

RESEARCH ARTICLE

Fast and stable modification of the Gauss-Newton method for low-rank signal estimation

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Summary

The weighted nonlinear least-squares problem for low-rank signal estimation is considered. The problem of constructing a numerical solution that is stable and fast for long time series is addressed. A modified weighted Gauss-Newton method, which can be implemented through the direct variable projection onto a space of low-rank signals, is proposed. For a weight matrix which provides the maximum likelihood estimator of the signal in the presence of autoregressive noise of order p the computational cost of iterations is $O(Nr^2 + Np^2 + rN \log N)$ as N tends to infinity, where N is the time-series length, r is the rank of the approximating time series. Moreover, the proposed method can be applied to data with missing values, without increasing the computational cost. The method is compared with state-of-the-art methods based on the variable projection approach in terms of floating-point numerical stability and computational cost.

KEYWORDS:

low-rank approximation, time series, Hankel matrix, variable projection, Gauss-Newton method, iterative methods

1 | INTRODUCTION

In this study we consider the ‘signal plus noise’ observation scheme:

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

Denote by $\mathbf{X} = (x_1, \dots, x_N)^T$, $\mathbf{S} = (s_1, \dots, s_N)^T$ and $\boldsymbol{\epsilon} = (\epsilon_1, \dots, \epsilon_N)^T$ the vectors of observations, signal values and 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 \mathbf{S} can be written in the parametric form as a finite sum

$$s_n = \sum_{k=1}^d P_{m_k}(n) \exp(\alpha_k n) \sin(2\pi\omega_k n + \phi_k), \quad (1)$$

where $P_{m_k}(n)$ are polynomials in n of degree m_k . In signal processing applications, the signal in the form (1) is usually a sum of sine waves¹ or a sum of damped sinusoids². The problem of estimating the unknown signal values s_n is as important as the problem of estimating the parameters in the explicit form (1). We will be concentrated on the signal estimation.

Certainly, there are many numerical methods for estimating signals in the form (1) in the ‘signal plus noise’ observation scheme. Our aim is to construct a method, which is accurate and fast for large series lengths N and also is competitive. It would be

a great advantage if the constructed method could deal with time series with gaps keeping algorithms' efficiency characteristics. The case of autoregressive noise is of special interest.

We will solve the problem of signal estimation in a class of signals, which is wider than that given in (1) and has a different parameterization from the explicit one. To describe the class of signals, we need some definitions. The rank of a signal \mathbf{S} is defined as follows. For a given integer L , $1 < L < N$, called the window length, we define the embedding operator $T_L : \mathbb{R}^N \rightarrow \mathbb{R}^{L \times (N-L+1)}$, which maps \mathbf{S} into a Hankel matrix, by

$$T_L(\mathbf{S}) = \begin{pmatrix} s_1 & s_2 & \dots & s_{N-L+1} \\ s_2 & s_3 & \dots & \vdots \\ \vdots & \vdots & \dots & s_{N-1} \\ s_L & s_{L+1} & \dots & s_N \end{pmatrix}. \quad (2)$$

The columns of $T_L(\mathbf{S})$ are sequential lagged vectors; this is why $T_L(\mathbf{S})$ is often called the *trajectory matrix* of \mathbf{S} . We say that the signal \mathbf{S} has rank $r < N/2$ if $\text{rank } T_{r+1}(\mathbf{S}) = r$. It is known that $\text{rank } T_{r+1}(\mathbf{S}) = r$ if and only if $\text{rank } T_L(\mathbf{S}) = r$ for any L such that $\min(L, N-L+1) > r$ (see³, Corollary 5.1 for the proof).

For a sufficiently large time-series length N , the signal in the form (1) has rank r , which is determined by the parameters m_k , α_k and ω_k ⁴. For example, the signal with values s_n has rank $r = 2$ for a sum of two exponentials $s_n = c_1 \exp(\alpha_1 n) + c_2 \exp(\alpha_2 n)$, a sine wave $s_n = c \sin(2\pi\omega n + \phi)$, where $0 < \omega < 0.5$, or a linear function $s_n = an + b$. Thus, the model fixes the rank r but does not fix the form of the signal, i.e., the number of terms and the orders of the polynomials in (1).

The considered model of signals, where the Hankel matrix $T_L(\mathbf{S})$ is rank-deficient, is one of the standard models in many areas, signal processing^{1,5}, speech recognition⁶, control theory and linear systems^{2,7} among others.

Let us state the optimization problem for estimating the signal. 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 in its closure $\overline{\mathcal{D}_r}$. It is well-known that $\overline{\mathcal{D}_r}$ consists of series of rank not larger than r (this result can be found in⁸, Remark 1.46 for the complex case; the real-valued case is considered in⁴).

Thus, in what follows, we study the weighted least-squares (WLS) problem

$$\mathbf{Y}^* = \arg \min_{\mathbf{Y} \in \overline{\mathcal{D}_r}} \|\mathbf{X} - \mathbf{Y}\|_{\mathbf{W}}, \quad (3)$$

where \mathbf{W} is a symmetric positive-definite weight matrix, $\|\mathbf{Z}\|_{\mathbf{W}}^2 = \mathbf{Z}^T \mathbf{W} \mathbf{Z}$. If noise ϵ is Gaussian with covariance matrix $\mathbf{\Sigma}$ and zero mean, the WLS estimate with the weight matrix $\mathbf{W} = \mathbf{\Sigma}^{-1}$ is the maximum likelihood estimator (MLE). The same is true if \mathbf{W} is scaled by a constant. In the case when noise is an autoregressive process of order p (AR(p)), the matrix \mathbf{W} is $(2p+1)$ -diagonal⁹, p.534.

Although the common case is the case of a positive definite matrix \mathbf{W} , the problem (3), where \mathbf{W} is positive semi-definite, is of considerable interest. For example, the case of a diagonal matrix \mathbf{W} with several zero diagonal elements corresponds to the problem of low-rank approximation for time series with missing values if the noise is white. Let us consider the case of a general weight matrix and time series with missing values. Let a symmetric positive definite matrix \mathbf{W}_0 be given for the whole time series including gaps. Then the weight matrix \mathbf{W} is constructed from \mathbf{W}_0 by setting the columns and rows with indices equal to entries of missing values to zero. Note that if \mathbf{W} is not positive-definite, then $\|\cdot\|_{\mathbf{W}}$ is semi-norm and the problem (3) may become ill-posed. In particular, the topology of $\overline{\mathcal{D}_r}$ is not consistent with the semi-norm and therefore the minimum in (3) should be changed to infimum, which can be not achieved at time series in $\overline{\mathcal{D}_r}$.

Different approaches for solving (3). The optimization problem (3) is non-convex with many local minima¹⁰. The problem (3) is commonly considered as a structured (more precisely, Hankel) low-rank approximation problem (SLRA, HSLRA)^{7,11,12}. A well-known subspace-based method for solving (3) is called 'Cadzow iterations'¹ 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 norm¹³. The Cadzow method has two drawbacks: first, the properties of the limiting point of the Cadzow iterations are unknown¹⁴ and second, it tries to solve the problem (3) with a weight matrix which generally differs from the given \mathbf{W} . Therefore, it is not optimal (the method does not provide the MLE), even for the case of white Gaussian noise¹⁵. The reason is that the problems are commonly stated in SLRA as matrix approximation problems, while the original problem (3) is stated in terms of time series.

Many methods have been proposed to solve HSLRA, including the Riemannian SVD¹⁵, Structured total least-norm¹⁶, Newton-like iterations¹⁷, proximal iterations¹⁸, symbolic computations¹⁰, stochastic optimization¹⁹, fixed point iterations¹⁴, a penalization approach²⁰.

Since we consider the problem of WLS time series approximation, which generally differs from the problem of matrix approximation due to different weights (see e.g. ²¹), let us use as a benchmark the effective and general approach of Markovsky and Usevich ^{22, 23}, which is based on the variable projection principle ²⁴ combined with the Gauss-Newton method for solving the optimization subproblem; we call it VPGN. The method of ^{22, 23} is able to deal with the problem in the form (3), i.e., exactly with the given weight matrix; 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. Thus, the VPGN method can be considered as a start-of-art method of low-rank time series approximation. Nevertheless, the approach has a couple of disadvantages. First, the Cholesky factorization is used for solving least-squares subproblems to obtain a fast algorithm; unfortunately, this squares the condition number (more stable decompositions like QR factorization are slower). Then, the VPGN method is efficient only if the inverse of the weight matrix is banded. Note that the approach of Markovsky and Usevich can be applied to the case of rank-deficient matrices \mathbf{W} in ²⁵ and ^{7, Section 4.4}. However, it is not clear how to implement the algorithm, which proposed in these papers, effectively in terms of computational costs. In ⁴, a version S-VPGN, which improves the stability of several steps of VPGN is considered; however, it does not overcome these drawbacks.

The proposed approach. Let us consider another approach to solving the problem (3); the considered approach is similar to VPGN but different. It is discussed in Section 2.1 that each time series \mathbf{S} in $\overline{\mathcal{D}}_r$ is characterized by a vector $\mathbf{a} \in \mathbb{R}^{r+1}$, which provides the coefficients of a generalized linear recurrence relation (GLRR) governing the time series, i.e. $\mathbf{a}^T T_{r+1}(\mathbf{S})$ is the zero vector. For each \mathbf{a} , we can consider the space $\mathcal{Z}(\mathbf{a})$ of signals governed by the GLRR with the given coefficients. Iterative algorithms that use the variable projection method for solving the problem (3) include the projection onto $\mathcal{Z}(\mathbf{a})$ as a subproblem.

In this paper, we propose to overcome the drawbacks of the methods of ^{22, 23} and ⁴ in the following manner. First, the proposed modification helps to avoid computing the pseudoinverse of the Jacobian matrix (compare (16) and (18)). Then, as well as in ⁴ (and unlike ²³), the projection is calculated directly onto the space $\mathcal{Z}(\mathbf{a})$ and is not obtained through projecting on its orthogonal complement $\mathcal{Q}(\mathbf{a})$. Finally, for calculating the projection, we use fast algorithms with improved numerical stability (the compensated Horner scheme, see Remark 5). As a result, the proposed method sometimes can be just slightly slower and is much faster in many real-life scenarios, but also is more stable (see Section 5 with the comparison results). Moreover, the algorithm with direct projections onto the space $\mathcal{Z}(\mathbf{a})$ can be extended to the case of a degenerate weight matrix \mathbf{W} (in particular, to the case of missing values) without loss of effectiveness (see Section 4.3); compare with that in ²⁵, where projections to the subspace $\mathcal{Q}(\mathbf{a})$ are used and the computational cost considerably increases for degenerate weight matrices.

Structure of the paper. In Section 2 we briefly discuss the parameterization of \mathcal{D}_r and its properties and introduce necessarily notation. In Section 3 we describe the known (VPGN) and the new proposed (MGN) iterative methods for solving the optimization problem (3). The algorithm VPGN is described in the way different from that in ²³, since the description in ²³ is performed for general SLRA problems, whereas we consider a particular case of time series. Section 4 presents the algorithms with the implementations of VPGN and MGN. In Section 5 we compare computational costs and numerical stability of the VPGN and MGN algorithms. Section 6 concludes the paper.

Main notation. In this paper, we use lowercase letters (a, b, \dots) and also L, K, M, N for scalars, bold lowercase letters ($\mathbf{a}, \mathbf{b}, \dots$) for vectors, bold uppercase letters ($\mathbf{A}, \mathbf{B}, \dots$) for matrices, and the calligraphic font for sets. Formally, time series are vectors; however, we use the uppercase sans serif font ($\mathbf{A}, \mathbf{B}, \dots$) for time series to distinguish them from ordinary vectors. Additionally, $\mathbf{I}_M \in \mathbb{R}^{M \times M}$ is the identity matrix, $\mathbf{0}_{M \times k}$ denotes the $M \times k$ zero matrix, $\mathbf{0}_M$ denotes the zero vector in \mathbb{R}^M , \mathbf{e}_i is the i -th standard basis vector.

