MODIFIED GAUSS-NEWTON METHOD IN LOW-RANK SIGNAL ESTIMATION*

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Abstract. The paper is devoted to the solution of a weighted non-linear least-squares problem for low-rank signal estimation, which is related Hankel structured low-rank approximation problems. The solution is constructed by a modified weighted Gauss-Newton method. The advantage of the suggested method is the possibility of its stable and fast implementation. The method is compared with a known method, which uses the variable-projection approach, by stability, accuracy and computational cost. For the weighting matrix, which corresponds to autoregressive processes of order $p$, the computational cost is $O(Nr^2 + Np^2 + rN \log N)$, where $N$ is the time series length, $r$ is the rank of approximating time series. For the proof of the suggested method, useful properties of the space of series of rank $r$ are studied.

Key words. linear recurrence relation, Hankel structured low-rank approximation, signal estimation, Gauss-Newton optimization, variable projection

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1. Introduction. In this study we consider the 'signal plus noise' observation scheme:

$$x_n = s_n + \epsilon_n, \quad n = 1, 2, \ldots, N.$$  

Denote by $X = (x_1, \ldots, x_N)^T$, $S = (s_1, \ldots, s_N)^T$ and $\epsilon = (\epsilon_1, \ldots, \epsilon_N)^T$ the vectors of observations, of signal values and of errors respectively. We will refer to vectors of observations in $\mathbb{R}^N$ as time series (or shortly series, since the observations are not necessarily temporal; e.g., they can be spatial).

We assume that the signal $S$ can be written in the parametric form as a finite sum

$$s_n = \sum_k P_{m_k}(n) \exp(\alpha_k n) \sin(2\pi \omega_k n + \phi_k),$$

where $P_{m_k}(n)$ are polynomials in $n$ of degree $m_k$. In signal processing applications, the signal in the model (1.1) is usually a sum of sine waves [3] or a sum of damped sinusoids [20]. The problem of estimation of the signal values is as important as the problem of estimation of parameters in the form (1.1). Both problems can be solved by the same approach, but we are concentrated on the signal estimation.

Let $S \in \mathbb{R}^N$ be a set, which contains a class of signals in the form (1.1) of low complexity (to be defined later). Consider the weighted least-squares problem (WLS) with a positive definite symmetric weight matrix $W \in \mathbb{R}^{N \times N}$

$$Y^* = \arg\min_{Y \in S} \|X - Y\|_W,$$

where $\|Z\|_W^2 = Z^T W Z$. If noise $\epsilon$ is Gaussian with covariance matrix $\Sigma$ and zero mean, then the WLS estimate with the weight matrix $W = \Sigma^{-1}$ is the Maximum Likelihood estimate (MLE). The same is true if the covariance matrix is scaled by a constant.

Let us consider different approaches for solving (1.2). The chances for success in solving problems of this kind depend on the parametrization of the problem. For the search of parameters in (1.1) by the parametric least squares method (non-linear parametric regression), one should fix an explicit parametric form of (1.1) in $S$. Here we consider another approach to the choice of $S$ and its parametrization, based on the so-called signal rank.

Let us introduce necessary notions. The rank of a signal $S$ is defined as follows. For a given integer $L$, we define the embedding operator $T_L : \mathbb{R}^N \to \mathbb{R}^{L \times (N-L+1)}$, which maps $S$ into the

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Hankel $L \times (N - L + 1)$ matrix, by

\[
T_L(S) = \begin{pmatrix}
  s_1 & s_2 & \ldots & s_{N-L+1} \\
  s_2 & s_3 & \ldots & \vdots \\
  \vdots & \vdots & \ddots & \vdots \\
  s_L & s_{L+1} & \ldots & s_N
\end{pmatrix}.
\]

The columns of $T_L(S)$ are lagged vectors, this is why $T_L(S)$ is often called trajectory matrix. We say that the signal $S$ has rank $r < N/2$ if rank $T_{r+1}(S) = r$. It is known that rank $T_{r+1}(S) = r$ if and only if rank $T_L(S) = r$ for any $L$ such that $\min(L, N - L + 1) > r$ (see [16, Corollary 5.1] for the proof of a precise statement).

For a sufficiently large series length $N$, the signal in the form (1.1) has rank $r$, which is determined by the parameters $m_k, \alpha_k$ and $\omega_k$. For example, the series with signal values $s_n$ has rank $r = 2$ for a sum of two exponentials $s_n = c_1 \exp(\alpha_1 n) + c_2 \exp(\alpha_2 n)$ or a sine wave $s_n = c \sin(2\pi\omega n + \phi)$, or a linear function $s_n = an + b$.

Let us consider the set $S$ in (1.2), which fixes the rank $r$ but does not fix the form of the signal, i.e., the number of terms and degrees of polynomials in (1.2). The model of signal, where the Hankel matrix $T_L(S)$ is rank-deficient, is one of common models in many areas, signal processing [3, 27], speech recognition [8], control theory and linear systems [20, 21] among others.

Denote $\mathcal{D}_r$ the set of series of rank $r$. Since the set $\mathcal{D}_r$ is not closed, we will seek for the solution of (1.2) in its closure, i.e., $S = \overline{\mathcal{D}_r}$. It is well-known that $\overline{\mathcal{D}_r}$ consists of series of rank $\leq r$ (this result can be found in [17, Remark 1.46] for the complex case; the real-valued case is proved similarly).

Thus, in what follows, we consider the problem

\[
Y^* = \arg \min_{Y \in \mathcal{D}_r} \|X - Y\|_W.
\]

Let us consider different approaches for solving (1.4). This problem is NP-hard [11]. The optimization problem (1.4) is non-convex with many local minima [24].

The problem (1.4) is commonly considered as a structured (more precisely, Hankel) low-rank approximation problem (SLRA, HSLRA) [4, 22, 21]. A well-known subspace-based method for solving (1.4) is called ‘Cadzow iterations’ [3] and belongs to the class of alternating-projection methods. The method of Cadzow iterations can be extended to a class of oblique Cadzow iterations in the norm, which differs from the Euclidean norm [10]. The method has two drawbacks: first, the properties of the limiting point of the Cadzow iterations are unknown [1] and second, it tries to solve the problem (1.4) with a weight matrix which generally differs from the given $W$. Therefore, it is not optimal (the method does not provide the MLE), even for the case of white Gaussian noise [7]. The reason is that the problems are commonly stated in HLRA as matrix approximation problems, while the original problem (1.4) is stated in terms of time series.

Many methods have been proposed to solve HSLRA, including the Riemannian SVD [7], Structured total least-norm [19], Newton-like iterations [25], proximal iterations [5], symbolic computations [24], stochastic optimization [9], fixed point iterations [1], a penalization approach [18].

Among the most promising is the approach of Markovsky and Usevich [29, 30], which is based on the principle of variable projection [12]. The method from [29, 30] is able to deal with the problem in the form (1.4), i.e., with proper weights; moreover, it is elaborated in general form for a wide class of structured matrices and at the same time its iteration complexity scales
linearly with the length of data for a class of weight matrices. Nevertheless, the approach has a number of disadvantages: Cholesky factorization is used for solving least squares subproblems (and thereby doubles the condition number), the method is efficient only if the inverse of the weight matrix is banded.

In this paper, we propose to overcome these difficulties, mainly in several ways. First, we consider a modified Gauss-Newton iteration method by using a special parametrization of the problem; this modification helps to avoid computing the pseudoinverse of the Jacobian matrix. Then, unlike [30], the projection is calculated on the image space of signals governed by linear relations with given coefficients \((Z(A))\) and not on the kernel space \(Q(A)\), see Section 2.1 for notation. Finally, for calculation of the projection, we use fast algorithms with improved stability. As a result, our method is not slower and is much faster in some scenarios, but also is more stable.

We also study the other properties of the problem including properties of \(D_r\) in the considered parametrization. The obtained results can be useful beyond the scope of this paper. In particular, the induced parametric form of the tangent subspace in a given point of \(D_r\) can be useful for investigation of local properties of the problem solution. Also, the effective algorithm for calculation of projection to the space of series governed by a specific linear recurrence relation, which is suggested in Section 4, can be used in different algorithms within HSLRA.

Structure of the paper. In Section 2 we consider a parametrization of \(D_r\) and its properties, which help to construct effective algorithms. In Section 3 we describe the known (VPGN) and the new suggested (MGN) iterative methods for solution of the optimization problem (1.4). The algorithm VPGN is described in the way different from that in [30], since the description in [30] is performed for general SLRA problems and therefore it is difficult to apply it to the particular case of HLRA for time series. In Section 4 we suggest effective algorithms for implementation of key steps of the algorithms. Section 5 presents the algorithms with implementations of VPGN and MGN. In Section 6 we compare computational costs and numerical stability of the VPGN and MGN algorithms. Section 7 concludes the paper. Long proofs and supplementary details of the algorithms are put up to Appendix.

Main notation. In this paper, we use lowercase letters \((a, b, \ldots)\) and also \(L, K, M, N\) for scalars, uppercase letters \((A, B, \ldots)\) for vectors, bold uppercase letters \((\mathbf{A}, \mathbf{B}, \ldots)\) for matrices, the uppercase sans serif font \((\mathbf{A}, \mathbf{B}, \ldots)\) for time series, and the calligraphic font for sets.

2. Parametrization of series of finite rank.

2.1. Linear recurrence relations. It is well known [15, Theorem 3.1.1] that any series of the form (1.1) satisfies a linear recurrence relation (LRR) of some order \(m\):

\[
s_i = \sum_{k=1}^{m} b_k s_{i-k}, b_m \neq 0, i = 1, \ldots, N - m.
\]

One time series can be governed by many different LRRs. The LRR of minimal order \(r\) (it is unique) is called minimal. The corresponding time series has rank \(r\). The minimal LRR uniquely defines the form of (1.1) and the parameters \(m_k, \alpha_k, \omega_k\).

The equations (2.1) can be expressed in the vector form as \(A^T T_{m+1}(S) = 0\), where \(A = (b_m, \ldots, b_1, -1)^T \in \mathbb{R}^{r+1}\). The vector \(A\) corresponding to the minimal LRR \((m = r + 1)\) and the first \(r\) values of the series \(S\) uniquely determine the whole series \(S\). Therefore, \(r\) coefficients of an LRR of order \(r\) and the first \(r\) values of the series (\(2r\) parameters altogether) can be chosen as parameters of a series of rank \(r\).

However, this parametrization does not describe the whole set \(D_r\).

Let us generalize LRRs. We say that a series satisfies a generalized LRR (GLRR) of order \(m\) if \(A^T T_m(S) = 0\) for some \(A \in \mathbb{R}^m, A \neq 0\). As before, we can consider the GLRR of minimal
order. The difference between a GLRR and an ordinary LRR is that the last coefficient in a GLRR is not necessarily non-zero and therefore the GLRR does not necessary set a recurrence. However, at least one of the coefficients in a GLRR should be non-zero. The GLRR corresponds exactly to the first characteristic polynomial in [16, Definition 5.4].

The following properties clarify the structure of the spaces \( \mathcal{D}_r \) and \( \overline{\mathcal{D}}_r \):

- \( \mathcal{D}_r = \{ Y : \exists A \in \mathbb{R}^{r+1}, A \neq 0 : A^T \mathcal{T}_m(S) = 0 \} \) or, equivalently, \( Y \in \mathcal{D}_r \) iff there exists a GLRR\((A)\) of order \( r \), which governs \( Y \).
- \( Y \in \mathcal{D}_r \) iff there exists a GLRR\((A)\) of order \( r \), which governs \( Y \), and this GLRR is minimal.

2.2. Subspace approach. Let \( \mathcal{Z}(A) \) be the space of time-series of length \( N \) governed by a GLRR\((A)\), \( A \in \mathbb{R}^{r+1} \); that is, \( \mathcal{Z}(A) = \{ S : A^T \mathcal{T}_{r+1}(S) = 0 \} \). Therefore \( \overline{\mathcal{D}}_r = \bigcup_A \mathcal{Z}(A) \).

