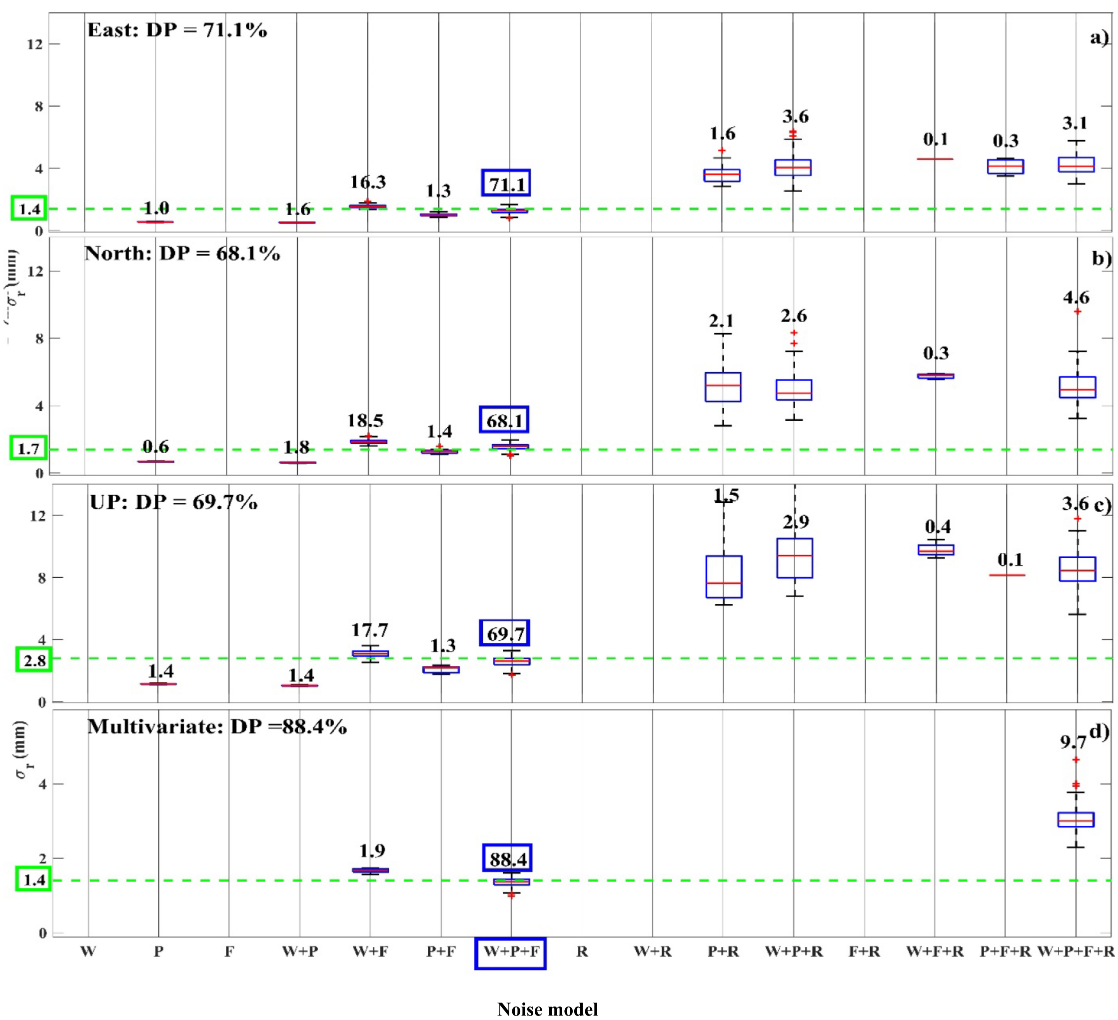

Fig. 6 Rate uncertainty value for case III in univariate analysis for East, North and Up directions for the identified noise models vs. multivariate analysis: East (**a**), North (**b**), Up (**c**) and Multivariate for East component is (**d**)

opposite scenario, if there is noise present in the time series data but it is not considered in the stochastic model, it leads to a bias in the uncertainty of the rate estimation. For example, all-time series mainly include white noise.

Advantages of multivariate analysis

GNSS time series analysis using multivariate model has been shown to have significant impact on functional model identification. For example, the reader refers to signal detection (Amiri-Simkooei 2009) and offset detection (Amiri-Simkooei et al. 2019). The fact that different time series can be correlated suggests that estimating these series individually may not be realistic. In NNLS-VCE, we employ multivariate analysis to estimate rate uncertainties. This involves analyzing three coordinate time series simultaneously for various cases of study.

In Fig. 4, multivariate analysis was conducted to consider all three components (east, north and up) simultaneously as the observation matrix. The results showed that the identification power for all three components was 99.5%. As the noise structure detected is consistent for all three coordinate components in every case of study, the results presented as multivariate are specifically related to the east component in all cases.