Denote \mathbf{b}_C the vector consisting of the elements of a vector \mathbf{b} with indices in a set C . For matrices, denote $\mathbf{B}_{C, \cdot}$ the matrix consisting of rows of a matrix \mathbf{B} with indices in C and $\mathbf{B}_{\cdot, C}$ the matrix consisting of columns of a matrix \mathbf{B} with indices in C .

Finally, we put a brief list of main common symbols and acronyms.

LRR is a linear recurrence relation.

GLRR(\mathbf{a}) is a generalized LRR with the coefficients given by \mathbf{a} .

$\overline{\mathcal{D}}_r$ is the set of time series of rank r .

$\underline{\mathcal{D}}_r$ is the set of time series of rank not larger than r .

$\mathcal{Z}(\mathbf{a}) \in \mathbb{R}^N$ is the set of time series of length N governed by the minimal GLRR(\mathbf{a}); $\mathbf{Z}(\mathbf{a})$ is a matrix consisting of its basis vectors.

$\mathcal{Q}(\mathbf{a})$ is the orthogonal complement to $\mathcal{Z}(\mathbf{a})$; $\mathbf{Q}(\mathbf{a})$ is the matrix consisting of its special basis vectors (see Section 2.2).

$\mathbf{W} \in \mathbb{R}^{N \times N}$ is a weight matrix.

$(\mathbf{F})_{\mathbf{W}}^\dagger$ is the weighted pseudoinverse matrix; \mathbf{F}^\dagger stands for $(\mathbf{F})_{\mathbf{I}_N}^\dagger$.

\mathbf{J}_S is the Jacobian matrix of a map S .

$T_M : \mathbb{R}^N \rightarrow \mathbb{R}^{M \times (N-M+1)}$ is the embedding operator, which constructs the M -trajectory matrix.

$H_\tau : \mathbb{R}^r \rightarrow \mathbb{R}^{r+1}$ is the operator, which inserts -1 in the position τ .

$\Pi_{\mathcal{L}, \mathbf{W}}$ is the \mathbf{W} -orthogonal projection onto \mathcal{L} , $\Pi_{\mathbf{L}, \mathbf{W}}$ is the \mathbf{W} -orthogonal projection onto the column space $\text{colspace}(\mathbf{L})$; if \mathbf{W} is the identity matrix, it is omitted in the notation.

$S_\tau^*(\mathbf{a}) = \Pi_{\mathcal{Z}(H_\tau(\mathbf{a}), \mathbf{W})} \mathbf{X}$, where $\mathbf{a} \in \mathbb{R}^r$.

2 | PARAMETERIZATION OF LOW-RANK SERIES

In this section, we introduce the notations and describe the results of⁴ which we will use further.

2.1 | Generalized linear recurrence relations

It is well known^{26, Theorem 3.1.1} that for sufficiently large N , a time series in the form (1) satisfies a linear recurrence relation (LRR) of some order m :

$$s_n = \sum_{k=1}^m b_k s_{n-k}, n = m+1, \dots, N; b_m \neq 0. \quad (4)$$

One time series can be governed by many different LRRs. The LRR of minimal order r (it is unique) is called minimal. If $r < N/2$, the corresponding time series has rank r . The minimal LRR uniquely defines the form of (1) and the parameters m_k, α_k, ω_k .

The relations (4) can be expressed in vector form as $\mathbf{a}^T T_{m+1}(\mathbf{S}) = \mathbf{0}_{N-m}^T$, where $\mathbf{a} = (b_m, \dots, b_1, -1)^T \in \mathbb{R}^{m+1}$. The vector \mathbf{a} corresponding to the minimal LRR ($m = r + 1$) and the first r values of the series \mathbf{S} uniquely determine the whole series \mathbf{S} . Therefore, r coefficients of an LRR of order r and r initial values ($2r$ parameters altogether) can be chosen as parameters of a series of rank r . However, this parameterization does not describe the whole set. For example, $\mathbf{S} = (1, 1, 1, 1, 1, 2)^T$ has rank 2 and does not satisfy an LRR of order $m < N - 1$.

Let us generalize LRRs. We say that a time series satisfies a generalized LRR (GLRR) of order m if $\mathbf{a}^T T_{m+1}(\mathbf{S}) = \mathbf{0}_{N-m}^T$ for some non-zero $\mathbf{a} \in \mathbb{R}^{m+1}$; we call this linear relation $\text{GLRR}(\mathbf{a})$. If $a_{m+1} = -1$, the same relation is called $\text{LRR}(\mathbf{a})$. As well as for LRRs, the minimal GLRR can be introduced. The difference between a GLRR and an ordinary LRR is that the last coefficient in the GLRR is not necessarily non-zero and therefore the GLRR does not necessarily set a recurrence. However, at least one of the coefficients of the GLRR should be non-zero.

Let us demonstrate the difference between LRRs and GLRRs by an example. Let $\mathbf{S} = (s_1, \dots, s_N)^T$ be a signal and $\mathbf{a} = (a_1, a_2, a_3)^T$. Then $\text{GLRR}(\mathbf{a})$ and $\text{LRR}(\mathbf{a})$ mean the same: $a_1 s_i + a_2 s_{i+1} + a_3 s_{i+2} = 0$ for $i = 1, \dots, N - 2$. For $\text{LRR}(\mathbf{a})$, we state that $a_3 = -1$ (or just not equal to 0). Then this linear relation becomes a recurrence relation since $s_{i+2} = a_1 s_i + a_2 s_{i+1}$. For $\text{GLRR}(\mathbf{a})$, we assume that some of a_i is not zero (or equal to -1). It may be a_1 or a_2 or a_3 . For example, $\mathbf{S} = (1, 1, 1, 1, 1, 2)^T$ satisfies the $\text{GLRR}(\mathbf{a})$ with $\mathbf{a} = (1, -1, 0)^T$.

Thus, we consider the parameterization with the help of $\text{GLRR}(\mathbf{a})$; in fact, the same approach is used in^{22, 23}. In what follows, we assume that $2r < N$.

The following properties clarify the difference between the spaces \mathcal{D}_r and its closure $\overline{\mathcal{D}_r}$: (a) $\overline{\mathcal{D}_r} = \{\mathbf{Y} : \exists \mathbf{a} \in \mathbb{R}^{r+1}, \mathbf{a} \neq \mathbf{0}_{r+1} : \mathbf{a}^T T_{r+1}(\mathbf{S}) = \mathbf{0}_{N-r}^T\}$ or, equivalently, $\mathbf{Y} \in \overline{\mathcal{D}_r}$ if and only if there exists a $\text{GLRR}(\mathbf{a})$ of order r , which governs \mathbf{Y} ; (b) $\mathbf{Y} \in \mathcal{D}_r$ if and only if there exists a $\text{GLRR}(\mathbf{a})$ of order r , which governs \mathbf{Y} , and this GLRR is minimal.

2.2 | Subspace approach

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

Define the operator $\mathbf{Q} : \mathbb{R}^{r+1} \rightarrow \mathbb{R}^{M \times (N-r)}$ as

$$(\mathbf{Q}(\mathbf{a}))^T = \begin{pmatrix} a_1 & a_2 & \dots & \dots & a_{r+1} & 0 & \dots & 0 \\ 0 & a_1 & a_2 & \dots & \dots & a_{r+1} & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & 0 \\ 0 & \dots & 0 & a_1 & a_2 & \ddots & \ddots & a_{r+1} \end{pmatrix}. \quad (5)$$

Then the other convenient form of $\mathcal{Z}(\mathbf{a})$ is $\mathcal{Z}(\mathbf{a}) = \{\mathbf{S} : \mathbf{Q}^T(\mathbf{a})\mathbf{S} = \mathbf{0}_{N-r}\}$.

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

2.3 | Parameterization

Let us describe the details of the considered parameterization. Consider a series $\mathbf{S}_0 \in \mathcal{D}_r$, which satisfies a minimal GLRR(\mathbf{a}_0) of order r defined by a non-zero vector $\mathbf{a}_0 = (a_1^{(0)}, \dots, a_{r+1}^{(0)})^T$. Let us fix τ such that $a_\tau^{(0)} \neq 0$. Since GLRR(\mathbf{a}_0) is invariant to multiplication by a constant, we assume that $a_\tau^{(0)} = -1$. This condition on τ is considered to be valid hereinafter. Let us build a parameterization of \mathcal{D}_r in the vicinity of \mathbf{S}_0 ; parameterization depends on the index τ . Note that we can not construct a global parameterization, since for any index τ there exists a point \mathbf{a} of \mathcal{D}_r , such that the τ -th element of \mathbf{a} is zero.

In the case of a series governed by an ordinary LRR(\mathbf{a}), $\mathbf{a} \in \mathbb{R}^{r+1}$, since the last coordinate of \mathbf{a} is equal to -1 , the series is uniquely determined by the first r elements of \mathbf{a} and r initial values of the series. Then, applying the LRR to the initial data, which are taken from the series that is governed by the LRR, we restore this series. In the case of an arbitrary series in \mathcal{D}_r , the approach is similar but a bit more complicated. For example, we should take the boundary data ($\tau - 1$ values at the beginning, and $r + 1 - \tau$ values at the end) instead of the r initial values at the beginning of the series.

Denote $\mathcal{I}(\tau) = \{1, \dots, N\} \setminus \{\tau, \dots, N - r - 1 + \tau\}$ and $\mathcal{K}(\tau) = \{1, \dots, r + 1\} \setminus \{\tau\}$ two sets of size r . The set $\mathcal{I}(\tau)$ consists of the indices of the series values (we call them boundary data), which are enough to find all the series values with the help of the vector $\mathbf{a}_{\mathcal{K}(\tau)} \in \mathbb{R}^r$ consisting of the elements of a vector $\mathbf{a} \in \mathbb{R}^{r+1}$ with indices in $\mathcal{K}(\tau)$; that is, $\mathbf{a}_{\mathcal{K}(\tau)} = (a_1, \dots, a_{\tau-1}, a_{\tau+1}, a_{r+1})^T$.

To simplify notation, let us introduce the operator $H_\tau : \mathbb{R}^r \rightarrow \mathbb{R}^{r+1}$, which acts as follows. Let $\hat{\mathbf{a}} \in \mathbb{R}^r$ and $H_\tau(\hat{\mathbf{a}}) = \mathbf{a}$. Then $\mathbf{a} = (a_1, \dots, a_{r+1})^T$ is such that $\mathbf{a}_{\mathcal{K}(\tau)} = \hat{\mathbf{a}}$ and $a_\tau = -1$; that is, $\hat{\mathbf{a}} \in \mathbb{R}^r$ is extended to $\mathbf{a} \in \mathbb{R}^{r+1}$ by inserting -1 in the τ -th position. In this notation, $\mathbf{a}_{\mathcal{K}(\tau)} = H_\tau^{-1}(\mathbf{a})$.