Let \( Q^{M,d} \) be the operator \( \mathbb{R}^{d+1} \to \mathbb{R}^{M \times (M-d)} \), which is defined by

\[
Q^{M,d}(B) = \begin{pmatrix}
        b_1 & 0 & \cdots & 0 \\
        b_2 & b_1 & 0 & \cdots \\
        \vdots & b_2 & \ddots & 0 \\
        b_{d+1} & \cdots & \cdots & b_1 \\
        0 & b_{d+1} & \cdots & b_2 \\
        \vdots & 0 & \ddots & \vdots \\
        0 & \cdots & 0 & b_{d+1}
\end{pmatrix},
\]

where \( B = (b_1, \ldots, b_{d+1})^T \in \mathbb{R}^{d+1} \). Then the other convenient form of \( \mathcal{Z}(A) \) is \( \mathcal{Z}(A) = \{ S : Q^T(A)S = 0 \} \), where \( Q = Q^{N,r} \); i.e., \( \mathcal{Z}(A) \) is the left nullspace of \( Q(A) \).

The following notation will be used below: \( Q(A) = \text{colspace}(Q(A)) \) and by \( Z(A) \) we denote a matrix whose column vectors form a basis of \( \mathcal{Z}(A) \).

2.3. Parametrization. Consider a series \( S_0 \in \mathcal{D}_r \), which satisfies a minimal GLRR\((A_0)\) of order \( r \) defined by a non-zero vector \( A_0 = (a_0^{(0)}, \ldots, a_{r+1}^{(0)})^T \). Let us fix \( \tau \) such that \( a_0^{(\tau)} \neq 0 \). Since GLRR\((A_0)\) is invariant to multiplication by a constant, we assume that \( a_0^{(0)} = -1 \). This condition on \( \tau \) is considered to be valid hereinafter. Let us build a parametrization of \( \mathcal{D}_r \) in a vicinity of \( S_0 \); parametrization depends on the index \( \tau \).

In the case of a series governed by an ordinary LRR\((A)\), \( A \in \mathbb{R}^{r+1} \), since the last coordinate of \( A \) is equal to -1, the series is uniquely determined by the vector \( A \) containing \( r \) parameters and \( r \) initial values. Then, applying the LRR to initial data, which are taken from the series, we restore this series.

In the case of a series from \( \mathcal{D}_r \), the approach is similar but a bit more complicated. For example, we should take the boundary data \((\tau-1 \text{ values at the beginning, and } r+1-\tau \text{ values at the end}) \) instead of the \( r \) initial values at the beginning of the series; also, the GLRR is not in fact recurrent (we keep notation to show that LRRs are a particular case of GLRRs).

Denote \( I(\tau) = \{1, \ldots, N\} \setminus \{\tau, \ldots, N-r-1+\tau\} \) and \( K(\tau) = \{1, \ldots, r+1\} \setminus \{\tau\} \) two sets of size \( r \). The set \( I(\tau) \) consists of numbers of series values (we call them boundary data), which are enough to find all the series values with the help of \( A \) (more precisely, by elements of \( A \) with numbers from \( K(\tau) \)).

Let \( B_\mathcal{C} \) denote the vector consisting the elements of a vector with the numbers from \( \mathcal{C} \). In particular, \( A_{K(\tau)} \in \mathbb{R}^r \) defines the vector consisting of elements of a vector \( A \in \mathbb{R}^{r+1} \) with the numbers from \( K(\tau) \).
Theorem 2.1 defines the parametrization, which will be used in what follows. From now, the same notation $S$ is used for both the parameterizing mapping and for the series itself.

**Theorem 2.1.** Let $A_0 \in \mathbb{R}^{r+1}$, $a_r^{(0)} = -1$, and $S_0 \in \mathcal{D}_r$ satisfy the GLRR($A_0$). Then there exists a unique one-to-one mapping $S : \mathbb{R}^{2r} \rightarrow \mathcal{D}_r$ between a vicinity of the point $((S_0)_{\mathcal{I}(r)}, (A_0)_{\mathcal{K}(r)})^T \subset \mathbb{R}^{2r}$ and intersection of a vicinity of $S_0$ with the set $\mathcal{D}_r$, which satisfies the following relations:

- for $S = S(S_0(\tau), A(\tau))$, $(S)_{\mathcal{I}(\tau)} = S_0(\tau)$;
- $S \in \mathcal{D}_r$ is governed by the GLRR($A$) such that $A_{\mathcal{K}(\tau)} = A(\tau)$ and $a_r = -1$.

The following proposition presents an explicit form of the parameterizing mapping $S$ from Theorem 2.1. It is convenient to prove Theorem 2.1 and Proposition 2.2 together.

Let us denote $G_C$: the matrix consisting of rows of a matrix $G$ with the numbers from $C$ and $G_{\mathcal{L}}$ the matrix consisting of columns of a matrix $G$ with the numbers from $\mathcal{L}$. In particular, $Z_{\mathcal{I}(\tau),} : \in \mathbb{R}^{r \times r}$ defines the matrix consisting of rows of a matrix $Z \in \mathbb{R}^{N \times r}$ with the numbers from $\mathcal{I}(\tau)$.

**Proposition 2.2.** Let $A_0 \in \mathbb{R}^{r+1}$, $a_r^{(0)} = -1$, and $Z_0 \in \mathbb{R}^{N \times r}$ consist of basis vectors of $Z(A_0)$.

1. Consider $(S_0(\tau), A(\tau))^T \in \mathbb{R}^{2r}$ and define $A \in \mathbb{R}^{(r+1)}$ such that $A_{\mathcal{K}(\tau)} = A(\tau)$ and $a_r = -1$. Denote $\Pi_{Z(A)}$ the orthogonal projection onto $Z(A)$. Then for $Z = \Pi_{Z(A)}Z_0$, $G = Z(Z_{\mathcal{I}(\tau),})^{-1}$, the mapping $S$ introduced in Theorem 2.1, has the explicit form

\[
S(S_0(\tau), A(\tau)) = GS_0(\tau).
\]

2. The mapping, inverse to $S$, is given by the following relations: $S_0(\tau)(S) = (S)_{\mathcal{I}(\tau)}$ and

\[
A(\tau)(S) = (-\hat{A}/\hat{a}_r)_{\mathcal{K}(\tau)},
\]

where $\hat{A} = \hat{A}(S) = (\hat{a}_1, \ldots, \hat{a}_{r+1})^T = (I_{r+1} - \Pi_{\mathcal{L}(S)})A_0$, $\mathcal{L}(S) = \text{colspace}(T_{r+1}(S))$, $\Pi_{\mathcal{L}(S)}$ is the orthogonal projection onto $\mathcal{L}(S)$.

**Proof.** See the proof of this proposition and Theorem 2.1 in Section 8.1.1 of Appendix. □

Thus, for different series $S_0 \in \mathcal{D}_r$, we have different parameterizations of $\mathcal{D}_r$ in vicinities of $S_0$. Moreover, for a fixed $S_0$, there is a variety of parameterizations provided by different choices of the index $\tau$.

**2.4. Smoothness of parametrization and derivatives.**

**Theorem 2.3.** Let $A_0 \in \mathbb{R}^{r+1}$, $a_r^{(0)} = -1$, and $S_0 \in \mathcal{D}_r$ satisfy the GLRR($A_0$). Then the parametrization $S(S_0(\tau), A(\tau))$, which is introduced in Theorem 2.1 and Proposition 2.2, is a smooth diffeomorphism between a vicinity of the point $((S_0)_{\mathcal{I}(\tau)}, (A_0)_{\mathcal{K}(\tau)})^T \subset \mathbb{R}^{2r}$ and intersection of a vicinity of $S_0$ with the set $\mathcal{D}_r$.

**Proof.** See the proof in Section 8.1.2 of Appendix. □

Let us consider derivatives of the parameterizing mapping. Let the series $S$ belong to a sufficient small vicinity of $S_0$ and be parameterized as $S = S(S_0(\tau), A(\tau))$. Denote $J_S = J_S(S_0(\tau), A(\tau)) \in \mathbb{R}^{N \times 2r}$ the Jacobian matrix of $S(S_0(\tau), A(\tau))$.

By definition, the tangent subspace at the point $S$ is $\text{colspace} J_S(S_0(\tau), A(\tau))$, where $S = S(S_0(\tau), A(\tau))$. The tangent subspace is invariant with respect to the choice of a certain parametrization of $\mathcal{D}_r$ in the vicinity of $S$. 


Define by \( A^2 \) the acyclic convolution of \( A \) with itself:

\[
A^2 = (a_i^{(2)}) \in \mathbb{R}^{2r+1}, \quad a_i^{(2)} = \sum_{j=\max(1,i-r)}^{\min(i,r+1)} a_j a_{i-j+1}.
\]

**Theorem 2.4.** The tangent subspace to \( D_r \) at the point \( S \) has dimension \( 2r \) and is equal to \( Z(A^2) \).

_Proof._ See the proof in Section 8.1.3 of Appendix.

### 3. Optimization

Let us consider different methods for solving the problem (1.4). First, note that we search for a local minimum. Then, since the objective function is smooth in the considered parametrization, we can apply the conventional weighted version of the Gauss-Newton method (GN) [23]. This approach appears to be non-stable and has a high computational cost. In [30], the variable-projection method (VP) is used for the solution of the minimization problem. When the reduced minimization problem is solved again by the Gauss-Newton method, we call it VPGN.

We suggest a similar (but different) approach called Modified Gauss-Newton method (MGN), which appears to have some advantages in comparison with VPGN, which is one of the best methods for solution of (1.4); in particular, MGN is more stable.

After a brief discussion of the problem (1.4) we start with the description of the methods GN and VP for a general problem; then we apply these methods to (1.4) and finally present the new method MGN.

Note that the considered methods are used for solving a weighted least-squares problem and therefore we consider there weighted version, omitting ‘weighted’ in their titles.

Let us introduce notation, which is used in this section. Define the weighted pseudoinverse matrix \((F)^\dagger_W = (F^\top W F)^{-1} F^\top W \) for some matrix \( F = \mathbb{R}^{N \times p} \) [26], which arises in the solution of a linear weighted least-squares problem \( \min_P \| Y - FP \|^2_W \) with \( Y \in \mathbb{R}^N \), since its solution is equal to \( P_{\min} = (F)^\dagger_W Y \). In particular case \( W = I_N \) (ordinary pseudoinverse) let us denote \((F)^\dagger_{I_N}\) as \( F^\dagger \). Let us also define the projection (it is oblique if \( W \) is not the identity matrix) onto the column space \( F \) of a matrix \( F \) as \( \Pi_F W = F (F)^\dagger W \). If it is not important which particular basis is considered, then we use the notation \( \Pi_{F,W} \).

#### 3.1. Properties of the optimization problem (1.4)

The following lemma shows that the global minimum of (1.4) belongs to \( D_r \) in the majority of \( X \). Therefore, it is sufficient to find it in the set of series of exact rank \( r \).

**Lemma 3.1.** Let \( X \notin \overline{D_r \setminus D_r} \). Then any point of global minimum in the problem (1.4) belongs to \( D_r \).

_Proof._ See the proof in Section 8.1.4 of Appendix.

Thus, in the chosen parametrization of \( D_r \), the problem (1.4) in the vicinity of \( S_0 \) has the form

\[
Y^* = \arg\min_P \| X - S(P) \|_W,
\]

where \( P = (S(\tau), A(\tau)) \).

Since \( S(P) \) is a differentiable function of \( P \) due to (2.3) for an appropriate choice of \( \tau \), numerical methods like the Gauss-Newton method can be applied for solution of (3.1).

The following theorem helps to detect if the found solution is a local minimum. Recall that \( Z(A^2) \) determines the tangent subspace (Theorem 2.4).
LEMMA 3.2 (Necessary conditions of local minimum). If the series $X_0 \in D$, governed by a GLRR($A_0$), provides a local minimum in (1.4), then $\Pi_{Z(A_0^*)}w(X - X_0) = 0$.

Proof. Let us take appropriate index $\tau$ together with parametrization $S(S(\tau), A(\tau))$ introduced in Theorem 2.1. Objective function $\|X - S(S(\tau), A(\tau))\|_w^2$ is smooth in the vicinity of $((S_0)I(\tau), (A_0)I(\tau))^T \in \mathbb{R}^{2r}$ due to Theorem 2.3.

Substituting an objective function into [23, Theorem 2.2] while considering result of Theorem 2.4 proves the lemma. \qed

Note that Lemma 3.2 provides the necessary condition only. According to [23, Theorem 2.3], sufficient conditions include positive definiteness of the Hessian of the objective function. At the moment, we can check it only numerically.

### 3.2. Methods for solving a general nonlinear least squares problem

Let us $X \in \mathbb{R}^N$ be a given vector and consider a general WLS minimization problem

\[ \arg \min_P \|X - S(P)\|_W^2, \tag{3.2} \]

where $P \in \mathbb{R}^p$ is the vector of parameters, $S : \mathbb{R}^p \to \mathbb{R}^N$ is some parametrization of a subset of $\mathbb{R}^N$, $S(P)$ is a differentiable vector–function of $P$, $W \in \mathbb{R}^{N \times N}$ is a positive definite symmetric matrix.