In case I, when using multivariate analysis instead of univariate analysis, we observed a significant improvement. The percentage of FP models has been reduced to only 0.5%, indicating a higher accuracy. Additionally, both the number and dispersion of these incorrect models have also been reduced. Specifically, in the "$W+P+F$" as FP noise model, the σ_r amount is estimated to be higher than the actual value (Fig. 4(d)). According to the information provided in Fig. 5, when utilizing multivariate analysis, the identification power achieves a high level of accuracy, reaching 99.8%. Only a small portion, specifically 0.2% of the model, was incorrectly identified (specifically the "W" and "$W+P+F$" models).

After comparing the results of multivariate and univariate analysis in Figs. 5 and 6, it becomes evident that multivariate analysis is the more preferable option. This preference can be attributed to several factors. Firstly, it is observed that the east, north and up time series exhibit noises with a similar structure, indicating a common underlying cause. The synergistic nature of these noise components further strengthens the case for multivariate analysis. By employing multivariate analysis, the probability of detecting noise is heightened, leading to increased σ_r accuracy as the results. This improved accuracy is particularly notable when dealing with more complex noise models that entail larger mean spectral indices. In summary, the effectiveness of multivariate analysis surpasses that of univariate analysis, as observed in Figs. 5 and 6. Its ability to identify and account for common noise structures and its superiority in handling complex noise models make it the preferred choice.

As the complexity of the noise model increases, the application of multivariate analysis becomes more remarkable compared to univariate analysis. In Fig. 6, the input noise model undergoes further complexity as it includes three distinct noises, referred to as case III. In this case, the average power detection of the correct noise model for the three coordinate components is 67%. When comparing Fig. 6 to 5, despite both figures having an average spectral index of 0.5 for the true noise model, the presence of three distinct noises simultaneously has resulted in a decrease of approximately 23% in the detection power during univariate analysis.

According to Fig. 6(d), in the case III, it was found that the use of multivariate analysis greatly enhances the detection power, reaching an impressive 88.5%. This highlights the significant impact of multivariate analysis in dealing with complex noise models. Additionally, through this analysis, it was determined that the FP noise models consisted of combinations of variables, namely, "$W+F$" and "$W+P+F+R$", with probabilities of 1.9% and 9.7%, respectively. The "$W+P+F+R$" noise model, with an average spectral index of 0.87, is positioned above the index line. On the other hand, the "$W+F$" noise model, with an average spectral index of 0.5, is situated closer to the index line. Despite the fact that the average spectral index of "$W+F$" and "$W+P+F+R$" noise models is both 0.5, the box plot in the multivariate analysis shows that, in the case of the "$W+P+F+R$" noise model, the index line has been intersected at the most probable position.

Based on the information provided in Fig. 7, it can be observed that in case IV, the power detection of univariate analysis in three components has significantly decreased to an average of 29.3%. Additionally, the index line has been predominantly affected by not only the correct model ("$W+P+F+R$") but also the wrongly identified models of "$W+F+R$" and "$P+F+R$", which were mistakenly considered as the FP models. With the utilization of multivariate analysis method, the identification power has improved to 83.7% (Fig. 7(d)). Additionally, the number of incorrect models has been reduced to only three. Among these models, the noise model stands out as it intersects the index line with the highest probability.

Conclusions

Researchers have been paying significant attention to identifying and estimating the presence of white and colored noises in integrated GNSS time series. The most well-known noise model for GNSS time series horizontal components is "$W+F$," which is commonly used as the default stochastic model in most analyses. Additionally, some researchers