Let $\mathbf{Z} = \mathbf{Z}(\mathbf{a})$ be a matrix consisting of basis vectors of $\mathcal{Z}(\mathbf{a})$ and $\mathbf{G}(\hat{\mathbf{a}}) = \mathbf{Z}(\mathbf{Z}_{\mathcal{I}(\tau), :})^{-1}$; here $\mathbf{Z}_{\mathcal{I}(\tau), :} \in \mathbb{R}^{r \times r}$, $\mathbf{G}(\hat{\mathbf{a}}) \in \mathbb{R}^{N \times r}$. It follows from the explicit form of the parameterization given in⁴ that the parameterization mapping $S_\tau : \mathbb{R}^{2r} \rightarrow \mathcal{D}_r$ has the form

$$\mathbf{S} = S_\tau(\dot{\mathbf{s}}, \hat{\mathbf{a}}) = \mathbf{G}(\hat{\mathbf{a}})\dot{\mathbf{s}}. \quad (6)$$

Note that $\mathbf{G}(\hat{\mathbf{a}})$ does not depend on the choice of basis vectors of $\mathcal{Z}(\mathbf{a})$ used for forming \mathbf{Z} . The expression $\mathbf{G}(\hat{\mathbf{a}})\dot{\mathbf{s}}$ gives the linear combination of the chosen basis vectors such that $\dot{\mathbf{s}} = (\mathbf{S})_{\mathcal{I}(\tau)}$. Thus, $\mathbf{S} \in \mathcal{Z}(\mathbf{A})$ and has boundary data $\dot{\mathbf{s}}$.

Note that for different series $\mathbf{S}_0 \in \mathcal{D}_r$ we may have different parameterizations of \mathcal{D}_r in vicinities of \mathbf{S}_0 . Moreover, for a fixed \mathbf{S}_0 , there is a variety of parameterizations provided by different choices of the index τ .

3 | OPTIMIZATION

Let us consider different numerical methods for solving the problem (3). First, note that we search for a local minimum. Then, since the objective function is smooth in the considered parameterization, one can apply the conventional weighted version of the Gauss-Newton method (GN), see²⁷ for details. However, this approach appears to be numerically unstable and has a high computational cost.

In²³, the variable-projection method (VP) is used for solving the minimization problem. When the reduced minimization problem is solved again by the Gauss-Newton method, we will refer to it as VPGN.

We propose a similar (but different) approach called Modified Gauss-Newton method (MGN), which appears to have some advantages in comparison with VPGN that is one of the best methods for solving the problem (3). Below we will show that the MGN algorithm consists of different numerical sub-problems to be solved, which are more well-conditioned than in the VPGN

case (see²⁸, where different properties of problems such as stability and well-conditioning are discussed); thereby, MGN allows a better numerically stable implementation.

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

Let us introduce the notation, which is used in this section. For a matrix $\mathbf{F} = \mathbb{R}^{N \times p}$, define its weighted pseudoinverse²⁹ $(\mathbf{F})_{\mathbf{W}}^{\dagger} = (\mathbf{F}^T \mathbf{W} \mathbf{F})^{-1} \mathbf{F}^T \mathbf{W}$; this pseudoinverse arises in the solution of the weighted linear least-squares problem $\min_{\mathbf{p}} \|\mathbf{y} - \mathbf{F}\mathbf{p}\|_{\mathbf{W}}^2$ with $\mathbf{y} \in \mathbb{R}^N$, since its solution is equal to $\mathbf{p}_{\min} = (\mathbf{F})_{\mathbf{W}}^{\dagger} \mathbf{y}$. In the particular case $\mathbf{W} = \mathbf{I}_N$, $(\mathbf{F})_{\mathbf{W}}^{\dagger}$ is the ordinary pseudoinverse; we will denote it \mathbf{F}^{\dagger} . Denote the projection (it is oblique if \mathbf{W} is not the identity matrix) onto the column space \mathcal{F} of a matrix \mathbf{F} as $\mathbf{\Pi}_{\mathbf{F}, \mathbf{W}} = \mathbf{F} (\mathbf{F})_{\mathbf{W}}^{\dagger}$. If it is not important which particular basis of \mathcal{F} is considered, we use the notation $\mathbf{\Pi}_{\mathcal{F}, \mathbf{W}}$.

Remark 1. If the matrix \mathbf{F} is complex, the above formulas and considerations are still valid with the change of the transpose \mathbf{F}^T to the complex conjugate \mathbf{F}^H .

The structure of this section is as follows. After a brief discussion of the problem (3), we start with the description of the methods GN and VP for a general optimization problem; then we apply these methods to (3) and finally present the new method MGN.

3.1 | Approaches for solving a general nonlinear least-squares problem

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

$$\mathbf{p}^{\star} = \arg \min_{\mathbf{p}} \|\mathbf{x} - \mathcal{S}(\mathbf{p})\|_{\mathbf{W}}^2, \quad (7)$$

where $\mathbf{p} \in \mathbb{R}^p$ is the vector of parameters, $\mathcal{S} : \mathbb{R}^p \rightarrow \mathbb{R}^N$ is some parameterization of a subset of \mathbb{R}^N such that $\mathcal{S}(\mathbf{p})$ is a differentiable vector-function of \mathbf{p} , $\mathbf{W} \in \mathbb{R}^{N \times N}$ is a positive (semi-)definite symmetric matrix.

If the problem (7) is nonlinear, iterative methods with linearization at each iteration are commonly used, such as the Gauss-Newton method or its variations²⁷. One of the 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 value and does not affect near the minimum. Therefore, in the paper, we consider the Gauss-Newton method without regularization. We use the weighted Gauss-Newton method, which is a straightforward extension of the unweighted version with $\mathbf{W} = \mathbf{I}_N$.

3.1.1 | Gauss-Newton method

One iteration of the Gauss-Newton algorithm with step γ is

$$\mathbf{p}_{k+1} = \mathbf{p}_k + \gamma (\mathbf{J}_{\mathcal{S}}(\mathbf{p}_k))_{\mathbf{W}}^{\dagger} (\mathbf{x} - \mathcal{S}(\mathbf{p}_k)), \quad (8)$$

where $\mathbf{J}_{\mathcal{S}}(\mathbf{p}_k)$ is the Jacobian matrix of $\mathcal{S}(\mathbf{p})$ at \mathbf{p}_k . Note that the iteration step (8) is uniquely defined for any positive semi-definite matrix, see Remark 6. The choice of step γ is a separate problem. For example, one can apply the backtracking line search starting from $\gamma = 1$ and then decreasing the step if the next value is worse (that is, if the value of the objective functional increases).

An additional aim of the WLS problem is to find the approximation $\mathcal{S}(\mathbf{p}^{\star})$ of \mathbf{x} , where \mathbf{p}^{\star} is the solution of (7). Then we can write (8) in the form of iterations of approximations:

$$\mathcal{S}(\mathbf{p}_{k+1}) = \mathcal{S} \left(\mathbf{p}_k + \gamma (\mathbf{J}_{\mathcal{S}}(\mathbf{p}_k))_{\mathbf{W}}^{\dagger} (\mathbf{x} - \mathcal{S}(\mathbf{p}_k)) \right). \quad (9)$$

The following remark explains the approach, which underlies the Modified Gauss-Newton method proposed in this paper (see Section 3.3).

Remark 2. The iteration step (9) can be varied by means of the change of $\mathcal{S}(\mathbf{p}_{k+1})$ to $\tilde{\mathcal{S}}(\mathbf{p}_{k+1})$, where $\tilde{\mathcal{S}}(\mathbf{p}_{k+1})$ is such that $\|\mathbf{x} - \tilde{\mathcal{S}}(\mathbf{p}_{k+1})\|_{\mathbf{W}} \leq \|\mathbf{x} - \mathcal{S}(\mathbf{p}_{k+1})\|_{\mathbf{W}}$. This trick is reasonable if $\tilde{\mathcal{S}}(\mathbf{p}_{k+1})$ can be calculated faster and/or in a more stable way than $\mathcal{S}(\mathbf{p}_{k+1})$.

3.1.2 | Variable projection

Let $\mathbf{p} = \begin{pmatrix} \mathbf{b} \\ \mathbf{c} \end{pmatrix} \in \mathbb{R}^p$, $\mathbf{b} \in \mathbb{R}^{p_1}$, $\mathbf{c} \in \mathbb{R}^{p_2}$. Consider the (weighted) least-squares problem (7), where $S(\mathbf{p})$ is linear in \mathbf{c} and the nonlinear part is defined by $\mathbf{G}(\mathbf{b}) \in \mathbb{R}^{N \times p_2}$:

$$S(\mathbf{p}) = \mathbf{G}(\mathbf{b})\mathbf{c}.$$

This problem can be considered as a problem of projecting the data vector \mathbf{x} onto a given set:

$$\min_{\mathbf{y} \in D} \|\mathbf{x} - \mathbf{y}\|_{\mathbf{W}}, \quad \text{where } D = \left\{ \mathbf{G}(\mathbf{b})\mathbf{c} \mid \begin{pmatrix} \mathbf{b} \\ \mathbf{c} \end{pmatrix} \in \mathbb{R}^p \right\}. \quad (10)$$

Here $\{\varphi(z) \mid z \in C\}$ means the set of values of $\varphi(z)$ for $z \in C$. The variable projection method takes advantage of the known explicit solution of the subproblem:

$$C^*(\mathbf{b}) = \arg \min_{\mathbf{c}} \|\mathbf{x} - \mathbf{G}(\mathbf{b})\mathbf{c}\|_{\mathbf{W}} = (\mathbf{G}(\mathbf{b}))_{\mathbf{W}}^{\dagger} \mathbf{x}.$$

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

$$S^*(\mathbf{b}) = \arg \min_{\mathbf{s} \in \mathcal{G}(\mathbf{b})} \|\mathbf{x} - \mathbf{s}\|_{\mathbf{W}} = \Pi_{\mathcal{G}(\mathbf{b}), \mathbf{W}} \mathbf{x}. \quad (11)$$

Thus, we can reduce the problem (10) to the projection onto a subset $D^* \subset D$ and thereby to the optimization in the nonlinear part of parameters only:

$$\min_{\mathbf{y} \in D^*} \|\mathbf{x} - \mathbf{y}\|_{\mathbf{W}} \quad \text{with } D^* = \{S^*(\mathbf{b}) \mid \mathbf{b} \in \mathbb{R}^{p_1}\}. \quad (12)$$

This is called ‘‘variable projection’’ principle (see²⁴ for the case of the Euclidean norm).

3.2 | Known iterative methods for low-rank approximation

Let us turn from a general nonlinear least-squares problem (7) to the specific problem (3).

A variation from the standard way of the use of iterative methods is that the parameterization $S_{\tau}(\mathbf{p})$, $\mathbf{p} = (\mathbf{s}, \mathbf{a})$ (which is based on τ) is changed at each iteration in a particular way. At $(k + 1)$ -th iteration, the parameterization is constructed in the vicinity of $\mathbf{a}_0 = \mathbf{a}^{(k)}$. The index τ , which determines the parameterization, is chosen in such a way to satisfy $a_{\tau}^{(0)} \neq 0$. We propose the following approach to the choice of τ . Let τ be the index of the maximum absolute entry of \mathbf{a}_0 . Since the parameterization is invariant to the multiplication of \mathbf{a}_0 by a constant, it can be assumed that $a_{\tau}^{(0)} = -1$ and $|a_i^{(0)}| \leq 1$ for any i , $1 \leq i \leq r + 1$.

3.2.1 | Weighted Gauss-Newton method

The Gauss-Newton algorithm can be applied to the problem (3) in a straightforward manner, taking into consideration that the parameterization S_{τ} may be changed at each iteration. The Gauss-Newton iteration has the form $\mathbf{p}_{k+1} = \mathbf{p}_k + \gamma (\mathbf{J}_{S_{\tau}}(\mathbf{p}_k))_{\mathbf{W}}^{\dagger} (\mathbf{X} - S_{\tau}(\mathbf{p}_k))$.

To apply the method, $S_{\tau}(\mathbf{p}_k)$ and the Jacobian matrix $\mathbf{J}_{S_{\tau}}(\mathbf{p}_k)$ should be calculated. Formally, their computing can be implemented; however, the direct calculation is not numerically stable and very time-consuming.