If the problem (3.2) is non-linear, iterative methods with linearization at each iteration are commonly used, such as Gauss-Newton methods or its variations [23, Section]. One of commonly used variations is the Levenberg-Marquardt method, which is a regularized version of the Gauss-Newton method. This regularization improves the method far from the minimum and does not improve near the minimum. Therefore, in the paper, we consider the Gauss-Newton method. We use a weighted Gauss-Newton method, which is a straightforward extension of the unweighted version.

#### 3.2.1. Gauss-Newton method

One iteration of the Gauss-Newton algorithm with step $\gamma$ is

\[ P_{k+1} = P_k + \gamma (J_S(P_k))^\dagger W (X - S(P_k)), \tag{3.3} \]

where $J_S(P_k)$ is the Jacobian matrix of $S(P)$ at $P_k$.

Choice of the step $\gamma$ is a separate problem. For example, one can start at $\gamma = 1$ and then decrease the step if the next value is worse (that is, the value of the objective functional increases).

An additional aim of the Weighted Least Squares problem is to find the approximation $S(P^*)$ of $X$, where $P^*$ is the solution (3.2). Then we can write (3.3) in the form of iterations of approximations:

\[ S(P_{k+1}) = S(P_k) + \gamma (J_S(P_k))^\dagger W (X - S(P_k)). \tag{3.4} \]

The following remark explains the approach, underlying the Modified Gauss-Newton method proposed in this paper.

**Remark 1.** Iterations (3.4) can be changed by means of the change of $S(P_{k+1})$ to $\tilde{S}(P_{k+1})$, where $\tilde{S}(P_{k+1})$ is such that $\|X - \tilde{S}(P_{k+1})\|_W \leq \|X - S(P_{k+1})\|_W$. This trick is reasonable if $\tilde{S}(P_{k+1})$ can be calculated faster and/or in a more stable way than $S(P_{k+1})$.

#### 3.2.2. Variable projection

Let $P = \begin{pmatrix} B \\ C \end{pmatrix} \in \mathbb{R}^p$, $B \in \mathbb{R}^{p_1}$, $C \in \mathbb{R}^{p_2}$. Consider the (weighted) least-squares problem (3.2), where $S(P)$ is linear in $C$:

\[ S(P) = G(B)C. \tag{3.5} \]
This problem can be considered as a problem of projecting the data vector $X$ onto a given set:

$$
\min_{Y \in \mathcal{D}} \|X - Y\|_W, \quad \text{where} \quad \mathcal{D} = \left\{ G(B)C \mid \begin{pmatrix} B \\ C \end{pmatrix} \in \mathbb{R}^p \right\}.
$$

Here $\{\varphi(z) \mid z \in C\}$ means the set of values of $\varphi(z)$ for $z \in C$. Let us take the advantage of the fact that the solution of the subproblem

$$
C^*(B) = \arg \min_C \|X - G(B)C\|_W
$$

is known: $C^*(B) = (G(B))^\dagger W X$.

Denote $S^*(B) = G(B)C^*(B)$, $\mathcal{G}(B) = \{G(B)C \mid C \in \mathbb{R}^{p_2}\}$. Then

$$(3.6) \quad S^*(B) = \arg \min_{S \in \mathcal{G}(B)} \|X - S\|_W.$$

Thus, we can reduce our problem to projection onto a subset $\mathcal{D}^* \subset \mathcal{D}$:

$$(3.7) \quad \min_{Y \in \mathcal{D}^*} \|X - Y\|_W \quad \text{with} \quad \mathcal{D}^* = \{S^*(B) \mid B \in \mathbb{R}^{p_1}\}.$$

This is called “variable projection” principle (see [12] for the case of the Euclidean norm).

3.3. Known methods for (1.4). Let us turn from a general nonlinear least squares problem (3.2) to our specific problem (1.4) in the form (3.1).

3.3.1. Weighted Gauss-Newton method for (1.4). We consider a modification of the standard Gauss-Newton method, where the parametrization $P = (S_\tau, A_\tau)$ (which is based on $\tau$) is changed at each iteration in a particular way. At $(k + 1)$-th iteration the parametrization is constructed in a vicinity of $A_0 = A^{(k)}$. The index $\tau$, which defines the parametrization, is chosen in such way to satisfy $a_\tau^{(0)} \neq 0$. We suggest the following approach to the choice of $\tau$ to improve the stability of calculations. Let $\tau$ correspond to the maximum absolute value of $A_0$. Since the parametrization is invariant to the multiplication of $A_0$ by a constant, it can be assumed that $a_\tau^{(0)} = -1$ and $|a_i^{(0)}| \leq 1$ for any $i$, $1 \leq i \leq r + 1$.

$$(3.8) \quad P_{k+1} = P_k + \gamma (J_S(P_k))^\dagger W (X - S(P_k)).$$

To apply the method, Jacobian matrix $J_S(P_k)$ and the value $S(S_\tau, A_\tau)$ should be calculated. Formally, these calculations can be implemented; however, the direct calculation is not stable and very time-consuming.

3.3.2. Variable projection for (1.4) (VPGN). Since $S(P)$ for solution of (1.4) has the form (3.5), we can apply the variable projection method. That is, $S(P) = S(S_\tau, A_\tau)$ and according to (2.3), $S_\tau$ is presented in $S(S_\tau, A_{\tau})$ in linear manner.

As well as in (2.3), we consider the problem (1.4) in vicinity of the series $S_0 \in \mathcal{D}_r$ and assume that $S_0$ is governed by GLRR$(A_0)$ with $a_\tau^{(0)} = -1$. Note that in the vicinity of $A_0$, the $A$ is uniquely determined by $A_\tau$; and vice versa ($A_{\tau} \in \mathbb{R}^r$ is extended to $A \in \mathbb{R}^{r+1}$ by supplement of $-1$ at the $\tau$ position).

Substitute in (3.7) $\mathcal{D} = \overline{\mathcal{D}}_r$, $\mathcal{D}^* = \mathcal{D}_r^*, B = A_\tau$, $G(B) = G$, where $G = \left(Z Z_{I_\tau}^{-1} \right)$ (see (2.3)), $C^*(B) = (G)^\dagger W X$, $G(B)C^*(B) = \Pi_{\mathcal{Z}(A)} W(X) \overset{\text{def}}{=} S^*(A_{\tau})$. Then we obtain the
equivalent problem for projection of the elements from the set $\overline{D}_r$ to the subset $D_r^*$, where the parameter $S_{(r)}$ is eliminated:

$$\text{(3.9)} \quad Y^* = \arg \min_{Y \in D_r^*} \|X - Y\|_W \quad \text{with} \quad D_r^* = \{\Pi_{\mathcal{Z}(A)}, w(X) \mid A_{(r)} \in \mathbb{R}^r\}.$$  

Therefore, we can present the problem (3.9) in terms of the parameter $A_{(r)}$ only:

$$\text{(3.10)} \quad A_{(r)}^* = \arg \min_{A_{(r)} \in \mathbb{R}^r} \|X - S^*(A_{(r)})\|_W,$$

Thus, for numerical solution of (1.4), it is sufficient to consider iterations for the nonlinear part of the parameters. This is the approach used in [29, 30].

Let us denote $J_{S^*}(A_{(r)})$ Jacobian matrix of $S^*(A_{(r)})$. Then iterations of the ordinary (weighted) Gauss-Newton method for the problem (3.10) have the form

$$\text{(3.11)} \quad A_{(r)}^{(k+1)} = A_{(r)}^{(k)} + \gamma \left( J_{S^*}(A_{(r)}^{(k)}) \right)^\dagger (X - S^*(A_{(r)}^{(k)})).$$

The explicit form of $J_{S^*}(A_{(r)}^{(k)})$ can be found in (8.2) in Appendix.

### 3.4. Modified Gauss-Newton method for (1.4) (MGN)

In this section we suggest the new iterative method for the problem (1.4), which is a modified Gauss-Newton method.

Let us return to the problem with full set of parameters $(S_{(r)}, A_{(r)})$ and apply the approach, which is described in Remark 1, with $\overline{S}(P) = S^*(A_{(r)}) = S^*(A_{(r)})$. We can do it, since (3.6) is valid with $\mathcal{G}(A) = \mathcal{Z}(A)$. Thus, we can consider $S^*(A_{(r)}^{(k+1)}) \in D_r^*$ as the result of the $(k+1)$th iteration instead of $S^*(A_{(r)}^{(k+1)}) \in \overline{D}_r$. It appears (see Section 4) that then we can perform more stable calculations. The suggested modification is similar to variable projections, since we can omit a part of parameters $S_{r_{(r)}}$ and obtain the following iterations:

$$\text{(3.12)} \quad A_{(r)}^{(k+1)} = A_{(r)}^{(k)} + \gamma \left( J_{S^*}(S_{(r)}^{(k)}, A_{(r)}^{(k)}) \right)^\dagger (X - S^*(A_{(r)}^{(k)})),$$

where $S_{(r)}^{(k)}$ are taken as corresponding boundary values of $S^*(A_{(r)}^{(k)})$.

As well as in the Variable Projection method with iterations (3.11), $S^*(A_{(r)}^{(k+1)}) \in D_r^*$ for each $k$.

The following theorem presents the form of iterations (3.12), which is suitable for stable implementation.

**Theorem 3.3.** The iterations (3.12) are equivalent to

$$\text{(3.13)} \quad A_{(r)}^{(k+1)} = A_{(r)}^{(k)} + \gamma M_k Q^T(A_{(r)}^{(k)}) \Pi_{\mathcal{Z}(A^{(k)})}, w(X - \Pi_{\mathcal{Z}(A^{(k)})}, w(X))$$

and $S_{k+1} = S^*(A_{(r)}^{(k+1)})$, $M_k = -S_{(r)}^{(k+1)}$, where $S = \mathcal{T}_{r+1}(S^*(A_{(r)}))$ is the $(r+1)$-trajectory matrix of $S^*(A_{(r)}^{(k)})$.

**Proof.** See the proof in Section 8.1.5 of Appendix. \qed

Thus, we constructed the modification (3.13) of the iterations (3.12) in such way that to reduce its complexity to computation of projections to $\mathcal{Z}(A)$ and $\mathcal{Z}(A^2)$. Algorithms for their computation is described in Section 4. The whole algorithm of the suggested MGN method is described in Algorithm 5.5.
4. Calculation of $Z(A)$ and $Z(A^2)$. For implementation of the iteration step (3.13) of the suggested optimization algorithm MGN, we need effective algorithms of calculation of orthonormal bases of $Z(A)$ and $Z(A^2)$, where $Z(B)$ is the space of series governed by GLRR($B$). Note that we can also use the obtained algorithms to improve stability of iteration step (3.11) of the VPGN method. As before, we denote $Z(B)$ a matrix, whose columns form a basis of $Z(B)$. In this section, we consider construction of an orthonormal basis to calculate the projections in (3.13) with improved precision.

4.1. Circulant matrices and construction of $Z(A)$. Let us start with the construction of $Z(A)$. Despite the series are real-valued, we construct a complex-valued basis, since this does not affect bases of $Z$. As before, we denote $Z$ $(\sum_{j=0}^{N-1} x_j e^{-\frac{i2\pi kj}{N}})$ with improved precision.

$Z(A)$ can be rank-deficient; e.g. in the case of the linear series when $A = (1, -2, 1)^T$. Lemma 4.1 shows that the leading coefficient is non-zero.

Then $V \in Z(A)$ iff $C(A)V \in \text{span}(e_{N-r+1}, \ldots, e_N)$. If $C(A)$ has full rank, then we can find the basis vectors $V_k$ by solving the systems of linear equations $C(A)V_k = e_{N-k+1}$, $k = 1, \ldots, r$, with the help of the Fourier transform [6], and then applying orthonormalization to $V_r = [V_1 : \ldots : V_r]$.

Denote $F_N$ and $F_N^{-1}$ the Fourier transform and inverse Fourier transform for series of length $N$, respectively. That is, if define $X = (x_0, \ldots, x_{N-1})^T \in \mathbb{C}^N$ and $F_N(X) = Y = (y_0, \ldots, y_{N-1})^T \in \mathbb{C}^N$, then $y_k = \frac{1}{\sqrt{N}} \sum_{j=0}^{N-1} x_j \exp(-\frac{2\pi i j k}{N})$. Define the (inverse) Fourier transform applied to a matrix as the matrix consisting of (inverse) Fourier transforms of columns. That is, $F_N(X) = [F_N(X_1) : \ldots : F_N(X_r)]$, where $X = [X_1 : \ldots : X_r]$; the same for $F_N^{-1}(Y)$.