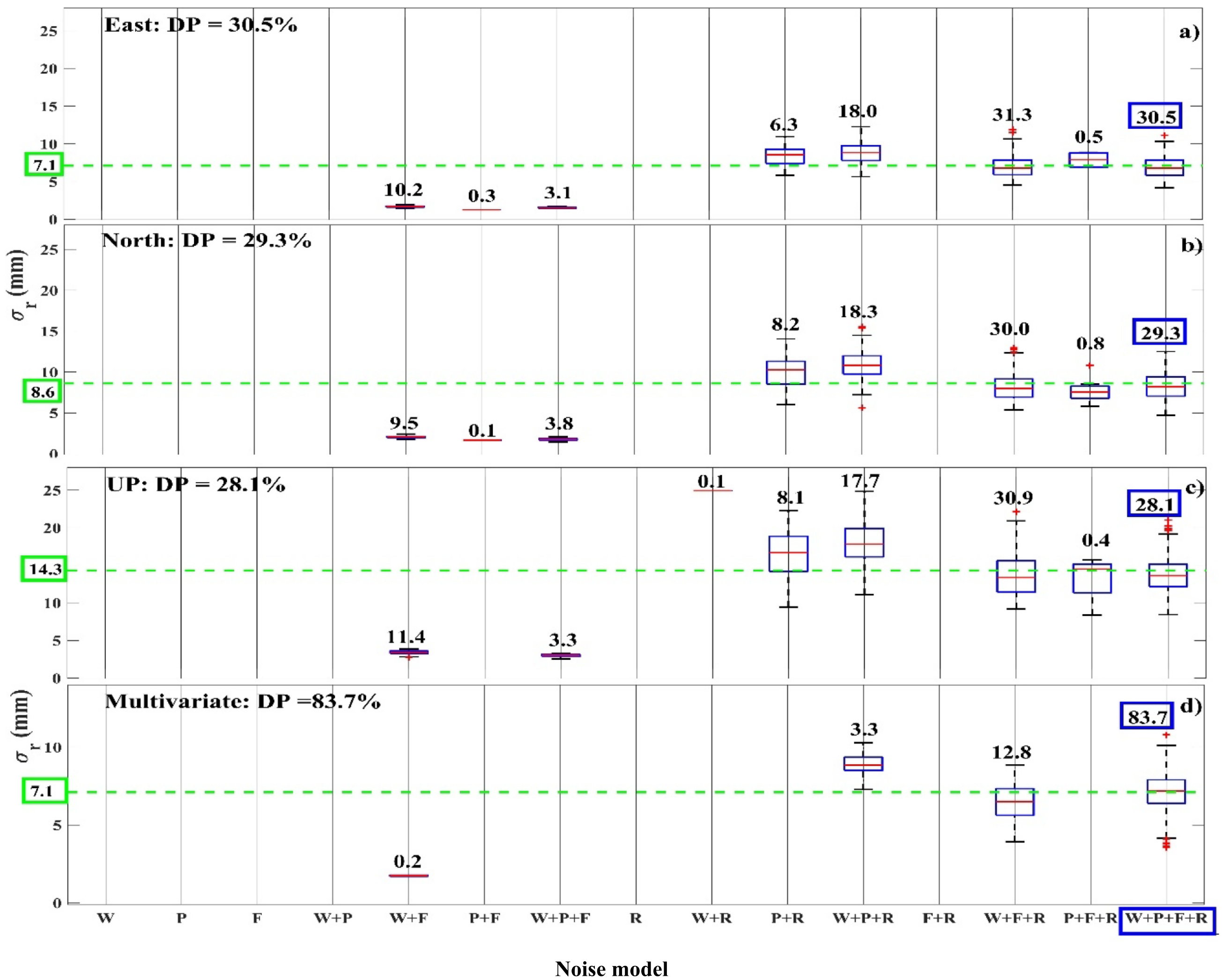

Fig. 7 Rate uncertainty value for case IV in univariate analysis for East, North and Up directions for the identified noise models vs. multivariate analysis: East (**a**), North (**b**), Up (**c**) and Multivariate for East component is (**d**)

have utilized the noise model "$W+P$" for processing GPS time series of horizontal components. The presence of noise in GNSS time series was examined through simulations (Table 1). Using the NNLS-VCE method, the study identified and estimated the existing noise in the time series. Comparing Figs. 4 and 5, it was observed that when the stochastic model is "$W+P$" but the time series includes flicker noise, the estimated accuracy rate is lower than the actual value. Taking into account the "$W+F$" noise model, if the spectral noise index in a time series is less than 1, the rate accuracy will be overestimated. There is more RW noise in the vertical time series of GNSS compared to the horizontal coordinate. By using multivariate analysis in the NNLS-VCE method, if RW noise exists, it can be identified alongside other noises by processing a 10-year time series with a probability close to 85%. The analysis considered "$W+P+F+R$" as the potential noise model, where the NNLS-VCE method expects the corresponding variance of an unlikely noise component to become zero.

In the NNLS-VCE method, in addition to univariate analysis, the possibility of multivariate analysis exists. When the noise model is complex, the percentage of estimation for multivariable analysis increases. The percentage of correct model identification for univariate and multivariate scenarios in case I, II, III and IV are as follows: 98.5% vs. 99.5%, 90.5% vs. 99.8%, 69.5% vs. 88.4% and 29.3% vs. 98.5%, respectively. In all cases, the probability of identifying a noise model in multivariate analysis significantly increases due to the co-addition of coordinate time series in an observational station. Among the influential parameters on identifying the stochastic noise model in time series analysis are the type of noise present in the time series, the number of noises present in the time series, and the length of the processed time series. As the number of noises increases and the accumulative spectral indices of colored noises surpass the spectral index of white noise, it becomes more challenging to accurately identify the noise model. In the context of multivariate analysis, the NNLS-VCE method has a higher likelihood of identifying a significant number of noises with complex structures.

Selecting a stochastic model erroneously as a noise model impacts the rate uncertainty values and leads to overestimation or underestimation of the actual rate uncertainty values. In the NNLS-VCE method, if there is no noise present in the time series, its amplitude is estimated as zero and it is removed from the stochastic model. This leads to a significant reduction in the number of false-positive models in multivariate analysis.

Declarations

Conflict of interest The authors declare that they have no conflict of interest.

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