3.2.2 | Gauss-Newton method with variable projection

The explicit form of the parameterization $S_{\tau}(\mathbf{p}) = S_{\tau}(\mathbf{s}, \mathbf{a})$ given in (6), where \mathbf{s} is presented in $S_{\tau}(\mathbf{s}, \mathbf{a})$ in a linear manner, allows one to apply the variable projection principle.

Assume that S_0 is governed by a GLRR(\mathbf{a}_0) with $a_{\tau}^{(0)} = -1$ and consider the problem (3) in the vicinity of the series $S_0 \in D_r$.

Substitute in (12) $D = \overline{D}_r$, $D^* = D_r^* \subset \overline{D}_r$, where $D_r^* = \{\Pi_{Z(H_{\tau}(\mathbf{a})), \mathbf{W}} \mathbf{X} \mid \mathbf{a} \in \mathbb{R}^r\}$, $\mathbf{b} = \mathbf{a}$, $\mathbf{G}(\mathbf{b}) = \mathbf{G}$, where $\mathbf{G} = \mathbf{Z}(\mathbf{Z}_{I(\tau), :})^{-1}$ (see (6)), $C^*(\mathbf{b}) = (\mathbf{G})_{\mathbf{W}}^{\dagger} \mathbf{X}$. Then

$$S_{\tau}^*(\mathbf{a}) = \Pi_{Z(\mathbf{a}), \mathbf{W}}(\mathbf{X}) \quad (13)$$

where $\mathbf{a} = H_{\tau}(\mathbf{a})$, and we obtain the equivalent problem for projecting the elements of the set \overline{D}_r to the subset D_r^* , where the parameter \mathbf{s} is eliminated:

$$\mathbf{Y}^* = \arg \min_{\mathbf{Y} \in D_r^*} \|\mathbf{X} - \mathbf{Y}\|_{\mathbf{W}}. \quad (14)$$

or, the same,

$$\hat{\mathbf{a}}^* = \arg \min_{\hat{\mathbf{a}} \in \mathbb{R}^r} \|\mathbf{X} - \mathbf{S}_\tau^*(\hat{\mathbf{a}})\|_{\mathbf{W}}, \quad (15)$$

Thus, for the numerical solution of the equation (3), it is sufficient to consider iterations for the nonlinear part of the parameters. This is the VP approach used in^{22, 23}.

Let us denote $\mathbf{J}_{\mathbf{S}_\tau^*}(\hat{\mathbf{a}})$ the Jacobian matrix of $\mathbf{S}_\tau^*(\hat{\mathbf{a}})$. Then the iterations of the Gauss-Newton method for solving the problem (15) have the form

$$\hat{\mathbf{a}}^{(k+1)} = \hat{\mathbf{a}}^{(k)} + \gamma \left(\mathbf{J}_{\mathbf{S}_\tau^*}(\hat{\mathbf{a}}^{(k)}) \right)_{\mathbf{W}}^\dagger (\mathbf{X} - \mathbf{S}_\tau^*(\hat{\mathbf{a}}^{(k)})). \quad (16)$$

The VPGN algorithm together with an explicit form of $\mathbf{J}_{\mathbf{S}_\tau^*}(\hat{\mathbf{a}}^{(k)})$ is presented in⁴; its iteration step is described in Algorithm 4.

3.3 | Modified Gauss-Newton method for low-rank approximation

In this section, we propose a new iterative method for the problem (3), which is a modified Gauss-Newton method.

Let us return to the problem with the full set of parameters $(\hat{\mathbf{s}}, \hat{\mathbf{a}})$ and apply the approach that is described in Remark 2, with $\tilde{\mathbf{S}}(\mathbf{p}) = \mathbf{S}_\tau^*(\hat{\mathbf{a}})$. We can do it, since $\mathbf{S}_\tau^*(\hat{\mathbf{a}}) = \Pi_{\mathcal{Z}(H_\tau(\hat{\mathbf{a}}), \mathbf{W})} \mathbf{X}$ and therefore (11) is valid with $\mathcal{G}(\hat{\mathbf{a}}) = \mathcal{Z}(H_\tau(\hat{\mathbf{a}}))$. Thus, we can consider $\mathbf{S}_\tau^*(\hat{\mathbf{a}}^{(k+1)}) \in \mathcal{D}_r^*$ as the result of the $(k+1)$ -th iteration instead of $\mathbf{S}_\tau(\hat{\mathbf{s}}^{(k+1)}, \hat{\mathbf{a}}^{(k+1)}) \in \overline{\mathcal{D}}_r$. It appears (see⁴) that then we can use more stable numerical calculations for the iteration implementation. The proposed modification is similar to variable projections, since we can omit the part $\hat{\mathbf{s}}$ of parameters.

Thus, we introduce the MGN iteration in the form

$$\hat{\mathbf{a}}^{(k+1)} = \hat{\mathbf{a}}^{(k)} + \gamma \left(\left(\mathbf{J}_{\mathbf{S}_\tau}(\hat{\mathbf{s}}^{(k)}, \hat{\mathbf{a}}^{(k)}) \right)_{\mathbf{W}}^\dagger (\mathbf{X} - \mathbf{S}_\tau^*(\hat{\mathbf{a}}^{(k)})) \right)_{:, \{r+1, \dots, 2r\}}, \quad (17)$$

where $\hat{\mathbf{s}}^{(k)}$ are the corresponding boundary data taken from $\mathbf{S}_\tau^*(\hat{\mathbf{a}}^{(k)})$, i.e. $\hat{\mathbf{s}}^{(k)} = (\mathbf{S}_\tau^*(\hat{\mathbf{a}}^{(k)}))_{I(\tau)}$. As well as in the variable projection method with the iteration step (16), $\mathbf{S}_\tau^*(\hat{\mathbf{a}}^{(k+1)}) \in \mathcal{D}_r^*$ for each k .

Theorem 3.1. Let $\mathbf{W}^{1/2} \mathbf{J}_{\mathbf{S}_\tau}(\hat{\mathbf{s}}^{(k)}, \hat{\mathbf{a}}^{(k)})$ have full rank. Denote $\mathbf{S} = T_{r+1}(\Pi_{\mathcal{Z}(H_\tau(\hat{\mathbf{a}}^{(k)}), \mathbf{W})} \mathbf{X})$, $\mathbf{M} = -(\mathbf{S}_{\mathcal{K}(\tau), :})^T$. Then the iteration step (17) is equivalent to

$$\hat{\mathbf{a}}^{(k+1)} = \hat{\mathbf{a}}^{(k)} + \gamma \left((\mathbf{I}_N - \Pi_{\mathcal{Z}(H_\tau(\hat{\mathbf{a}}^{(k)}), \mathbf{W})}) \hat{\mathbf{F}}_{\mathbf{a}} \right)_{\mathbf{W}}^\dagger (\mathbf{X} - \mathbf{S}_\tau^*(\hat{\mathbf{a}}^{(k)})), \quad (18)$$

where $\hat{\mathbf{F}}_{\mathbf{a}} \in \mathbb{C}^{N \times 2r}$ is an arbitrary matrix satisfying the equality $\mathbf{Q}^T(H_\tau(\hat{\mathbf{a}}^{(k)})) \hat{\mathbf{F}}_{\mathbf{a}} = \mathbf{M}$.

Let us fix the iteration number k . Denote by $\mathbf{F}_{\mathbf{s}} = (\mathbf{J}_{\mathbf{S}_\tau})_{:, \{1, \dots, r\}}$ the first r columns of the Jacobian matrix $\mathbf{J}_{\mathbf{S}_\tau} = \mathbf{J}_{\mathbf{S}}(\hat{\mathbf{s}}^{(k)}, \hat{\mathbf{a}}^{(k)})$, and by $\mathbf{F}_{\mathbf{a}} = (\mathbf{J}_{\mathbf{S}_\tau})_{:, \{r+1, \dots, 2r\}}$ the last r columns of $\mathbf{J}_{\mathbf{S}_\tau}$.

Before proving the theorem, let us write down the statements of several propositions of⁴.

By definition, the tangent space at the point \mathbf{S} coincides with $\text{colspace}(\mathbf{J}_{\mathbf{S}_\tau}(\hat{\mathbf{s}}, \hat{\mathbf{a}}))$. Note that the tangent space is invariant with respect to the choice of a certain parameterization of \mathcal{D}_r in the vicinity of \mathbf{S} .

Define by \mathbf{a}^2 the acyclic convolution of \mathbf{a} with itself:

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

Lemma 1 (⁴). $\mathbf{Q}^T(\mathbf{a}) \mathbf{F}_{\mathbf{s}} = \mathbf{0}_{(N-r) \times r}$; $\text{colspace}(\mathbf{F}_{\mathbf{s}}) = \mathcal{Z}(\mathbf{a})$.

Lemma 2 (⁴). $\mathbf{Q}^T(\mathbf{a}) \mathbf{F}_{\mathbf{a}} = -(\mathbf{S}_{\mathcal{K}(\tau), :})^T$, where $\mathbf{S} = T_{r+1}(\mathbf{S})$; $\text{colspace}(\mathbf{F}_{\mathbf{a}}) \subset \mathcal{Z}(\mathbf{a}^2)$.

Theorem 3.2 (⁴). The tangent space of \mathcal{D}_r at the point \mathbf{S} has dimension $2r$ and is equal to $\mathcal{Z}(\mathbf{a}^2)$.

Proof of Theorem 3.1. Let us rewrite the weighted pseudoinverse in the (17) as

$$\left((\mathbf{J}_{\mathbf{S}_\tau}(\hat{\mathbf{s}}^{(k)}, \hat{\mathbf{a}}^{(k)}))_{\mathbf{W}}^\dagger (\mathbf{X} - \mathbf{S}_\tau^*(\hat{\mathbf{a}}^{(k)})) \right)_{:, \{r+1, \dots, 2r\}} = \left((\mathbf{W}^{1/2} \mathbf{J}_{\mathbf{S}_\tau}(\hat{\mathbf{s}}^{(k)}, \hat{\mathbf{a}}^{(k)}))^\dagger \mathbf{W}^{1/2} (\mathbf{X} - \mathbf{S}_\tau^*(\hat{\mathbf{a}}^{(k)})) \right)_{:, \{r+1, \dots, 2r\}}.$$

Applying the Frisch-Waugh-Lovell theorem³⁰ about the partitioned regression to the obtained pseudoinverse for regressors $\mathbf{W}^{1/2}\mathbf{F}_s$ and $\mathbf{W}^{1/2}\mathbf{F}_a$, we get the following sequence of equalities:

$$\begin{aligned} \left((\mathbf{W}^{1/2}\mathbf{J}_{S_\tau}(\hat{\mathbf{s}}^{(k)}, \hat{\mathbf{a}}^{(k)}))^\dagger \mathbf{W}^{1/2}(\mathbf{X} - S_\tau^*(\hat{\mathbf{a}}^{(k)})) \right)_{:, \{r+1, \dots, 2r\}} &= \\ (\mathbf{I}_N - \mathbf{\Pi}_{\mathbf{W}^{1/2}\mathbf{F}_s}) \mathbf{W}^{1/2}\mathbf{F}_a &^\dagger (\mathbf{I}_N - \mathbf{\Pi}_{\mathbf{W}^{1/2}\mathbf{F}_s}) \mathbf{W}^{1/2}(\mathbf{X} - S_\tau^*(\hat{\mathbf{a}}^{(k)})) = \\ (\mathbf{I}_N - \mathbf{\Pi}_{\mathcal{Z}(H_\tau(\hat{\mathbf{a}}^{(k)}), \mathbf{W})}) \mathbf{F}_a &^\dagger (\mathbf{I}_N - \mathbf{\Pi}_{\mathcal{Z}(H_\tau(\hat{\mathbf{a}}^{(k)}), \mathbf{W})})(\mathbf{X} - \mathbf{\Pi}_{\mathcal{Z}(H_\tau(\hat{\mathbf{a}}^{(k)}), \mathbf{W})}\mathbf{X}). \end{aligned}$$