Define $g_A(z) = \sum_{k=0}^{r} a_k z^k$ the complex polynomial with coefficients $A = (a_1, \ldots, a_{r+1})^T$; we do not assume that the leading coefficient is non-zero.

The following lemma is the direct application of the theorem about the solution of a linear system of equation given by a circulant matrix [6].

**Lemma 4.1.** Denote $V_r = F_N^{-1}(A_g^{-1}R_r)$, where $R_r = F_N([e_{N-r} : \ldots : e_N])$ and $A_g = \text{diag}((g_A(\omega_0), \ldots, g_A(\omega_{N-1}))^T)$ for $\omega_j = \exp(\frac{2\pi i j}{N})$. Then $Q^T(A)V_r = 0$. Herewith, the diagonal of the matrix $A_g$ consists of the eigenvalues of the circulant matrix $C(A)$.

Remark 2. 1. We can take the matrix $Z$, $Q^T(A)Z = 0$, with orthonormalized columns by orthonormalization of the columns of $V_r$ defined in Lemma 4.1. Let us write it as $Z = \text{orthonorm}(V_r)$.

2. Since $F_N^{-1}$ is a transformation which keeps orthonormality, the matrix calculated as $Z = F_N^{-1}(\text{orthonorm}(A_g^{-1}R_r))$ has orthonormal columns.

4.2. Condition improvement of circulant matrix. However, $C(A)$ can be rank-deficient; e.g. in the case of the linear series when $A = (1, -2, 1)^T$. Lemma 4.1 shows that the eigenvalues
of \( C(A) \) are values of the polynomial \( g_A(z) \) in the nodes of equidistant grid on the complex unit circle \( \mathbb{T} \): \( \mathcal{W} = \{ \exp(\frac{2\pi i}{N}), \ j = 0, \ldots, N - 1 \} \), \( \mathbb{T} = \{ z \in \mathbb{C} : |z| = 1 \} \), \( \mathcal{W} \subset \mathbb{T} \). Therefore, nondegeneracy of \( C(A) \) is equivalent to that there are no roots of the polynomial \( g_A(z) \) in \( \mathcal{W} \).

The following theorem helps to avoid the problem with zero eigenvalues. Let us define unitary matrix \( T_M(\alpha) = \text{diag}(1, e^{i\alpha}, \ldots, e^{i(M-1)\alpha})^T \), where \( \alpha \) is a real number.

**Lemma 4.2.** Let \( \alpha \) be a real value. If a series \( X \) satisfies GLRR(\( A \)), then the series \( \tilde{X} = T_N(\alpha)X \) satisfies the GLRR(\( \tilde{A}(\alpha) \)), where \( \tilde{A}(\alpha) = (T_{r+1}(-\alpha))A \). Moreover, if a series \( Y \) satisfies GLRR(\( A^2 \)), then the series \( \tilde{Y} = T_N(\alpha)Y \) satisfies the GLRR(\( (\tilde{A}(\alpha))^2 \)). In addition, the eigenvalues of \( C(\tilde{A}) \) are equal to \( g_{\tilde{A}}(\omega_j) = g_A(\tilde{\omega}_j) \), where \( \tilde{\omega}_j = \omega_je^{-i\alpha} \).

**Proof.** The lemma is proved by direct calculation and the following observation \( g_{A^2}(z) = (g_A(z))^2 \).

**Remark 3.** Let us take \( \alpha \in \mathbb{R}, -\pi/N < \alpha \leq \pi/N \) (since \( \alpha \) and \( \alpha + 2\pi/N \) yield the same results) such that \( C(\tilde{A}(\alpha)) \) is non-degenerate, and calculate an orthonormal basis \( \tilde{Z} \) using Lemma 4.1 such that \( Q^T(\tilde{A})\tilde{Z} = 0 \). Then \( Z = (T_N(-\alpha))\tilde{Z} \) is orthonormal matrix such that \( Q^T(A)Z = 0 \). Similarly, for \( \tilde{Z}_2 \) such that \( Q^T(\tilde{A}^2)\tilde{Z}_2 = 0 \), \( Z_2 = (T_N(-\alpha))\tilde{Z}_2 \), we have \( Q^T(A^2)Z_2 = 0 \).

The equality \( g_{\tilde{A}}(\omega_j) = g_A(\tilde{\omega}_j) \) means that the eigenvalues of \( C(\tilde{A}(\alpha)) \) can be calculated as values of the polynomial \( g_A(\omega) \) in \( \omega \in \mathcal{W}(\alpha) = \{ \omega_j^{\alpha}, \ j = 0, \ldots, N - 1 \} \), where \( \omega_j^{\alpha} = \exp(i \left( \frac{2\pi i}{N} - \alpha \right)) \), \( \mathcal{W}(\alpha) \) is rotated equidistant grid on \( \mathbb{T} \). Therefore, \( C(\tilde{A}(\alpha)) \) can be non-degenerate by choosing suitable \( \alpha \).

The aim of the choice of \( \alpha \) is to do the condition number of \( C(\tilde{A}(\alpha)) \) as small as possible. This can be approximately reduced to the problem of maximization of the smallest eigenvalue \( |\lambda_{\min}(\alpha)| = \min_{z \in \mathcal{W}(\alpha)} |g_A(z)| \) of \( C(\tilde{A}(\alpha)) \), since the maximal eigenvalue is not greater than \( \max_{z \in \mathbb{T}} |g_A(z)| \). In the exact arithmetic, any non-zero smallest eigenvalue corresponds to non-degeneracy. However, in practice, we need to do the condition number as small as possible for stability and accuracy of calculations.

**4.3. Algorithm.** By combining Lemmas 4.1, 4.2 with Remarks 2, 3, we obtain the Algorithm 4.1 of calculating \( Z \).

**Algorithm 4.1** Calculation of a basis of \( Z(A) \)

1. Find \( \alpha_0 = \text{arg} \max_{-\pi/N \leq \alpha < \pi/N} \min_{z \in \mathcal{W}(\alpha)} |g_A(z)| \) by means of a 1D numerical optimization method.
2. Calculate the vector \( A_g = (a_g,0, \ldots, a_g,N-1)^T \) consisting of eigenvalues of \( C(\tilde{A}) \) as \( a_g,j = g_A(\exp(i \left( \frac{2\pi j}{N} - \alpha_0 \right))) \), \( j = 0, \ldots, N - 1 \).
3. Calculate matrices \( R_r = \mathcal{F}(e_{N-r+1} : \ldots, e_N) \), \( L_r = A_g^{-1}R_r \), where \( A_g = \text{diag} A_g \).
4. Find a matrix \( U_r \in \mathbb{C}^{N \times r} \) consisting of orthonormalized columns of the matrix \( L_r \) (e.g., \( U_r \) can consist of the \( r \) leading left singular vectors of \( L_r \)).
5. Compute \( \tilde{Z} = \mathcal{F}^{-1}(U_r) \).
6. **Return** Matrix \( Z = (T_N(-\alpha_0))\tilde{Z} \), whose columns form an orthonormal basis of \( Z(A) \).

The multiplication in this algorithm can be viewed as a multiplication by a \( z \)-circulant matrix (see https://eudml.org/doc/275637), which is often used for inversion of structured matrices, but with different \( z \).

**4.4. Computational properties of an algorithm.** Let us discuss computational properties of the constructed algorithm. The following theorem shows the order of \( |\lambda_{\min}(\alpha)| \) (and therefore the order of the condition number of a matrix to be inverted) with respect to \( \alpha \) in dependence on the series length \( N \).
Theorem 4.3. Let $t$ be the maximal multiplicity of roots of the polynomial $g_A(z)$ on the unit circle $\mathbb{T}$. Let $\lambda_{\min}(\alpha)$ be the minimal eigenvalues of $C(\tilde{A}(\alpha))$.

1. For any real sequence $\alpha(N)$, $|\lambda_{\min}(\alpha)| = O(N^{-t}).$
2. For any sufficiently large $N$ there exists such real $\alpha(N)$ that $|\lambda_{\min}(\alpha)| = \Theta(N^{-t}).$

Proof. See the proof in Section 8.1.6 of Appendix.

Theorem 4.3 shows that the order $N^{-t}$ can be reached and it is the exact order.

Let us turn to the calculation of $Z(A^2)$. Note that $g_{A^2}(z) = (g_A(z))^2$; this helps to construct more precise algorithm than Algorithm 4.1 applied to $A^2$. Algorithm 4.2 is constructed taking into account Remark 4.

Remark 4. Let us apply Lemma 4.1 to GLRR($A^2$): denote $R_{2r} = F_N([e_{N-2r+1} : \ldots : e_N])$, $L_{2r} = A_g^{-2}R_{2r}$, $V_{2r} = F_N^{-1}L_{2r}$. Also, apply the approach from Remark 2 to GLRR($A^2$). Since $Z(A) \subset Z(A^2)$, we have that colspace $V_r \subset$ colspace $V_{2r}$ and therefore colspace $L_r \subset$ colspace $L_{2r}$. Thus, the orthonormalization of the ill-conditioned matrix $L_{2r}$ can be changed to orthonormalization of the matrix $(I_N - \Pi_{U_r,1_N})L_{2r}$ of rank $r$; the latter can be implemented in a stable way due to orthonormalization of $L_r$ (with the result $U_r$), which has been performed in Algorithm 4.1.

Algorithm 4.2 Calculation of a basis of $Z(A^2)$

1. Compute $\alpha_0$, $A_g$, $U_r$ in the same way as in Algorithm 4.1
2. Calculate $R_{2r} = F_N([e_{N-2r+1} : \ldots : e_N])$, $L_{2r} = A_g^{-2}R_{2r}$
3. Calculate $\tilde{L}_{2r} = (I_N - \Pi_{U_r,1_N})L_{2r}$
4. Find a matrix $U_{2r} \in \mathbb{C}^{N \times r}$ consisting of orthonormalized columns of the matrix $\tilde{L}_{2r}$ (e.g, $U_{2r}$ can consist of the $r$ leading left singular vectors of $\tilde{L}_{2r}$).
5. Compute $\tilde{Z}_2 = F_N^{-1}[U_r : U_{2r}]$
6. return Matrix $Z = (T_N(-\alpha_0))\tilde{Z}_2$, whose columns form an orthonormal basis of $Z(A^2)$.

Since the system of linear equations with a circulant matrix is reduced to the system of linear equations with a diagonal matrix, Algorithm 4.2 is implemented with the same order of stability as Algorithm 4.1.

The following remarks are related to possible improvement of the suggested algorithms.

Remark 5. Calculation of bases of $Z(A)$ and $Z(A^2)$ is an ill-conditioned problem if the polynomial $g_A(z)$ has roots close to the unit circle $\mathbb{T}$, see Theorem 4.3. Therefore, Algorithms 4.1 and 4.2 can give unstable results in practice. We suggest to use error-free arithmetics and compensated Horner scheme [14, Algorithm CompHorner]. Details can be found in Appendix (Section 8.3).
5. Algorithms of Modified Gauss-Newton and Variable Projection Gauss-Newton methods.

5.1. Calculation of weighted projection to subspaces with a given basis. The MGN (3.13) and VPGN (3.11) methods use projections $\mathbf{I}_Z \mathbf{W} \mathbf{X}$, where a matrix $Z$ belongs to $\mathbb{R}^{N \times r}$ or $\mathbb{R}^{N \times 2r}$. We assume that if the matrix $W$ is $(2p + 1)$-diagonal, then it presented in the form of Cholesky decomposition $W = C^T C$; here $C$ is an upper triangular matrix with $(p + 1)$ diagonals. If however $W^{-1}$ is $(2p + 1)$-diagonal, then we consider the representation $W = \hat{C}^{-1}(\hat{C}^{-1})^T$, where $W^{-1} = \hat{C}^T \hat{C}$ is the Cholesky decomposition of $W^{-1}$.

Remark 6. As we mentioned in Section 3.2.1, calculation of $(CZ)^\dagger$ or $(\hat{C})^{-1}Z^\dagger$ is reduced to solution of weighted least-squares method and therefore can be performed with the help of the QR or SVD decomposition of the matrix $CZ$ or $(\hat{C})^{-1}Z$ respectively.