Since $\mathbf{I}_N - \mathbf{\Pi}_{\mathcal{Z}(H_\tau(\hat{\mathbf{a}}^{(k)}), \mathbf{W})}$ is a projector, $(\mathbf{I}_N - \mathbf{\Pi}_{\mathcal{Z}(H_\tau(\hat{\mathbf{a}}^{(k)}), \mathbf{W})})^2 = \mathbf{I}_N - \mathbf{\Pi}_{\mathcal{Z}(H_\tau(\hat{\mathbf{a}}^{(k)}), \mathbf{W})}$. Thus, we obtain the following iteration equivalent to (17):

$$\hat{\mathbf{a}}^{(k+1)} = \hat{\mathbf{a}}^{(k)} + \gamma (\mathbf{I}_N - \mathbf{\Pi}_{\mathcal{Z}(H_\tau(\hat{\mathbf{a}}^{(k)}), \mathbf{W})}) \mathbf{F}_a^\dagger (\mathbf{I}_N - \mathbf{\Pi}_{\mathcal{Z}(H_\tau(\hat{\mathbf{a}}^{(k)}), \mathbf{W})}) \mathbf{X}. \quad (19)$$

By Lemma 2, $\mathbf{Q}^T(H_\tau(\hat{\mathbf{a}}^{(k)}))\mathbf{F}_a = \mathbf{M}$. By the theorem's conditions, $\mathbf{Q}^T(H_\tau(\hat{\mathbf{a}}^{(k)}))\hat{\mathbf{F}}_a = \mathbf{M}$. Thus, $\mathbf{Q}^T(H_\tau(\hat{\mathbf{a}}^{(k)}))(\mathbf{F}_a - \hat{\mathbf{F}}_a) = \mathbf{0}_{(N-r) \times r}$. Since $\mathcal{Q}(\mathbf{a})$ is the orthogonal complement to $\mathcal{Z}(\mathbf{a})$, $(\mathbf{I}_N - \mathbf{\Pi}_{\mathcal{Z}(H_\tau(\hat{\mathbf{a}}^{(k)}), \mathbf{W})})(\mathbf{F}_a - \hat{\mathbf{F}}_a) = \mathbf{0}_{N \times r}$, which finishes the proof. \square

Remark 3. In the case when $S_\tau(\hat{\mathbf{s}}^{(k)}, \hat{\mathbf{a}}^{(k)}) \in \mathcal{D}_r$, the Jacobian matrix $\mathbf{J}_{S_\tau}(\hat{\mathbf{s}}^{(k)}, \hat{\mathbf{a}}^{(k)})$ has full rank, according to Theorem 3.2. This is sufficient for validity of the condition of Theorem 3.1 if \mathbf{W} has full rank. In the case of a rank-deficient matrix \mathbf{W} , the condition of Theorem 3.1 is discussed in Remark 6 with $\mathbf{F} = \mathbf{J}_{S_\tau}(\hat{\mathbf{s}}^{(k)}, \hat{\mathbf{a}}^{(k)})$.

Thus, we have constructed the equivalent version (18) of the iteration step (17) in such a way to reduce its complexity to the computational costs of computing the projections to $\mathcal{Z}(H_\tau(\hat{\mathbf{a}})) = \mathcal{Z}(\mathbf{a})$ and calculating the matrices $\hat{\mathbf{F}}_a$ for different \mathbf{a} . A numerically robust algorithm for calculating the iteration step (18) is given in Algorithm 5.

4 | ALGORITHMS OF THE VPGN AND MGN METHODS

The common scheme of the VPGN and MGN algorithms is given in Algorithm 1.

Algorithm 1 The common scheme of VPGN and MGN

Input: $\mathbf{X} \in \mathbb{R}^N$, $\mathbf{a}_0 \in \mathbb{R}^{r+1}$, a stopping criterion STOP.

- 1: Set $k = 0$, $\mathbf{b}^{(0)} = \mathbf{a}_0$.
 - 2: **repeat**
 - 3: Choose τ such that $b_\tau^{(k)} \neq 0$; for example, find $\tau = \arg \max_i |b_i^{(k)}|$. Calculate $\mathbf{a}^{(k)} = -\mathbf{b}^{(k)}/b_\tau^{(k)}$ to obtain $a_\tau^{(k)} = -1$ and take $\hat{\mathbf{a}}^{(k)} = H_\tau^{-1}(\mathbf{a}^{(k)})$.
 - 4: Calculate $\mathbf{S}_k = S_\tau^*(\hat{\mathbf{a}}^{(k)})$, where $S_\tau^*(\hat{\mathbf{a}}^{(k)}) = \mathbf{\Pi}_{\mathcal{Z}(\hat{\mathbf{a}}^{(k)}), \mathbf{W}}\mathbf{X}$.
 - 5: Calculate the direction $\Delta_k = \Delta(\hat{\mathbf{a}}^{(k)}, \mathbf{S}_k)$.
 - 6: Choose the size γ_k and perform the step of size γ_k in the descent direction given by Δ_k . For example, find $\gamma_k = \gamma$, $0 \leq \gamma \leq 1$, such that $\|\mathbf{X} - S_\tau^*(\hat{\mathbf{a}}^{(k)} + \gamma\Delta_k)\|_{\mathbf{W}} \leq \|\mathbf{X} - S_\tau^*(\hat{\mathbf{a}}^{(k)})\|_{\mathbf{W}}$ by the backtracking line search method²⁷, Section 3.1.
 - 7: Set $\hat{\mathbf{a}}^{(k+1)} = \hat{\mathbf{a}}^{(k)} + \gamma_k\Delta_k$, $\mathbf{b}^{(k+1)} = H_\tau(\hat{\mathbf{a}}^{(k+1)})$.
 - 8: Set $k = k + 1$.
 - 9: **until** STOP
 - 10: **return** $\tilde{\mathbf{S}} = S_\tau^*(\hat{\mathbf{a}}^{(k)})$ as an estimate of the signal.
-

As it is shown in⁴, the calculation of the direction in step 5 is the ‘‘bottleneck’’ of the VPGN algorithm, since the calculation of S_τ^* in steps 4 and 6 can be stably implemented (see S-VPGN in⁴). Moreover, the computational cost of step 5 is very large for the case of banded weight matrices \mathbf{W} , which correspond to autoregressive noise. The MGN method is designed to improve step 5.

Thus, we have Algorithm 1 with

$$\text{VPGN: } \Delta(\hat{\mathbf{a}}^{(k)}, \mathbf{S}_k) = \left(\mathbf{J}_{S_\tau^*}(\hat{\mathbf{a}}^{(k)}) \right)_{\mathbf{W}}^\dagger (\mathbf{X} - \mathbf{S}_k), \quad (20)$$

$$\text{MGN: } \Delta(\hat{\mathbf{a}}^{(k)}, \mathbf{S}_k) = \left((\mathbf{I}_N - \mathbf{\Pi}_{\mathcal{Z}(H_\tau(\hat{\mathbf{a}}^{(k)}), \mathbf{W})}) \hat{\mathbf{F}}_a \right)_{\mathbf{W}}^\dagger (\mathbf{X} - \mathbf{S}_k), \quad (21)$$

where $\mathbf{S}_k = \mathcal{S}_r^*(\hat{\mathbf{a}}^{(k)}) = \mathbf{\Pi}_{\mathcal{Z}(H_r(\hat{\mathbf{a}}^{(k)}), \mathbf{W})} \mathbf{X}$.

The stable versions of calculating the projection are described in⁴ (the algorithms S-VPGN and S-VPGN-H). All the version of VPGN still have a ‘‘bottleneck’’ in calculation of $\mathbf{J}_{\mathcal{S}_r^*}(\hat{\mathbf{a}}^{(k)})$, while the whole MGN algorithm can be stably implemented.

4.1 | Stable auxiliary algorithms

Algorithm 2 below contains the stable implementation of computing the basis for calculating the projection $\mathbf{\Pi}_{\mathcal{Z}(H_r(\hat{\mathbf{a}}^{(k)}), \mathbf{W})}$ ⁴. The step of MGN additionally contains the calculation of $\hat{\mathbf{F}}_{\mathbf{a}}$. Applying the technique of⁴, we can derive Algorithm 3 for calculating $\hat{\mathbf{F}}_{\mathbf{a}}$.

Let us briefly describe the approach of⁴. Denote

$$g_{\mathbf{a}}(z) = \sum_{k=0}^r a_{k+1} z^k \quad (22)$$

the complex polynomial with coefficients $\mathbf{a} = (a_1, \dots, a_{r+1})^T$; we do not assume that the leading coefficient is non-zero.

Let the circulant matrix $\mathbf{C}(\mathbf{a})$ be the extension of the partial circulant $\mathbf{Q}^T(\mathbf{a})$. Then the construction of a basis of $\mathcal{Z}(\mathbf{a})$ can be reduced to solving the system of linear equations

$$\mathbf{C}(\mathbf{a})\mathbf{v}_k = \mathbf{e}_{N-k+1}, \quad k = 1, \dots, r. \quad (23)$$

The eigenvalues of $\mathbf{C}(\mathbf{a})$ coincide with the values of the polynomial $g_{\mathbf{a}}(z)$ in nodes of the equidistant grid $\mathcal{W} = \left\{ \exp\left(\frac{i2\pi j}{N}\right), j = 0, \dots, N-1 \right\}$ on the complex unit circle $\mathbb{T} = \{z \in \mathbb{C} : |z| = 1\}$. Therefore, the nondegeneracy of $\mathbf{C}(\mathbf{a})$ is equivalent to that there are no roots of the polynomial $g_{\mathbf{a}}(z)$ in \mathcal{W} .

Let us define the unitary matrix

$$\mathbf{T}_M(\alpha) = \text{diag}\left((1, e^{i\alpha}, \dots, e^{i(M-1)\alpha})^T\right), \quad (24)$$

where α is a real number, M is a natural number.

Remark 4. In the exact arithmetic, an arbitrary small non-zero value of the smallest eigenvalue of a matrix provides its non-degeneracy. However, in practice, the numerical stability and accuracy of matrix calculations depend on the condition numbers of matrices. Therefore, the aim of the choice of a proper α is to do the condition number of $\mathbf{C}(\tilde{\mathbf{a}}(\alpha))$, where $\tilde{\mathbf{a}} = \tilde{\mathbf{a}}(\alpha) = (\mathbf{T}_{r+1}(-\alpha)) \mathbf{a}$, as small as possible. This minimization problem can be approximately reduced to the problem of maximization of the smallest eigenvalue $|\lambda_{\min}(\alpha)| = \min_{z \in \mathcal{W}(\alpha)} |g_{\mathbf{a}}(z)|$ of $\mathbf{C}(\tilde{\mathbf{a}}(\alpha))$, since the maximal eigenvalue is not larger than $\max_{z \in \mathbb{T}} |g_{\mathbf{a}}(z)|$.

Denote \mathcal{F}_N and \mathcal{F}_N^{-1} the Fourier transform and the inverse Fourier transform for series of length N , respectively. Define $\mathcal{F}_N(\mathbf{X}) = [\mathcal{F}_N(\mathbf{x}_1) : \dots : \mathcal{F}_N(\mathbf{x}_r)]$, where $\mathbf{X} = [\mathbf{x}_1 : \dots : \mathbf{x}_r]$; the same for $\mathcal{F}_N^{-1}(\mathbf{Y})$. Algorithm 2 exploits the fact that the operations with circulant matrices can be implemented by means of fast Fourier transform³¹.

Algorithm 2 Calculation of a basis of $\mathcal{Z}(\mathbf{a}) \subset \mathbb{C}^{N \times 4}$

Input: $\mathbf{a} \in \mathbb{R}^r$.

- 1: Find $\alpha_0 = \arg \max_{-\pi/N \leq \alpha < \pi/N} \min_{z \in \mathcal{W}(\alpha)} |g_{\mathbf{a}}(z)|$ by means of a 1D numerical optimization method.
 - 2: Calculate the vector $\mathbf{a}_g = (a_{g,0}, \dots, a_{g,N-1})^T$ consisting of the eigenvalues of $\mathbf{C}(\tilde{\mathbf{a}})$ by $a_{g,j} = g_{\mathbf{a}}\left(\exp\left(i\left(\frac{2\pi j}{N} - \alpha_0\right)\right)\right)$, $j = 0, \dots, N-1$, where $\tilde{\mathbf{a}} = (\mathbf{T}_{r+1}(-\alpha)) \mathbf{a}$; $\mathbf{A}_g = \text{diag}(\mathbf{a}_g)$.
 - 3: Calculate the matrices $\mathbf{R}_r = \mathcal{F}_N([\mathbf{e}_{N-r+1} : \dots : \mathbf{e}_N])$ and $\mathbf{L}_r = \mathbf{A}_g^{-1} \mathbf{R}_r$.
 - 4: Compute \mathbf{U}_r : find \mathbf{O}_r such that $\mathbf{L}_r \mathbf{O}_r$ consists of orthonormal columns (\mathbf{O}_r can be found by either the QR factorization or the SVD); calculate $\mathbf{B} = \mathbf{R}_r \mathbf{O}_r$ and $\mathbf{U}_r = \mathbf{A}_g^{-1} \mathbf{B}$.
 - 5: Compute $\tilde{\mathbf{Z}} = \mathcal{F}_N^{-1}(\mathbf{U}_r)$.
 - 6: **return** $\mathbf{Z} = (\mathbf{T}_N(-\alpha_0)) \tilde{\mathbf{Z}} \in \mathbb{C}^{N \times r}$, whose columns form an orthonormal basis of $\mathcal{Z}(\mathbf{a})$, α_0 and \mathbf{A}_g .
-

Let us now turn to calculating the matrix $\hat{\mathbf{F}}_{\mathbf{a}}$. According to Theorem 3.1, it is sufficient to find an arbitrary matrix such that $\mathbf{Q}^T(\mathbf{a}) \hat{\mathbf{F}}_{\mathbf{a}} = \mathbf{M}$, where $\mathbf{M} \in \mathbb{R}^{(N-r) \times r}$ is defined in Theorem 3.1. Therefore, it is sufficient to solve the following systems of linear

equations:

$$\mathbf{C}(\mathbf{a})\hat{\mathbf{F}}_{\mathbf{a}} = \begin{pmatrix} \mathbf{M} \\ \mathbf{0}_{r \times r} \end{pmatrix}. \quad (25)$$

The following lemma is a direct application of the theorem about the solution of a linear system of equations given by a circulant matrix³².

Lemma 3. Define $\hat{\mathbf{F}}_{\mathbf{a}} = \mathcal{F}_N^{-1}(\mathbf{A}_g^{-1}\hat{\mathbf{R}}_r)$, where $\hat{\mathbf{R}}_r = \mathcal{F}_N \left(\begin{pmatrix} \mathbf{M} \\ \mathbf{0}_{r \times r} \end{pmatrix} \right)$. Then $\mathbf{Q}^T(\mathbf{a})\hat{\mathbf{F}}_{\mathbf{a}} = \mathbf{M}$, i.e. $\hat{\mathbf{F}}_{\mathbf{a}}$ satisfies the conditions of Theorem 3.1.

Remark 4 together with Lemma 3 provide Algorithm 3.

Algorithm 3 Calculation of a matrix $\hat{\mathbf{F}}_{\mathbf{a}}$ in (18)

Input: $\mathbf{a} \in \mathbb{R}^r$ and a series $\mathbf{S} \in \mathbb{R}^N$ governed by the GLRR(\mathbf{a}).

- 1: Compute α_0, \mathbf{A}_g using steps 1 and 2 of Algorithm 2.
 - 2: Construct $\mathbf{M} = -(\mathbf{S}_{\mathcal{K}(\tau)}, :)^T$, where $\mathbf{S} = T_{r+1}(\mathbf{S})$.
 - 3: Calculate $\tilde{\mathbf{M}} = \begin{pmatrix} (\mathbf{T}_{N-r}(\alpha_0))\mathbf{M} \\ \mathbf{0}_{r \times r} \end{pmatrix}$.
 - 4: Calculate $\hat{\mathbf{R}}_r = \mathcal{F}_N(\tilde{\mathbf{M}})$ and $\tilde{\mathbf{F}}_{\mathbf{a}} = \mathcal{F}_N^{-1}(\mathbf{A}_g^{-1}\hat{\mathbf{R}}_r)$.
 - 5: **return** $\hat{\mathbf{F}}_{\mathbf{a}} = (\mathbf{T}_N(-\alpha_0))\tilde{\mathbf{F}}_{\mathbf{a}} \in \mathbb{C}^{N \times 2r}$.
-

Remark 5. In⁴, an enhanced version of Algorithm 2 using the compensated Horner scheme of³³ is considered. In the version with the compensated Horner scheme, this scheme is applied to calculating the values of the polynomial g and multiplication $\mathbf{R}_r\mathbf{O}_r$. It is shown that this way of calculations considerably improves the stability of the projection algorithm. The construction of Algorithm 3 allows one to improve its stability by the change of the first step ‘‘Compute α_0, \mathbf{A}_g using Algorithm 2’’ to its enhanced version.

4.2 | Algorithms for the iteration step in VPGN and MGN

Thus, both VPGN and MGN are particular cases of Algorithm 1 with different directions of the line search given by formulas 20 and 21 and presented in Algorithms 4 and 5.

Algorithm 4 Calculating the direction in VPGN

Input: $\mathbf{X} \in \mathbb{R}^N, \hat{\mathbf{a}}^{(k)} \in \mathbb{R}^{r+1}$.

- 1: Calculate $\mathbf{S}_k = \mathbf{S}_\tau^*(\hat{\mathbf{a}}^{(k)})$ as $\mathbf{S}_k = \mathbf{\Pi}_{\mathcal{Z}(\hat{\mathbf{a}}^{(k)}), \mathbf{W}}\mathbf{X}$.
 - 2: Calculate $\mathbf{J}_{\mathbf{S}_\tau^*}(\hat{\mathbf{a}}^{(k)})$.
 - 3: Calculate $\Delta_k = \left(\mathbf{J}_{\mathbf{S}_\tau^*}(\hat{\mathbf{a}}^{(k)}) \right)_{\mathbf{W}}^\dagger (\mathbf{X} - \mathbf{S}_k)$.
 - 4: **return** Δ_k
-

The technique for calculating the projector $\mathbf{\Pi}_{\mathcal{Z}(\hat{\mathbf{a}}), \mathbf{W}}$ developed in⁴ uses the basis consisting of the vectors found by Algorithm 2. This technique supplemented by Algorithm 3 allows one to create fast and stable implementation of MGN (Algorithm 5). The calculation of $\mathbf{J}_{\mathbf{S}_\tau^*}(\hat{\mathbf{a}}^{(k)})$ does not allow for both a fast and stable implementation of VPGN, even if Algorithm 2 is used for calculating the projector $\mathbf{\Pi}_{\mathcal{Z}(\hat{\mathbf{a}}), \mathbf{W}}$ (the S-VPGN algorithm in⁴).

Algorithm 5 Calculating the direction in MGN

-
- Input:** $\mathbf{X} \in \mathbb{R}^N$, $\hat{\mathbf{a}}^{(k)} \in \mathbb{R}^{r+1}$.
- 1: Calculate $\mathbf{S}_k = \mathcal{S}_\tau^*(\hat{\mathbf{a}}^{(k)})$ as $\mathbf{S}_k = \mathbf{\Pi}_{\mathcal{Z}(\hat{\mathbf{a}}^{(k)}, \mathbf{W})} \mathbf{X}$.
 - 2: Calculate $\hat{\mathbf{F}}_{\hat{\mathbf{a}}^{(k)}}$ by Algorithm 3 with $\mathbf{a} = \hat{\mathbf{a}}^{(k)}$ and $\mathbf{S} = \mathbf{S}_k$.
 - 3: Calculate $\Delta_k = \left((\mathbf{I}_N - \mathbf{\Pi}_{\mathcal{Z}(\hat{\mathbf{a}}^{(k)}, \mathbf{W})}) \hat{\mathbf{F}}_{\hat{\mathbf{a}}^{(k)}} \right)^\dagger_{\mathbf{W}} (\mathbf{X} - \mathbf{S}_k)$.
 - 4: **return** Δ_k
-

4.3 | The case of degenerate $(2p + 1)$ -diagonal \mathbf{W}

Let us show how Algorithm 5 in MGN can be implemented for a time series with missing values. Let a symmetric positive-definite matrix \mathbf{W}_0 be given for the whole time series including missing entries. Then the weight matrix \mathbf{W} is constructed from \mathbf{W}_0 by setting the values of its columns and rows with indices equal to the entries of missing values to zero. In the case of AR(p) noise, the matrix \mathbf{W}_0 (and therefore \mathbf{W}) is $(2p + 1)$ -diagonal.

Thus, consider a $(2p + 1)$ -diagonal matrix \mathbf{W} which can be degenerate.

In the considered algorithms, there is a problem of calculating the weighted pseudoinverses and projections if the weight matrix \mathbf{W} is degenerate. Let us extend the definition of $(\mathbf{F})^\dagger_{\mathbf{W}}$ and $\mathbf{\Pi}_{\mathbf{F}, \mathbf{W}}$ for some matrix \mathbf{F} .

Consider a degenerate case when $\mathbf{F}^T \mathbf{W} \mathbf{F}$ is not positive definite or, the same, $\mathbf{W}^{1/2} \mathbf{F}$ is rank-deficient ($\mathbf{W}^{1/2}$ is the principal square root of \mathbf{W}). Then we can use a different representation for the weighted pseudoinverse: $(\mathbf{F})^\dagger_{\mathbf{W}} = (\mathbf{W}^{1/2} \mathbf{F})^\dagger \mathbf{W}^{1/2}$. This corresponds to the minimum-(semi)norm solution of the corresponding WLS problem $\min_{\mathbf{p}} \|\mathbf{y} - \mathbf{F}\mathbf{p}\|_{\mathbf{W}}^2$. Although the projection $\mathbf{\Pi}_{\mathbf{F}, \mathbf{W}}$ is generally not uniquely defined in the degenerate case, we will consider its uniquely defined version given by the formula $\mathbf{\Pi}_{\mathbf{F}, \mathbf{W}} = \mathbf{F} (\mathbf{F})^\dagger_{\mathbf{W}}$.

Remark 6. Note that the matrix $\mathbf{W}^{1/2} \mathbf{F}$ is rank-deficient if \mathbf{F} is rank-deficient. However, for a full-rank \mathbf{F} and a degenerate \mathbf{W} , $\mathbf{W}^{1/2} \mathbf{F}$ is not necessarily rank-deficient. For example, if the orthogonal projections of the columns of \mathbf{F} on $\text{colspace}(\mathbf{W})$ are linearly independent, then $\mathbf{W}^{1/2} \mathbf{F}$ is full-rank.