Algorithm 5.1 Calculation of $\mathbf{I}_Z \mathbf{W} \mathbf{X}$ with the help of $W = C^T C$ or $W^{-1} = \hat{C}^T \hat{C}$

1: if $W$ is $(2p + 1)$-diagonal then
2: Compute the vector $CX$ and the matrix $CZ$
3: Calculate $Q = (CZ)^\dagger(CX)$, see Remark 6
4: end if
5: if $W^{-1}$ is $(2p + 1)$-diagonal then
6: Compute the vector $(\hat{C}^{-1})^T X$ and the matrix $(\hat{C}^{-1})^T Z$
7: Calculate $Q = ((\hat{C}^{-1})^T Z)^\dagger((\hat{C}^{-1})^T X)$, see Remark 6
8: end if
9: return Return $ZQ$

5.2. Calculation of $\mathbf{I}_{Z(A)} \mathbf{W} \mathbf{X}$. Calculation of $\mathbf{I}_{Z(A)} \mathbf{W} \mathbf{X}$ can be performed with the use of specific features of $Z(A)$ (see Section 4) and without them, as it is suggested in [30].

Let us start from the algorithm used in [30]. Calculation of $\mathbf{I}_{Z(A)} \mathbf{W} \mathbf{X}$ in [30] is performed by means of the relation (8.1); it needs computation of matrices $\Gamma(A)$ and $\Gamma(A)^{-1}$. Below we write down the algorithm, which was used in the paper [30], with fast computation of $\Gamma(A)$ and the inverse.

Algorithm 5.2 Calculation of $\mathbf{I}_{Z(A)} \mathbf{W} \mathbf{X}$ by the method from [30]

1: Calculate $(r + p + 1)$-diagonal matrix $\hat{C}Q(A)$
2: Calculate $(2r + 2p + 1)$-diagonal matrix $\Gamma(A) = (\hat{C}Q(A))^\dagger(\hat{C}Q(A))$
3: Calculate $(p + r + 1)$-diagonal Cholesky decomposition of the matrix $\Gamma(A)$ for multiplication of $\Gamma(A)^{-1}$ by a vector form right-side.
4: return Return the result of (8.1) (see Appendix)

The theory described in Section 4 gives us an opportunity to improve Algorithm 5.2.

Algorithm 5.3 Calculation of $\mathbf{I}_{Z(A)} \mathbf{W} \mathbf{X}$ with the use of special properties of $Z(A)$

1: Compute the matrix $Z(A)$ consisting of basis vectors of $Z(A)$ by Algorithm 4.1 (or Algorithm 8.1 if an improved precision is necessary).
2: return Calculate $\mathbf{I}_{Z(A)} \mathbf{W} \mathbf{X}$ by means of Algorithm 5.1

The key difference between algorithms 5.3 and 5.2 is the usage of nullspace of matrix $Q(A)$, which is $Z(A)$, instead of image, which is $Q(A)$. 
5.3. VPNGN algorithm. Algorithm 5.4 implements the Gauss-Newton method for iterations (3.11), which were obtained in [30] by the Variable Projection approach. Note that the fast implementation of the suggested algorithm (calculation of $\Pi_{Z(A)}^\mathbf{w}$) is available if $\mathbf{W}^{-1}$ is $(2p + 1)$-diagonal.

Algorithm 5.4 Gauss-Newton method by Variable Projection and calculation of $S^*$ from [30] (VPGN)

1: Input: the series $\mathbf{X}$, the GLRR($A_0$)  
2: Find $\tau = \arg\max_{\sigma} \left|a^{(0)}_{\sigma}\right|$  
3: Calculate $S_0 = S^*(A^{(0)}_{\tau})$  
4: Set $k = 0$  
5: while Not STOP do  
6: Calculate $J_{S^*}(A^{(k)}_{\tau})$ by (8.2) with the help of steps 1–3 of Algorithm 5.2.  
7: Calculate $\Delta_k = (J_{S^*}(A^{(k)}_{\tau}))^\dagger \mathbf{w}(\mathbf{X} - S_k)$ by Algorithm 5.1.  
8: Find $\gamma_k = \arg\min_{0 \leq \gamma \leq 1} \|\mathbf{X} - S_k(A^{(k)}_{\tau} + \gamma \Delta_k)\|_W$ by a numerical 1D optimization method  
9: Set $A^{(k+1)}_{\tau} = A^{(k)}_{\tau} + \gamma_k \Delta_k$, $a^{k+1}_{\tau} = a^k_{\tau}$  
10: Calculate $S_{k+1} = S^*(A^{(k+1)}_{\tau})$  
11: Set $k = k + 1$  
12: end while  
13: return the series $S_k$

Note that $S^*(A^{(k)}_{\tau}) = \Pi_{Z(A^{(k)}_{\tau})}^\mathbf{w}$ can be calculated by either Algorithm 5.2 or Algorithm 5.3. The former algorithm is abbreviated as VPGN, while the latter algorithm is more stable and is abbreviated as S-VPGN.

5.4. Modified Gauss-Newton algorithm. Algorithm 5.5 implement iterations (3.13) of Modified Gauss-Newton algorithm, which is suggested in the paper.

Algorithm 5.5 Modified Gauss-Newton method (MGN)

1: Input: the series $\mathbf{X}$, the GLRR($A_0$)  
2: Find $\tau = \arg\max_{\sigma} \left|a^{(0)}_{\sigma}\right|$  
3: Calculate $S_0 = S^*(A^{(0)}_{\tau})$  
4: Set $k = 0$  
5: while Not STOP do  
6: Calculate $Z(\mathbf{(X^{(k)})^2})$ by Algorithm 4.2 (or 8.2 if an improved precision is necessary  
7: Calculate $\Delta_k = M_k^{k} \Pi_{Z(\mathbf{(X^{(k)})^2})}^\mathbf{w}(\mathbf{X} - S_k)$ by Algorithm 5.1.  
8: Find $\gamma_k = \arg\min_{0 \leq \gamma \leq 1} \|\mathbf{X} - S_k(A^{(k)}_{\tau} + \gamma \Delta_k)\|_W$ by a numerical 1D optimization method  
9: Set $A^{(k+1)}_{\tau} = A^{(k)}_{\tau} + \gamma_k \Delta_k$, $a^{k+1}_{\tau} = a^k_{\tau}$  
10: Calculate $S_{k+1} = S^*(A^{(k+1)}_{\tau})$  
11: Set $k = k + 1$  
12: end while  
13: return The series $S_k$

6. Comparison of algorithms. Let us compare Algorithms 5.4 and 5.5. For convenience, we present in Table 1 correspondence between notation used in this paper and notation from [29, 30].

6.1. Comparison by computational costs.

6.1.1. Design of comparison. We consider three algorithms:
Table 1
Correspondence between notation

| This paper     | Usevich & Markovsky |
|----------------|---------------------|
| X              | pD, nD              |
| N              | m, d                |
| r + 1          | n, R                |
| 1              | W                   |
| N − r          | Γ(A)                |

1. Method VPGN, where the projection is calculated by Algorithm 5.2 and the iteration step by Algorithm 5.4
2. Method S-VPGN, where the projection is calculated by Algorithm 5.3 and the iteration step by Algorithm 5.4
3. The suggested method MGN, where the projection is calculated by Algorithm 5.3 and the iteration step by Algorithm 5.5

6.1.2. Comparison of computational costs of Algorithms 5.2 and 5.3. Let us estimate the computational costs. We will calculate asymptotic costs as $N \to \infty$. Note that the cost of search of optimal rotation (optimal $\alpha_0$) in step 1 of Algorithm 4.1 is not included in the asymptotic cost of Algorithm 5.3.

- Let $W^{-1}$ be $(2p + 1)$-diagonal.
  Asymptotic cost of Algorithm 5.3 is $O(Nr^2 + Np^2 + rN \log N)$, since Algorithms 4.1 and 8.1 require $O(rN \log N + Nr^2)$, the calculation of projection by Algorithm 5.1 needs $O(Nr^2 + Np^2)$, the least-square method by means of the QR-decomposition takes $O(Nr^2)$ operations.
  Asymptotic cost of Algorithm 5.2 is $O(Nr^2 + Np^2)$.

- Let $W$ be $(2p + 1)$-diagonal, $p > 0$.
  Asymptotic cost of Algorithm 5.3 is $O(Nr^2 + Np^2 + rN \log N)$, analogously. There is no implementation of Algorithm 5.2 with linear in $N$ asymptotic complexity, since $\Gamma(A)$ is not a banded matrix.

6.1.3. Comparison of computational costs of Algorithms 5.5 and 5.4. Asymptotics for computational costs of one iteration of Algorithms 5.5 and 5.4 are as follows.

- Let $W^{-1}$ be $(2p + 1)$-diagonal.
  Asymptotic cost of one iteration of Algorithm 5.5 is $O(Nr^2 + Np^2 + rN \log N)$, since Algorithms 4.2 and 8.2 require $O(rN \log N + Nr^2)$, calculation of projection by Algorithm 5.1 needs $O(Nr^2 + Np^2)$; the least-square method by the QR-decomposition takes $O(Nr^2)$ operations.
  Asymptotic cost of one iteration of Algorithm 5.4 is $O(Nr^2 + Np^2)$; we takes into account that the Cholesky decomposition of the matrix $\Gamma(A_k)$ is performed once (for iteration) and requires $O(Nr^2 + Np^2)$, multiplication of $\Gamma^{-1}(A_k)$ by a vector costs $O(N(r + p))$.

- Let $W$ be $(2p + 1)$-diagonal, $p > 1$.
  Asymptotic cost of one iteration of Algorithm 5.5 is $O(Nr^2 + Np^2 + rN \log N)$, analogously.
  There is no implementation of Algorithm 5.4 with linear in $N$ asymptotic complexity, since $\Gamma(A)$ is not a banded matrix.

Thus, if the inverse weighting matrix $W^{-1}$ is $(2p + 1)$-diagonal, then the computational cost of the suggested MGN method is slightly larger in comparison with the VPGN method. However, if the weighting matrix itself $W$ is $(2p + 1)$-diagonal (this is the case of auto-regressive noise and therefore a natural assumption), then the computational cost of the MGN method is smaller by order.

6.2. Numerical comparison of optimization algorithms by stability. Let us construct an example, where a local solution of (1.4) is known, based on Lemma 3.2.
Lemma 6.1. Let $Y_N^\ast = (c_1x_1^2, \ldots, c_Nx_N^2)^T$, where $x_i$ is the equidistant grid at $[-1; 1]$ and $c_1$ is such that $\|Y_N^\ast\| = 1$, and $N_N = (c_3|x_1|, \ldots, c_3|x_N|)^T$ such that $\|\hat{N}_N\| = 1$. Then for $X_N = Y_N^\ast + N_N$, where $N_N = \hat{N}_N - \Pi_{Z(A_0^2)}w\hat{N}_N$, the solution of the problem (1.4) is achieved at $Y_N^\ast$.

We want to compare algorithms for solution of (1.4) by accuracy. To do it, we should generate the series $X_N$ numerically with high precision. The main difficulty is in calculation of $\Pi_{Z(A_0^2)}w$. The series $Y_N^\ast$ is governed by GLRR($A_0$), where $A_0 = (1, -3.3, -1)^T$. The GLRR($A_0$) governs polynomials of degree not greater than 2 [13]. Basis of $Z(A_0^2)$ consists of polynomials of degree from 0 to 5. Therefore, to calculate the projection, we use Legendre polynomials [2] of degree from 0 to 5 calculated in points $x_i$. Then the constructed basis is orthogonalized.

For simplicity, consider non-weighted case, when $W$ is the identity matrix. The comparison is performed for the methods VPGN, S-VPGN and MGN (see Section 6.1.1 for abbreviation description) for different $N$ from 20 to 50000; the compensated Horner scheme is used within the algorithms. Denote $\tilde{Y}^\ast$ the result of an algorithm participating in the comparison.

The main comparison was done by accuracy, that is, by Euclidean distance between $\tilde{Y}^\ast$ and $Y_N^\ast$. Additionally, we checked if the obtained solution $\tilde{Y}^\ast$ satisfies the final GLRR($A^\ast$), used in the algorithm. The measure of correspondence with the GLRR($A^\ast$) is the relative residual $\frac{\|Q^T(A^\ast)\tilde{Y}^\ast\|}{\|A^\ast\|}$.

The compared algorithms contain a method of local search in the direction $\Delta_k$. The method and the stopping criteria are not specified in the algorithms. The details of the used method are described in Appendix. It is important that the method together with the stopping criterion is stable with respect to the calculation precision.