Calculation of weighted projection onto subspace with a given basis

Consider the Cholesky decomposition $\mathbf{W} = \mathbf{C}^T \mathbf{C}$; here \mathbf{C} is an upper triangular matrix with p nonzero superdiagonals^{34, p. 180}.

The calculation of the pseudoinverse $(\mathbf{CZ})^\dagger$ can be reduced to solving a linear least-squares problem and therefore its computing can be performed with the help of either the QR factorization or the SVD of the matrix \mathbf{CZ} .

Although Algorithm 6 for calculating the projection can be applied to the case of positive semidefinite weight matrices, the general case of the Cholesky factorization of a degenerate matrix \mathbf{W} is complicated, see^{35, p. 201}.

Algorithm 6 Calculation of $(\mathbf{Z})^\dagger_{\mathbf{W}}$ and $\mathbf{\Pi}_{\mathbf{Z}, \mathbf{W}} \mathbf{x}$ with the use of $\mathbf{W} = \mathbf{C}^T \mathbf{C}$

-
- Input:** $\mathbf{Z} \in \mathbb{C}^{N \times r}$, $\mathbf{W} \in \mathbb{R}^{N \times N}$ and $\mathbf{x} \in \mathbb{C}^N$.
- 1: Compute the vector $\mathbf{C}\mathbf{x}$ and the matrix \mathbf{CZ} .
 - 2: Calculate $\mathbf{q} = (\mathbf{CZ})^\dagger (\mathbf{C}\mathbf{x})$.
 - 3: **return** $(\mathbf{Z})^\dagger_{\mathbf{W}} = \mathbf{q} \in \mathbb{R}^{r \times N}$ and $\mathbf{\Pi}_{\mathbf{Z}, \mathbf{W}} \mathbf{x} = \mathbf{Z}\mathbf{q} \in \mathbb{R}^N$.
-

However, there is a particular case of degenerate weight matrices, which correspond to a time series with missing values. In this case, the weight matrix \mathbf{W} has zero columns and rows corresponding to missing entries and thereby can be easily processed. Denote $\mathbf{u} \in \mathbb{R}^N$ the vector with ones at the places of observations and zeros at the places of missing values, $\mathbf{U} = \text{diag}(\mathbf{u})$. Then the matrix \mathbf{W} can be expressed as $\mathbf{W} = \mathbf{U}^T \mathbf{W}_0 \mathbf{U}$. Suppose that \mathbf{W}_0 is positive definite. Consider the Cholesky decomposition $\mathbf{W}_0 = \mathbf{C}_0^T \mathbf{C}_0$, where \mathbf{C}_0 is upper triangle, and set $\mathbf{C} = \mathbf{C}_0 \mathbf{U}$. Then $\mathbf{W} = \mathbf{C}^T \mathbf{C}$. Note that if \mathbf{C}_0 is upper triangular with p nonzero superdiagonals, then \mathbf{C} is also upper triangular and has p nonzero superdiagonals.

5 | COMPARISON OF THE VPGN AND MGN ALGORITHMS

Let us compare the VPGN method and the proposed MGN method from the computational viewpoint.

5.1 | Design of comparison

We consider several versions of the algorithms VPGN and MGN with the directions of line search given by Algorithm 4 and Algorithm 5 respectively. The method VPGN is suggested in²³. The difference between VPGN and S-VPGN is described in⁴; in S-VPGN, the projections $\mathbf{\Pi}_{\mathcal{Z}(\mathbf{a}), \mathbf{W}}$ are calculated in a more stable way using the techniques introduced in⁴ (see Algorithm 2 for calculating the special basis of $\mathcal{Z}(\mathbf{a})$ and Algorithm 6 for calculating the projection itself in the case of a banded \mathbf{W}). In MGN, the projections are always stably calculated. The addition of ‘-H’ at the end of the method abbreviations means that the Compensated Horner scheme is used for calculating the projections.

The source code (R and C++) for these algorithms can be found in³⁶, where the MGN and VPGN methods are implemented for the case of a common (not necessarily diagonal) weight matrix \mathbf{W} . The implementation of VPGN in³⁶ extends that of³⁷, which is suitable for diagonal weight matrices only, and has the same order of computational cost.

The comparison of VPGN, S-VPGN and S-VPGN-H was performed in⁴. This comparison demonstrated that the technique for the projection calculation, which was proposed in⁴, improves the algorithm numerical stability; however, this techniques cannot be applied to the calculation of Δ_k given in 20 and therefore does not allow one to considerably improve the VPGN method. The MGN method changes the iteration step in such a way (see 21) that the techniques developed in⁴ can be used for all steps of the optimization algorithm.

5.2 | Theoretical comparison

We start the comparison from comparing the algorithms by the computational costs. Then, we will compare the stability of the algorithms when the algorithms are comparable by the computational costs. This depends on the structure of the weight matrix \mathbf{W} . The special case of interest is the case when the weight matrix \mathbf{W} is $(2p + 1)$ -diagonal with a small p (this is the case of autoregressive noise of order p and therefore a natural assumption). Note that the special case when both \mathbf{W} and \mathbf{W}^{-1} are banded corresponds to the case of a diagonal matrix \mathbf{W} .

5.2.1 | Computational cost

Let us estimate computational costs in flops and study the asymptotic costs of one iteration as $N \rightarrow \infty$.

The MGN method

The computation cost of the MGN method differs from that of the S-VPGN method only by the cost of calculating $\mathbf{F}_{\mathbf{a}^{(k)}}$ instead of $\mathbf{J}_{S^*}(\hat{\mathbf{a}}^{(k)})$ (compare Algorithms 5 and 4), since the projection $\mathbf{\Pi}_{\mathcal{Z}(\hat{\mathbf{a}}^{(k)}), \mathbf{W}}$ is calculated by the same algorithms (with the cost $O(rN \log N + Nr^2 + Npr^4)$).

As it is shown in⁴, if \mathbf{W}^{-1} is $(2p + 1)$ -diagonal, the asymptotic cost of the calculation of $\mathbf{J}_{S^*}(\hat{\mathbf{a}}^{(k)})$ is $O(Nr^2 + Np^2)$ flops; for the case when \mathbf{W} is $(2p + 1)$ -diagonal, where $p > 0$, it takes $O(N^3)$. The calculation of $\mathbf{F}_{\mathbf{a}^{(k)}}$ is performed by Algorithm 3, which calls Algorithm 2. The S-VPGN method contains Algorithm 2 with the cost $O(rN \log N + Nr^2)$ for any form of \mathbf{W}^4 ; therefore, we need to discuss the cost of additional steps of Algorithm 3 only.

Algorithm 3 includes the first two steps of Algorithm 2; the other steps can be performed in $O(rN \log N)$ flops. Thus, the cost of Algorithm 3 is $O(rN \log N + Nr^2)$. Therefore, the asymptotic cost of one iteration of MGN given in Algorithm 5 is $O(Nr^2 + Np^2 + rN \log N)$, or $O(Np^2 + N \log N)$ for a fixed rank r .

Table 1 summarizes the computational costs for different methods.

Remark 7. Thus, if the inverse \mathbf{W}^{-1} of the weight matrix \mathbf{W} is $(2p + 1)$ -diagonal, then the computational cost of the proposed MGN method is slightly larger in comparison with the VPGN method. However, if the weight matrix \mathbf{W} is $(2p + 1)$ -diagonal and $p > 0$ (the case of autoregressive noise of order p), then the computational cost of the MGN method is significantly smaller by order. In the case of a diagonal matrix \mathbf{W} and a fixed r , the costs of MGN and VPGN are $O(N \log N)$ and $O(N)$ respectively.

TABLE 1 r -Rank approximation: Asymptotic computational costs in flops

Method	\mathbf{W} is $(2p + 1)$ -diagonal, $p > 0$	\mathbf{W}^{-1} is $(2p + 1)$ -diagonal
VPGN	$O(N^3)$	$O(Nr^2 + Np^2)$
S-VPGN, S-VPGN-H	$O(N^3)$	$O(Nr^2 + Np^2 + rN \log N)$
MGN, MGN-H	$O(Nr^2 + Np^2 + rN \log N)$	$O(Nr^2 + Np^2 + rN \log N)$

5.2.2 | Stability

It is discussed in⁴ that the main “stability bottlenecks” of the VPGN algorithms consists of solving the systems of linear equations. In fact, we say about inverting the matrices depending on \mathbf{a} , that is, on the coefficients of $\text{GLRR}(\mathbf{a})$ governing the signal. The stability is measured by the orders of the condition numbers of these matrices as the time-series length N tends to infinity.

For the MGN algorithm, the matrix \mathbf{A}_g is inverted in Algorithm 2. It was shown in⁴ that the order of the condition number of the matrix \mathbf{A}_g is N^t , where t is the maximal multiplicity of the roots of the characteristic polynomial $g(\mathbf{a})$ (22) on the unit circle. It is worth to mention that the use of the compensated Horner scheme increases the accuracy of computing the diagonal elements of \mathbf{A}_g and does not change its condition number.

For stability comparison, we consider the case when \mathbf{W}^{-1} is banded, since otherwise the computational cost of the VPGN algorithm is very large. Independent noise with a diagonal covariance matrix $\mathbf{\Sigma}$ corresponds to this case in practice; then $\mathbf{W} = \mathbf{\Sigma}^{-1}$ is diagonal. It was discussed in⁴ with reference to^{23, Section 6.2} that the condition number of the “bottleneck” matrix of the VPGN algorithm has order N^{2t} .

Therefore, the advantage of the MGN algorithm in the accuracy is more significant in the case of the existence of unit-modulus roots of large enough multiplicity. In the general form (1), the multiplicity of a root is determined by the order of the corresponding polynomial P_{m_k} and is equal to $m_k + 1$. The root has unit modulus if $\alpha_k = 0$. Therefore, the typical examples are polynomial signals and sinusoids with polynomial amplitude modulations.

5.3 | Numerical comparison

For the numerical comparison of the considered algorithms, we use the example of a quadratic signal constructed in⁴, where a local solution of (3) is known. Let us briefly describe this example. For constructing a solution of rank $r = 3$, the well-known theory explaining the relation of linear recurrence relations, characteristic polynomials, their roots and the explicit form of the series, see e.g. the book^{38, Section 3.2} with a brief description of this relation in the context of time series structure.

Let $\mathbf{Y}_N^* = (bt_1^2, \dots, bt_N^2)^T$, where $t_i, i = 1, \dots, N$, form the equidistant grid in $[-1; 1]$ and the constant b is such that $\|\mathbf{Y}_N^*\| = 1$. The series \mathbf{Y}_N^* satisfies the $\text{GLRR}(\mathbf{a}^*)$ for $\mathbf{a}^* = (1, -3, 3, -1)^T$. Since the last component of \mathbf{a}^* is equal to -1 , we can say that the series satisfies the $\text{LRR}(\mathbf{a}^*)$; the characteristic polynomial of this LRR has one unit root of multiplicity $t = 3$. Denote $\hat{\mathbf{R}}_N = (c|t_1|, \dots, c|t_N|)^T$, where the constant c is such that $\|\hat{\mathbf{R}}_N\| = 1$. Construct the observed series as $\mathbf{X}_N = \mathbf{Y}_N^* + \mathbf{R}_N$, where $\mathbf{R}_N = \hat{\mathbf{R}}_N - \mathbf{\Pi}_{\mathcal{Z}((\mathbf{a}^*)^2), \mathbf{W}} \hat{\mathbf{R}}_N$. Thus, the pair $\mathbf{X}_0 = \mathbf{Y}_N^*$ and $\mathbf{X} = \mathbf{X}_N$ satisfies the necessary conditions for local minima⁴. The sufficient condition was tested numerically for $N < 100$. Details of the example implementation see in⁴.