All algorithms started from the GLRR($A$), where $A = A_0 + 10^{-6}(1, 1, 1, 1)^T$. The results for distance to $Y_N^\ast$ are shown in Figure 1. The relative residuals are presented in Figure 2.

All three methods converged to the vicinity of $Y_N^\ast$. Algorithm S-VPGN does not show a significant improvement in the distance to the solution if we compare with VPGN; Algorithm MGN has considerably higher accuracy. Comparison by relative residuals shows that the algorithms S-VPGN and MGN are similar and considerably better than the algorithm VPGN.
Fig. 1. Comparison of algorithms by distance to the solution, for different $N$.

Fig. 2. Comparison of algorithms by relative residuals, for different $N$. 
7. Conclusion. In the paper we presented a new iterative algorithm (MGN, Algorithm 5.5) for numerical solution of the problem (1.4) and compared it with a state-of-art algorithm based on the variable projection approach (VPGN, Algorithm 5.4). We showed that the suggested algorithm MGN allows the implementation, which is more stable for the case of multiple roots of the characteristic polynomial (in particular, for polynomial series, where the multiplicity is equal to the polynomial degree plus one). This effect can be explained by the inversion of matrices with conditional number $O(N^t)$ in MGN (Theorem 4.3), where $t$ is the multiplicity, while the direct implementation of VPGN deals with matrices with conditional number $O(N^{2t})$ [30, Section 6.2]. Comparison of computational costs in Section 6.1.2 shows that the algorithm MGN has slightly larger costs for the case of banded inverse weighting matrix $W^{-1}$. However, in the case of autoregressive noise with covariance matrix $\Sigma$, the corresponding weighting matrix $W = \Sigma^{-1}$ is banded itself and $W^{-1}$ is not banded. Then the suggested algorithm MGN has much smaller computational cost than VPGN.

To construct and justify the new algorithm, properties of the space of series of finite rank were studied. These properties can be useful not only in the framework of the algorithm justification. In particular, we proved (Theorem 2.4) that the tangent subspace in the point $S$, which is governed by GLRR($A$), can be described in terms of GLRR($A^2$). This fact allows to construct first-order linear approximations to functions in a point from $D_r$. Then, in Section 4 we present a stable algorithm of projection of a series to the set $Z(A)$ of series, which are governed by the GLRR($A$). This can be useful for numerical solutions of different approximation problems related to the HLRA problems.
REFERENCES

[1] F. Andersson and M. Carlsson, Alternating projections on non-tangential manifolds, (2011), https://arxiv.org/abs/arXiv:1107.4055v1.
[2] S. L. Belousov, Tables of Normalized Associated Legendre Polynomials: Mathematical Tables Series, Pergamon, 2014.
[3] J. Cadzow, 1988, signal enhancement—a composite property mapping algorithm: Ieee transactions on acoustics, speech and signal processing, 36, 49–62. (1988).
[4] M. T. Chu, R. E. Funderlic, and R. J. Plemmons, Structured low rank approximation, Linear Algebra and its Applications, 366 (2003), pp. 157 – 172. Special issue on Structured Matrices: Analysis, Algorithms and Applications.
[5] L. Condat and A. Hirabayashi, Cadzow denoising upgraded: A new projection method for the recovery of dirac pulses from noisy linear measurements, Sampling Theory in Signal and Image Processing, 14 (2015), pp. 17–47.
[6] P. J. Davis, Circulant matrices, American Mathematical Soc., 2012.
[7] B. De Moor, Total least squares for affinely structured matrices and the noisy realization problem, IEEE Transactions on Signal Processing, 42 (1994), pp. 3104–3113.
[8] M. Dendrinos, S. Bakamidis, and G. Carayannis, Speech enhancement from noise: A regenerative approach, Speech Communication, 10 (1991), pp. 45–57, https://doi.org/10.1016/0167-6393(91)90027-q.
[9] J. Gillard and A. Zhigljavsky, Stochastic methods for hankel structured low rank approximation, in Proceedings of 21th International Symposium on Mathematical Theory of Networks and Systems, 2014, pp. 961–964.
[10] J. Gillard and A. Zhigljavsky, Weighted norms in subspace-based methods for time series analysis, Numerical Linear Algebra with Applications, 23 (2016), pp. 947–967.
[11] N. Gillis and F. Glineur, Low-rank matrix approximation with weights or missing data is np-hard, SIAM J. Matrix Anal. Appl., 32 (2011), pp. 1149–1165, https://doi.org/10.1137/110820361.
[12] G. Golub and V. Pereyra, Separable nonlinear least squares: the variable projection method and its applications, Inverse problems, 19 (2003), p. R1.
[13] N. Golyandina, V. Nekrutkin, and A. Zhigljavsky, Analysis of Time Series Structure: SSA and Related Techniques, Chapman&Hall/CRC, 2001.
[14] S. Graillat and V. Ménissier-Morain, Compensated horner scheme in complex floating point arithmetic, in Proceedings of the 8th Conference on Real Numbers and Computers, Santiago de Compostela, Spain, 2008, pp. 133–146.
[15] M. Hall, Combinatorial Theory, Wiley-Interscience, 1998.
[16] G. Heing and Rost, Algebraic Methods for Toeplitz-like Matrices and Operators (Operator Theory: Advances and Applications), Birkhäuser Verlag, 1985.
[17] A. Iarrobino, A. Iarrobino, V. Kanev, and S. Kleiman, Power Sums, Gorenstein Algebras, and Determinantal Loci, Lecture Notes in Mathematics, Springer Berlin Heidelberg, 1999.
[18] M. Ishteva, K. Usevich, and I. Markovsky, Factorization approach to structured low-rank approximation with applications, SIAM Journal on Matrix Analysis and Applications, 35 (2014), pp. 1180–1204.
[19] P. Lemmerling, N. Mastronardi, and S. Van Huffel, Fast algorithm for solving the hankel/toeplitz structured total least squares problem, Numerical Algorithms, 23 (2000), pp. 371–392, https://doi.org/10.1023/A:1019116520737.
[20] I. Markovsky, Structured low-rank approximation and its applications, Automatica, 44 (2008), pp. 891–909, https://doi.org/10.1016/j.automatica.2007.09.011.
[21] I. Markovsky, Low Rank Approximation: Algorithms, Implementation, Applications (Communications and Control Engineering), Springer, 2011.
[22] I. Markovsky, J. C. Willems, S. Van Huffel, and B. De Moor, Exact and approximate modeling of linear systems: A behavioral approach, vol. 11, SIAM, 2006.
[23] J. Nocedal and S. Wright, Numerical Optimization, Springer Science & Business Media, 2006.
[24] G. Ottaviani, P.-J. Spaenlehauer, and B. Sturmfels, Exact solutions in structured low-rank approximation, SIAM Journal on Matrix Analysis and Applications, 35 (2014), pp. 1521–1542, https://doi.org/10.1137/13094520X.
[25] E. Schost and P.-J. Spaenlehauer, Newton-like iteration for determinantal systems and structured low rank approximation, ACM Commun. Comput. Algebra, 47 (2014), pp. 96–97, https://doi.org/10.1145/2576802.2576811, http://doi.acm.org/10.1145/2576802.2576811.
[26] G. Stewart, On scaled projections and pseudoinverses, Linear Algebra and its Applications, 112 (1989), pp. 189–193, https://doi.org/10.1016/0024-3795(89)90594-6.
[27] D. Tufts and A. Sirah, Estimation of a signal waveform from noisy data using low-rank approximation to a data matrix, IEEE Transactions on Signal Processing, 41 (1993), pp. 1716–1721, https://doi.org/10.1109/78.212753.
[28] K. Usevich, Variable projection for affinely structured low-rank approximation in weighted 2-norms, Journal of Computational and Applied Mathematics, 272 (2014), pp. 430–448.
8. Appendix.

8.1. Proofs of propositions.

8.1.1. Proof of Theorem 2.1 and Proposition 2.2.

Proof. The first statement of Proposition 2.2 provides the parameterizing mapping if we prove correctness of (2.3), (2.4), uniqueness of $S$ satisfying relations of Theorem 2.1, prove that $S$ is an injective mapping and (2.4) is an inverse mapping to $S$.

Let us prove the correctness of (2.3). To begin with, we show that $Z_{I(τ)}$: is not singular and therefore invertible. This will be a consequence of non-singularity of $(Z_{0})_{I(τ)}$: for any basis of $Z(A_0)$.

Let us represent $A_0$ as $A_0 = (0, \ldots, 0, b_{r_m+1}, \ldots, b_1, 0, \ldots, 0)^T$, with $r_b$ zeroes at the beginning and $r_e$ zeroes at the end, $r_e + r_b + r_m = r$. Let us choose a matrix $Z_{0}^*$ such that $Z_{0}^* = \[Z_{\text{begin}} : Z_{\text{middle}} : Z_{\text{end}}\]$ consists of three blocks: $Z_{\text{begin}} = \begin{pmatrix} I_{r_b} & 0_{(N-r_b) \times r_b} \\ 0_{r_b \times r_m} & 0_{r_e \times r_m} \end{pmatrix}$, $Z_{\text{middle}} = \begin{pmatrix} 0_{r_e \times r_m} \\ Z_{\text{middle}} \end{pmatrix}$, $Z_{\text{end}} = \begin{pmatrix} 0_{(N-r_e) \times r_e} \\ I_{r_e} \end{pmatrix}$, where columns of $\hat{Z}_{\text{middle}} \in \mathbb{R}^{(N-r_b-r_e) \times r_m}$ form a basis of time-series of length $N - r_b - r_e$ governed by the LRR with coefficients $-b_2/b_1, \ldots, -b_{r_{m+1}}/b_1$. Since $\{1, \ldots, r_b\} \cup \{N-r_e+1, \ldots, N\} \subset I(τ)$ and any submatrix of size $r_m \times r_m$ of $\hat{Z}_{\text{middle}}$ is non-degenerate [28, Prop. 2.3], we obtain non-degeneracy of $(Z_{0}^*)_{I(τ)}$:.

Any other matrix which consists of basis vectors of $Z(A_0)$ can be represented in the form $Z_{0}^*P$ with a non-singular matrix $P \in \mathbb{R}^{r \times r}$. Therefore, matrix $(Z_{0}^*P)_{I(τ)}$: is also non-degenerate.

Now let us prove the non-degeneracy of $Z_{I(τ)}$: since $Z(A)$ is the subspace orthogonal to $Q(A)$, $\Pi_{Z(A)}$ can be represented as a continuous function $\Pi_{Z(A)} = I_N - \Pi_{Q(A)}$ of $A$, $A \neq 0$, where $Q(A)$ is defined in (2.2). Note that the determinant of $Z_{I(τ)}$: is a continuous function of $Z$. In turn, $Z$ continuously depends on $A_0$. Since $Z(A_0) = Z_0$ and the determinant of $(Z_0)_{I(τ)}$: is non-zero, there is a vicinity of $(A_0)_{K(τ)}$, such that the determinant of $Z_{I(τ)}$: is not zero; therefore, the matrix $Z_{I(τ)}$: is invertible.

The constructed mapping (2.3) does not depend on $Z_{0}$. Indeed, for any non-singular matrix $P \in \mathbb{R}^{r \times r}$: $(\Pi_{Z(A)}Z_0^*P)((\Pi_{Z(A)}Z_0^*P)_{I(τ)}:)^{-1} = ZZ^{-1}_{I(τ)}:$. Let us demonstrate that the properties of $S$, which are stated in Theorem 2.1, are fulfilled; i.e., show that $S \in D_r$, the series $S$ satisfies the GLRR($A$) and $(S)_{I(τ)} = S(τ)$. The series $S$ satisfies the GLRR($A$), since each column of the matrix $Z$ satisfies the GLRR($A$). To prove that $S \in D_r$, consider the matrix $T_{r+1}(S_0)$ and choose the submatrix of size $r \times r$ with non-zero determinant. Then take the submatrix $B$ of the matrix $T_{r+1}(S(S(r), A(τ)))$ with the same location. Its determinant is a continuous function of $(S(r), A(τ))$, since the function given in (2.3) is continuous. Therefore, there exists a vicinity of $(S(r), A(τ))$, where the determinant of $B$ is non-zero; thus, $S \in D_r$. The condition $(S)_{I(τ)} = S(τ)$ is fulfilled, since

$$(S)_{I(τ)} = \left(Z_{I(τ)}:Z^{-1}_{I(τ)}:ight)S(τ) = S(τ).$$

Let us explain the uniqueness of the mapping $S$ satisfying the relations of Theorem 2.1.

Let $S_2$ be a different mapping satisfying relations of Theorem 2.1, $\hat{S}_2 = S_2((S(r), A(τ))) \in D_r$. We know that $\hat{S}_2 \in Z(A)$. Therefore, columns of $Z$ contain a basis of $Z(A)$. Let $\hat{S}_2 = ZV$, $V \in \mathbb{R}^r$ be the coefficients of decomposition of $\hat{S}_2$ by the columns of $\hat{S}_2$. Then the following is fulfilled: $(ZV)_{I(τ)} = S(τ)$. However, $Z_{I(τ)}V = S(τ)$ together with invertibility of $Z_{I(τ)}$ leads to $V = Z^{-1}_{I(τ)}S(τ)$. Therefore, $\hat{S}_2 = \left(ZZ^{-1}_{I(τ)}\right)S(τ) = S$. \[\square\]
Let us prove that $S$ is an injective mapping. We choose two different sets of parameters $(S^{(1)}(r), A^{(1)}(r))$, $(S^{(2)}(r), A^{(2)}(r))$ in the vicinity of $((S_0)_{I(r)}, (A_0)_{K(r)})$ and consider $X_1 = S(S^{(1)}(r), A^{(1)}(r))$, $X_2 = S(S^{(2)}(r), A^{(2)}(r))$. If $S^{(1)}(r) \neq S^{(2)}(r)$, then $X_1 \neq X_2$, since $(X_1)_{I(r)} \neq (X_2)_{I(r)}$. Let $S^{(1)}(r) = S^{(2)}(r)$ be fulfilled, but $A^{(1)}(r) \neq A^{(2)}(r)$. Then a vector $V_1$ is orthogonal to colspace $T_{r+1}(X_1)$ iff $V_1 = c_1 A^{(1)}$, a vector $V_2$ is orthogonal to colspace $T_{r+1}(X_2)$ iff $V_2 = c_2 A^{(2)}$, where $A^{(1)}(r) \in \mathbb{R}^{r+1}$, $A^{(2)}(r) \in \mathbb{R}^{r+1}$, $a^{(1)}_r = -1$, $a^{(2)}_r = -1$, $c_1 \neq 0$, $c_2 \neq 0$ are arbitrary real numbers. But there is no $c_1$, $c_2$ such that $c_1 A^{(1)} = c_2 A^{(2)}$, hence $X_1 \neq X_2$.

Let us prove correctness of $(2.4)$. According to the statement of the proposition, $A^{(r)}(r)$ is a renormalization of $\hat{A}$ such that the $\tau$-th element becomes equal to $-1$. Let us prove the correctness of $A^{(r)}$, i.e., the possibility to renormalize $\hat{A}$. Consider the matrix $S = T_{r+1}(S)$, $S \in \mathbb{R}^{(r+1) \times (N-r)}$. Let $J$ be a subset of indices such that the submatrix $(S_0)_{i,J} \in \mathbb{R}^{(r+1) \times r}$ has rank $r$, where $S_0 = T_{r+1}(S_0)$. Then $\Pi_{\mathcal{L}(S)}$ can be represented as a continuous function $\Pi_{\mathcal{L}(S)} = \Pi_{S_{i,J}}$ in the vicinity of $S_0$; therefore, we can choose a vicinity in which $\hat{a}_\tau$ does not vanish.

Let us explain that $(2.4)$ gives the inverse mapping to $S$. Let $S = S(S^{(r)}, A^{(r)})$. Values $S^{(r)} = S_{I(r)}$ are taken directly from time series. The series $S$ is governed by GLRR($\hat{A}$) since the vector $\hat{A}$ is orthogonal to colspace ($T_{r+1}(S)$) by its definition. But the series $S$ is governed by GLRR($\hat{A}$); hence, $\hat{A}$ coincides with $\hat{A}$ up to normalization. Therefore, renormalization of $\hat{A}$ gives us the required $A^{(r)}$. This consideration concludes the proof.

### 8.1.2. Proof Theorem 2.3.

**Proof.** We need to show that $\Pi_{\mathcal{L}(S)}$ and $\Pi_{\mathcal{Z}}$ from Proposition 2.2 are smooth projections in the vicinity of $S_0$ and $Z_0$ respectively.

Since $(S_0)_{i,J}$ has full rank, $\Pi_{\mathcal{L}(S)} = S_{i,J}((S_{i,J})^T S_{i,J})^{-1} S_{i,J}^T$ is a smooth function in the vicinity of $S_0$. Since $Q(A)$ has full rank, see definition $(2.2)$,

$$\Pi_{\mathcal{Z}(A)} = I_N - Q(A) (Q^T(A) Q(A))^{-1} Q^T(A)$$

is smooth everywhere except $A = 0$.

It is clear that other operations mentioned in parametrization are smooth in the corresponding vicinities.

### 8.1.3. Proof of Theorem 2.4.

Let us start with a couple of lemmas.

It is convenient to separate the parameters $(2r$ arguments of the map $S$) into two parts, $S^{(r)}$ and $A^{(r)}$. Then $J_S = [F_S : F_A]$, where $F_S = (J_S)_{i:\{1, \ldots, r\}}$, $F_A = (J_S)_{i:\{r+1, \ldots, 2r\}}$.

**Lemma 8.1.** $Q(A)^T F_S = 0$; colspace $F_S = Z(A)$.

**Proof.** Let $F_S = [F_{S,1}, \ldots, F_{S,r}]$. Consider the equation $Q^T(A) S = 0$ and differentiate it with respect to $(S^{(r)})_{i(i)}$. We obtain $Q^T(A) F_{S,i} = 0$, which means that colspace $F_S \subset Z(A)$. The fact $(F_S)_{I(r,:)} = I$, completes the proof.

**Lemma 8.2.** $Q^T(A) F_A = -S^T_{K(\tau),i}$; where $S = T_{r+1}(S)$; colspace $F_A \subset Z(A^2)$.

**Proof.** Denote $F_A = [F_{A,1}, \ldots, F_{A,r}]$. By Lemma 8.1, $Q^T(A) S = 0$. Let us differentiate the equality with respect to $(a_{K(\tau)})_i$, i.e. $i$-th element of $a_{K(\tau)}$, $i = 1, \ldots, r$. Then we obtain $Q^T(e_j) S + Q(A) F_{A,j} = 0$, where $j$ is $i$-th element of $K(\tau)$. Note that $Q^T(e_j) S$ is the $j = K(\tau)_i$-th column of the transposed $(r+1)$-trajectory matrix $S^T$. Therefore, the equation $Q^T(A) F_A = -S^T_{K(\tau),i}$ is proved.
To prove the second part of lemma, let us consider the matrix $Q^{N-r,r}(A) \in \mathbb{R}^{N \times (N-r)}$. Due to the first statement, the following equation is true: $(Q^{N-r,r}(A))^T(Q^{N,r}(A))^T F_A = 0$. Then
\[
(Q^{N-r,r}(A))^T = \sum_{i=1}^{r+1} a_i (Q^{N-r,r}(e_i))^T, \quad (Q^{N,r}(A))^T = \sum_{j=1}^{r+1} a_j (Q^{N,r}(e_j))^T.
\]
Note that $(Q^{N-r,r}(e_i))^T(Q^{N,r}(e_j))^T = (Q^{N,2r}(e_{i+j-1}))^T$. Thus,
\[
(\sum_{i=1}^{r+1} \sum_{j=1}^{r+1} a_i a_j (Q^{N,2r}(e_{i+j-1}))^T) F_A = (Q^{N,2r}(\sum_{i=1}^{r+1} \sum_{j=1}^{r+1} a_i a_j e_{i+j-1}))^T F_A = 0,
\]
which is equivalent to $Q^T(A^2)F_A = 0$.

Now we can prove Theorem 2.4.

Proof. It follows from Lemma 8.2 that $Q^T(A^2)F_S = (Q^{N-r,r}(A))^TQ^T(A)F_S = 0$. Therefore, colspace $J_S \subset Z(A^2)$. Also, $S \in Z(A^2)$. Since we have a diffeomorphism at the point $S$, the Jacobian matrix $J_S$ has full rank $2r$. Hence, colspace $J_S = Z(A^2)$.

8.1.4. Proof of Lemma 3.1.

Proof. Assume contrary. Let $S^* = S_0$ be the point of global minimum in the problem (1.4). Let $S_0 \in D_{r_0}, r_0 < r$ so that $S_0$ satisfies a GLRR defined by $A_0 \in \mathbb{R}^{r_0+1}$, $A_0 = (a_1, \ldots, a_{r_0+1})^T$. Then we can construct $N$ linearly independent exponential series $S^{(i)}$ of length $N$, $S^{(i)} = (e^{\alpha_1}, e^{2\alpha_1}, \ldots, e^{N\alpha_1})^T$, governed by GLRRs($A^{(i)}$), $A^{(i)} = (e^{\lambda_i}, -1)$, where all $\lambda_i$ are different. Then for any real $\alpha$ we have $S_0 + \alpha S^{(i)} \in D_r$ since the series $S_0 + \alpha S^{(i)}$ is governed by the GLRR with $B_i = (e^{\alpha_1}a_1, e^{\lambda_i}a_2 - a_1, e^{\lambda_i}a_3 - a_2, \ldots, e^{\lambda_i}a_{r_0+1} - a_{r_0}, -a_{r_0+1})^T \in \mathbb{R}^{r_0+2}$.

Consider the weighted inner product $(\mathcal{Z}, Y)_W = \mathcal{Z}^T W Y$ and the corresponding norm $\| \cdot \|_W$. By the condition of the lemma, $X - S_0 \neq 0$. Consider inner products $\langle X - S_0, S^{(i)} \rangle_W, i = 1, 2, \ldots, N$. Since $S^{(i)}, i = 1, \ldots, N$, form a basis of $\mathbb{R}^N$, there exists an index $j$ such that $\langle X - S_0, S^{(j)} \rangle_W \neq 0$. Let us take $S_1 = S_0 + \frac{\langle X - S_0, S^{(j)} \rangle_W}{\mathcal{Z}^T W S^{(j)}} S^{(j)}$ governed by GLRR($B_i$) (hence, it belongs to $D_r$), and show that $\| X - S_1 \|_W < \| X - S_0 \|_W$.

\[
\langle X - S_0, X - S_0 \rangle_W - \langle X - S_1, X - S_1 \rangle_W = \frac{\langle X - S_0, S^{(j)} \rangle_W^2}{\langle S^{(j)}, S^{(j)} \rangle_W} > 0.
\]
We obtained a contradiction with the fact that $S_0 = S^*$ is a point of global minimum in the problem (1.4).

8.1.5. Proof of Theorem 3.3. Denote by $F_{S,k} = (J_{S,k})_{i,\{1,\ldots,r\}}$ first $r$ columns of Jacobian matrix $J_{S,k} = J_S(S^{(k)}_{(r)}, A^{(k)}_{(r)})$, and by $F_{A,k} = (J_{S,k})_{i,\{r+1,\ldots,2r\}}$ last $r$ columns of Jacobian matrix $J_{S,k}$.

Proof. The following equality is valid for any full-rank $F$ and positive definite $V$:
\[
(F)^\dagger V \Pi_F W = (F^T V F)^{-1} F^T V F (F^T W F)^{-1} F^T W = (F)^\dagger W.
\]
By Theorem 2.4, colspace $J_{S,k} = Z(A^2_k)$ and therefore $\Pi_{J_{S,k}} W = \Pi_{Z(A^2_k)} W$.

Let us choose $V$. We define $\tilde{Q}_k = Q = \left( Q^T(A_k) F^T_{S,k} W \right)$, which is a full rank matrix (see Lemma 8.1), and set $V = \tilde{Q}^T \tilde{Q}$. Let us probe that
\[
(\left( J_{S,k} \right)^\dagger V \Pi_{Z(A^2_k)} W (X - \Pi_{Z(A_k)} W (X)))_{i,\{r+1,\ldots,2r\}} = M_k^T Q^T(A_k) \Pi_{Z(A^2_k)} W (X - \Pi_{Z(A_k)} W (X)),
\]
where \( M_k = Q^T(A_k)F_{A,k} \) due to Lemma 8.2.

We prove this by means of the block-matrix techniques. Note that the calculation of the bottom half of the rows of \((J_{S,k})^T_V\) requires the calculation of the bottom half of \((J_{S,k}^T VJ_{S,k})^{-1}\) only.

Therefore, we have
\[
\hat{Q}J_{S,k} = \begin{pmatrix} 0 & M_k \\ F_{S,k}^T F_{S,k} & F_{S,k}^T F_{A,k} \end{pmatrix},
\]
\[
J_{S,k}^T VJ_{S,k} = \begin{pmatrix} (F_{S,k}^T F_{S,k})^T & (F_{S,k}^T F_{S,k})^T F_{A,k} \\ F_{S,k}^T F_{S,k} & M_k^T M_k + (F_{A,k}^T F_{A,k})^T F_{S,k}^T F_{A,k} \end{pmatrix},
\]
\[
((J_{S,k}^T VJ_{S,k})^{-1})_{z_i;\{r+1,\ldots,2r\}} = \left(- (M_k^T M_k)^{-1} (F_{S,k}^T F_{A,k}) \right) ((F_{S,k}^T F_{S,k})^T)^{-1} (M_k^T M_k)^{-1},
\]
\[
V = Q(A_k)Q^T(A_k) + F_{S,k} F_{S,k}^T, \quad J_{S,k}^T V = \left(M_k Q^T(A_k) + (F_{S,k}^T F_{S,k})^T F_{S,k}^T \right),
\]
\[
((J_{S,k}^T VJ_{S,k})^{-1})_{z_i;\{r+1,\ldots,2r\}} J_{S,k}^T V = \left((J_{S,k}^T VJ_{S,k})^{-1} J_{S,k}^T V \right)_{z_i;\{r+1,\ldots,2r\}} = (M_k^T M_k)^{-1} M_k^T Q^T(A_k) = M_k^T Q^T(A_k).
\]

8.1.6. Proof of Theorem 4.3.

Proof. Let us denote by \( \angle(x, y) \) the angle between two points on \( \mathbb{T} \), \( 0 \leq \angle(x, y) \leq \pi \). Let us prove the first part. Consider a root \( z_1 \in \mathbb{T} \) of multiplicity \( t \); then for any \( \alpha \) we have \( \min_{w \in W(\alpha)} \angle(w, z_1) \leq \frac{\pi}{N} \) by Dirichlet’s principle. Let us fix any \( 0 \leq \alpha_0 < 2\pi \), and choose \( w_0 = \arg \min_{w \in W(\alpha_0)} \angle(w, z_1) \). Evaluation of \( g_A(z) \) at point \( w_0 \) proves the first part, since \(|z_1 - w_0| = O(1/N)\).

To prove the second part, let us construct a piecewise estimate of \( g_A(z) \) for \( z \). Consider the decomposition \( g_A(z) = p_A(z)q_A(z) \), where the roots of \( p_A(z) \) belong to \( \mathbb{T} \) while the roots of \( q_A(z) \) do not. By construction, \( \inf_{z \in \mathbb{T}} |q_A(z)| > 0 \).

Let \( z_1, \ldots, z_k \) be the roots of \( p_A(z) \) with multiplicities \( t_1, \ldots, t_k \). We split the circle \( \mathbb{T} \) into \( k \) semi-open non-intersecting arcs \( S_1, \ldots, S_k, \mathbb{T} = \bigcup_{1 \leq i \leq k} S_i \), such that \( z_i \in S_i \) for any \( i \) and \( z_j \notin \overline{S_i} \) for any \( j \neq i \) (\( \overline{S_i} \) denotes closure of \( S_i \)), which leads to \( \inf_{z \in S_i} \left| \frac{p_A(z)}{(z - z_i)} \right| \) > 0.

To finish the proof we need to show that there exists \( 0 \leq \alpha = \alpha(N) < 2\pi \) such that \( \min_{w \in W(\alpha(N)), 1 \leq i \leq k} \angle(w, z_i) = \Theta(1/N) \). Let us denote for \( 0 \leq \mu < \pi/N \) and \( z \in \mathbb{T} \)
\[
B_{z,\mu} = \{0 \leq \alpha < 2\pi : \min_{w \in W(\alpha)} \angle(w, z) \leq \mu \}.
\]

The set \( B_{z,\mu} \) has the explicit form:
\[
B_{z,\mu} = \bigcup_{0 \leq j \leq N-1} \left\{ \arg \left( \exp \left( i \left( \frac{2\pi j}{N} + y \right)/z \right) \right) |_{-\mu \leq y \leq \mu} \right\}.
\]

Let us comment this expression. Consider \( \omega_j^{(\alpha)} = \exp \left( i \left( \frac{2\pi j}{N} - \alpha \right) \right) \), and choose \( \alpha_j \) such that \( \angle(\omega_j^{(\alpha_j)}, z) \leq \mu \). This means that the polar angle of their ratio \( \omega_j^{(\alpha_j)}/z \) belongs to the interval \([\mu, \mu]\), i.e. \( \omega_j^{(\alpha_j)}/z \in \exp \left( i|x| \right)|_{\mu \leq x \leq \mu} \). Let us perform equivalent transformations: \( \exp \left( i \left( \frac{2\pi j}{N} - \alpha \right) \right) \in \{ z \exp(i|x|) \}_{-\mu \leq x \leq \mu}, \exp \left( i \left( \alpha_j - \frac{2\pi j}{N} \right) \right) \in \{ \exp(iy) \}_{-\mu \leq y \leq \mu} \), where \( y = \)
the following transformations:

Expression (8.1) is obtained using formula \[23, 16.4, 16.15\]. To obtain \( \min_{w \in \mathcal{W}(\alpha)} \angle(w, z) \leq \mu \), \( \alpha \) should be equal to one of \( \alpha_0, \ldots, \alpha_j \). Union of all such sets for \( j = 0, \ldots, N - 1 \) gives us \( \mathcal{B}_{z,\mu} \).

The Lebesgue measure of \( \mathcal{B}_{z,\mu} \) is equal to \( \min \mathcal{B}_{z,\mu} = 2\mu N \) for \( \mu < \pi / N \). Let us take \( \mu = \frac{\pi}{2N} \) and consider \( \mathcal{B} = \bigcup_{1 \leq i \leq k} \mathcal{B}_{\mu, z_i} \). Since \( \mathrm{mes} \mathcal{B} \leq \pi \), we obtain \( \mathrm{mes} \mathcal{B} = \pi \) for \( \mathcal{B} = [0; 2\pi] \setminus \mathcal{B} \), which means that \( \mathcal{B} \) is not the empty set. Thus, we have proved that for any \( \alpha \in \mathcal{B} \)

\[
\min_{w \in \mathcal{W}(\alpha); 1 \leq i \leq k} \angle(w, z_i) > \frac{\pi}{2N\kappa}.
\]

Let us fix arbitrary \( \alpha_0 \in \mathcal{B} \) and consider any \( w \in \mathcal{W}(\alpha_0) \). Let \( i \) be such that \( w \in S_i \). For any \( i \), \( |w - z_i| = \Theta(1/N) \). Then \( |g_A(w)| = |q_A(w)| |PA(w)| |(w - z_i)^t| \geq C\Theta(N^{-t_i}) \), where \( C > 0 \) is some constant.

8.2. Formulas for calculation of the step (3.11) in VPGN. An explicit form of the step (3.11) is contained in [30, Proposition 3]. We present a new form for the Jacobian \( J_{S^*} \), which is more convenient for implementation.

**Lemma 8.3.** The projection \( \Pi_{Z(A),w} \) can be calculated as

\[
(8.1) \quad \Pi_{Z(A),w} X = W^{-1}Q(A)\Gamma^{-1}(A)Q^T(A)X,
\]

where \( \Gamma(A) = Q^T(A)W^{-1}Q(A) \).

The columns of \( J_{S^*}(A(r)) \) have the form

\[
(8.2) \quad (J_{S^*}(A(r)))_{:i} = -W^{-1}Q(A)\Gamma^{-1}(A)Q^T(e_{K_i})\Pi_{Z(A),w} X \quad - \Pi_{Z(A),w} W^{-1}Q(e_{K_i})\Gamma^{-1}(A)Q^T(A)X,
\]

where \( K = K(r) \).

**Proof.** The equality

\[
S^*(A(r)) = \Pi_{Z(A(r)),w}(X) \in \mathcal{D}^*_r(X)
\]

corresponds to the solution of the following quadratic problem:

\[
S^*(A(r)) = \arg \min_Y \left\{ \frac{1}{2} Y^T W Y - Y^T X \right\}.
\]

Expression (8.1) is obtained using formula [23, 16.4, 16.15].

Proof of equality (8.2) is done by taking derivatives of formula (8.1) by \( a_k \) and by applying the following transformations:

\[
(\Pi_{Z(A),w} X)_{:k} = -W^{-1}Q(e_k) (Q^T(A)W^{-1}Q(A))^{-1} Q^T(A)X
\]

\[
= -W^{-1}Q(A) (Q^T(A)W^{-1}Q(A))^{-1} Q^T(e_k)X + W^{-1}Q(A) (Q^T(A)W^{-1}Q(A))^{-1}
\]

\[
\times (Q^T(e_k)W^{-1}Q(A) + Q^T(A)W^{-1}Q(e_k)) (Q^T(A)W^{-1}Q(A))^{-1} Q^T(A)X
\]

\[
= -W^{-1}Q(A) (Q^T(A)W^{-1}Q(A))^{-1} Q^T(e_k)\Pi_{Z(A),w} X \quad - \Pi_{Z(A),w} W^{-1}Q(e_k) (Q^T(A)W^{-1}Q(A))^{-1} Q^T(A)X. \quad \square
\]
8.3. Compensated Horner scheme for basis calculation in Algorithms 4.1 and 4.2. Let us describe how the compensated Horner scheme can be used for calculation of bases of $Z(A)$ and $Z(A^2)$ with improved accuracy. The Horner scheme can be directly applied in Algorithms 4.1 and 4.2 for calculation of polynomials $g_A$.

Moreover, the Horner scheme can improve the accuracy of calculation of $U_r$ at step 4 of Algorithm 4.1; it is important if $L_r$ is ill-conditioned. Note that the same approach can be applied to calculation of $U_{2r}$ at step 4 of algorithm Algorithm 4.2. Let us consider the matrix $R_r$ calculated at step 3 of Algorithm 4.1. Since $(R_r)_{k,:} = (\exp(\frac{i2\pi r k}{N}), \exp(\frac{i2\pi(r-1) k}{N}), \ldots, \exp(\frac{i2\pi k}{N}))$, we can reduce the multiplication of $R_r$ by a vector to calculation of a polynomial of degree $r$ in the point $\exp(\frac{i2\pi k}{N})$. Therefore, we can accurately calculate the multiplication of $R_r$ by a vector with the help of the Horner scheme.

To use this property, let us consider a new way of calculation of $U_r$. Let $O_r$ be such that $L_r O_r$ consists of orthonormal columns; $O_r$ can be found by the SVD or QR decomposition. Then $U_r = A_g^{-1}(R_r O_r)$. This representation of $U_r$ allows to apply the Horner scheme to calculation of $R_r O_r$.

Algorithm 8.1 Calculation of a basis of $Z(A)$ using Compensated Horner Scheme

1: Compute $\alpha_0$ and $A_g$ by the same way as in steps 1 and 2 of Algorithm 4.1 except for the use of the algorithm CompHorner for calculation of values of polynomials $g_A$.
2: Compute $L_r$ and $R_r$ by the same way as in step 3 of Algorithm 4.1.
3: Compute $U_r$ in a new manner: find $O_r$ such that $L_r O_r$ consists of orthonormal columns; calculate $B = R_r O_r$ by means of the algorithm CompHorner; calculate $U_r = A_g^{-1}(B)$ directly by matrix multiplication.
4: return Matrix $Z$, which is calculated by the same way as in steps 5 and 6 of Algorithm 4.1.

Algorithm 8.2 Calculation of a basis of $Z(A^2)$ using Compensated Horner Scheme

1: Compute $\alpha_0$, $A_g$, $U_r$ by the same way as in steps 1, 2 and 3 of Algorithm 8.1.
2: Compute $R_{2r}$ and $L_{2r}$ by the same way as in steps 2 and 3 of Algorithm 4.2.
3: Compute $U_{2r}$ in a new manner: find $O_{2r}$ such that $L_{2r} O_{2r} \in R^{N \times r}$ consists of orthonormal columns; calculate $B = R_{2r} O_{2r}$ by means of the algorithm CompHorner; calculate $U_{2r} = (I_N - \Pi U_r I_N) A_g^{-2}(B)$ directly by matrix multiplication.
4: return Matrix $Z$, which is calculated by the same way as in steps 5 and 6 of Algorithm 4.2.