All computations are performed in double precision. When the compensated Horner scheme is used, the accuracy of calculations in double precision is the same as if the calculation would be in quadruple precision without the compensated Horner scheme.

5.3.1 | Stability

The comparison is performed for the methods VPGN, S-VPGN-H, MGN and MGN-H for different N from 100 to 50000. For simplicity, consider the non-weighted case, when \mathbf{W} is the identity matrix.

Denote $\tilde{\mathbf{Y}}^*$ the result of an algorithm participating in the comparison. We compare the algorithms by the accuracy, that is, by the Euclidean distance between $\tilde{\mathbf{Y}}^*$ and \mathbf{Y}_N^* (Fig. 1).

The algorithms were started from the $\text{GLRR}(\mathbf{a}_0)$, where $\mathbf{a}_0 = \mathbf{a}^* + 10^{-6}\mathbf{d}^T$ and each components of \mathbf{d} is randomly distributed in $[-1, 1]$. We used 100 simulations to obtain the averaged results. The iterations stop when the backtracking line search method

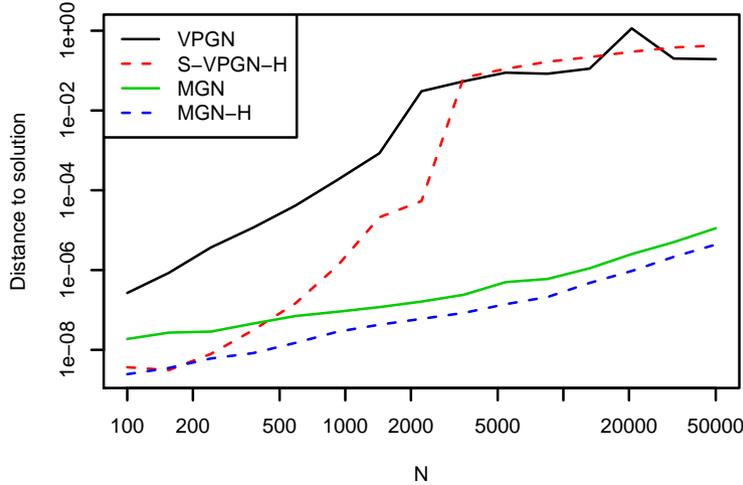


FIGURE 1 Comparison of algorithms by distance to the solution, for different N .

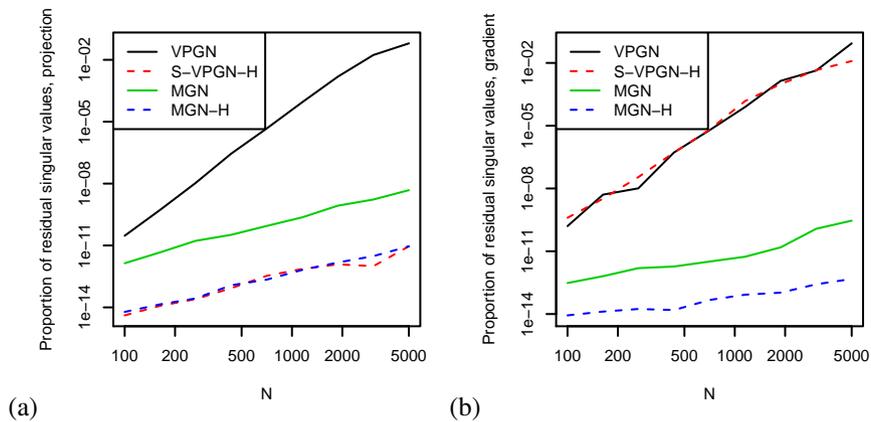


FIGURE 2 Shares of the residual eigenvalues, for different N ; (a) the projection to \overline{D}_r and (b) the Jacobian matrix with columns from a $2r$ -dimensional space.

(in step 6 of Algorithm 1) with decreasing search steps $\gamma = 1, 1/2, 1/4, \dots, 2^{-50}$ does not decrease the value of the objective function.

Figure 1 shows that the accuracy of MGN and MGN-H is asymptotically much better than the accuracy of VPGN and S-VPGN-H; moreover, the errors of VPGN and S-VPGN-H increases drastically for large N . Note that in exact arithmetic, VPGN and S-VPGN-H would produce the same results; the same is true for the pair of MGN and MGN-H.

Figure 2 explains the difference between the algorithms. In⁴, the projection algorithms for calculating $\mathbf{\Pi}_{\mathbf{Z}, \mathbf{W}} \mathbf{X}$ are compared by the difference with the true value. In Figure 2(a), the comparison of the computed projectors to the set of time series of rank not larger than r is performed by the proximity of their results to r -rank time series. Let \mathbf{Y}_N be the numerical result of the projection, choose $L = \lfloor N/2 \rfloor$ and denote $\{\sigma_i\}_{i=1}^L$ the singular values of the L -trajectory matrix $\mathbf{Y} = T_L(\mathbf{Y}_N)$. We measure the projector accuracy as $\sqrt{\sum_{i=r+1}^L \sigma_i^2} / \|\mathbf{Y}\|_F$, where $\|\mathbf{Y}\|_F^2 = \sum_{i=1}^L \sigma_i^2$ is the Frobenius norm. The projection $\mathbf{\Pi}_{\mathbf{Z}, \mathbf{W}} \mathbf{X}$ is performed in the same way in the algorithms S-VPGN-H and MGN-H. Therefore, their accuracies coincide. MGN does not use the Horner compensation scheme and therefore it is a bit worse. The algorithm used in VPGN is less numerically accurate.

The key difference between the VPGN and MGN algorithms is in the 5-th step of Algorithm 1, that is, in the way of calculation of the Jacobian matrix; this can be performed in MGN with improved accuracy. Since each column of the Jacobian matrix (that is, each gradient vector) has rank $2r$ (Theorem 3.2), we can check the accuracy of its calculation by summing the shares

$\sqrt{\sum_{i=2r+1}^L \sigma_i^2} / \|\mathbf{Y}\|_F$ for columns \mathbf{Y}_N of $\mathbf{J}_{S_\tau^*}(\hat{\mathbf{a}}^{(k)})$ for VPGN and of $(\mathbf{I}_N - \mathbf{\Pi}_{Z(H_\tau(\hat{\mathbf{a}}^{(k))), \mathbf{W}}) \hat{\mathbf{F}}_{\mathbf{a}}$ for MGN, see (20) and (21) and Algorithms 4 and 5.

Figure 2(b) confirms that VPGN and S-VPGN-H lack numerical stability when computing the direction (step 5 of Algorithm 1); recall that the multiplicity t equals 3 for this example (see discussion in Section 5.2.2). Figure 2(a) shows that VPGN produces a resultant series far from r -rank one, for large N . Both of these factors lead to that VPGN and S-VPGN-H perform worse than the MGN and MGN-H methods (a ‘‘plateau’’ visible in Figure 1 for VPGN and S-VPGN-H for $N > 2000$ is due to the fact that the distance can not be greater than the series norm).

5.3.2 | Computational cost

For effectively implemented algorithms, the computational speed should have the same order as the theoretical computational cost in flops. Let us numerically confirm Remark 7. We will consider the computational time for different implementations of Algorithms 4 and 5, which calculate the search directions. This time characterizes the computational speed of one iteration. We consider different time series lengths N and two types of the weight matrix \mathbf{W} , the identity matrix and a 3-diagonal matrix, which is the inverse of the covariance matrix of AR(1) with the coefficient 0.9 (the explicit form of this inverse can be found e.g. in³⁹). The speed is estimated with the help of the example described in Section 5.3.1.

The results for the CPU time are depicted in Fig. 3. Since we compare asymptotic behavior (as $N \rightarrow \infty$), we eliminate the constant time, which does not depend on N , in the following way. For each algorithm, we consider the CPU times for different values of N starting from 100 and then divide them by the CPU time for N equal 100. Note that if \mathbf{W} is diagonal, the computational times of the algorithms are asymptotically almost the same. However, if \mathbf{W} contains three diagonals, the computational times for the methods MGN and MGN-H are much smaller than that for the methods VPGN and S-VPGN-H.

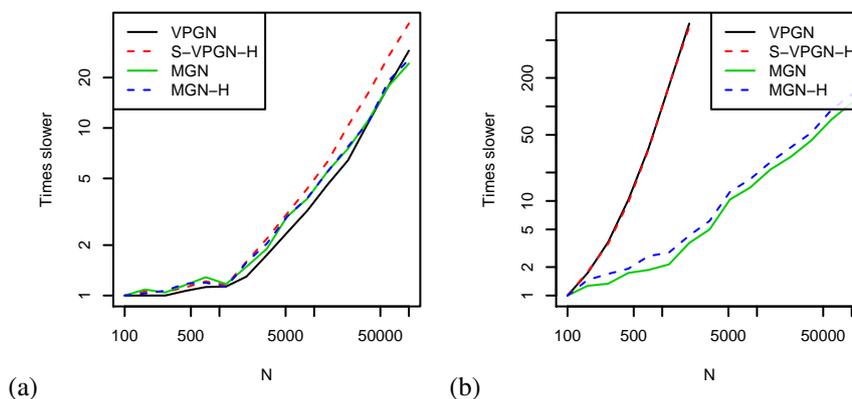


FIGURE 3 Comparison of algorithms by CPU times of one iteration for different N ; (a) diagonal \mathbf{W} and (b) 3-diagonal \mathbf{W} .

5.4 | Signal estimation using MGN: with and without gaps

Consider a time series \mathbf{Y}_{50} similar to the one considered in²⁰, which is the sum of a signal of rank $r = 4$ and Gaussian white noise. That is, let the signal \mathbf{S}_{50} have the following form: $\mathbf{S}_{50} = (s_1, \dots, s_{50})^T$, where

$$s_i = 0.9^i \cos\left(\frac{\pi}{5}i\right) + \frac{1}{5}1.05^i \cos\left(\frac{\pi}{12}i + \frac{\pi}{4}\right), \quad i = 1, \dots, 50, \quad (26)$$

and

$$\mathbf{Y}_{50} = \mathbf{S}_{50} + 0.2 \frac{\mathbf{R}_{50}}{\|\mathbf{R}_{50}\|} \|\mathbf{S}_{50}\|;$$

here the series \mathbf{R}_{50} consists of i.i.d. normal random variables with zero mean and unit variance. Note that since \mathbf{Y}_{50} contains a random component, we were not able to reproduce the time series studied in²⁰ exactly; we used `set.seed(15)` in R version 4.0.2, see³⁶.

Let us consider two versions of the time series Y_{50} , the first one is without missing data and the second time series with artificial gaps at positions $i = 10 \dots 19$ and $i = 35 \dots 39$, and construct two estimates of the signal by the MGN-H method. Since the noise is white, the identity matrix $\mathbf{W} = \mathbf{I}_{50}$ was taken for the case without gaps; for the case with gaps, we consider $\mathbf{W}_0 = \mathbf{I}_{50}$ and construct \mathbf{W} changing ones on the diagonal of \mathbf{W}_0 at the positions of missing data to zeros (see Section 4.3). For constructing the initial GLRR, we replace the missing entries by the mean value of the time series and then set the GLRR coefficients equal to $(r + 1)$ -th left singular vector of the SVD of the $(r + 1)$ -trajectory matrix $T_{r+1}(Y_{50})$.

The results are presented in Figure 4. The series Y_{50} is indicated by the black dots, the signal S_{50} is depicted by the blue line, and the obtained approximation \tilde{S} is shown by the red solid line. Note that in both cases \tilde{S} gives a fairly close estimate of S_{50} , despite even a large gap at $10 \dots 19$ in the case with missing values.

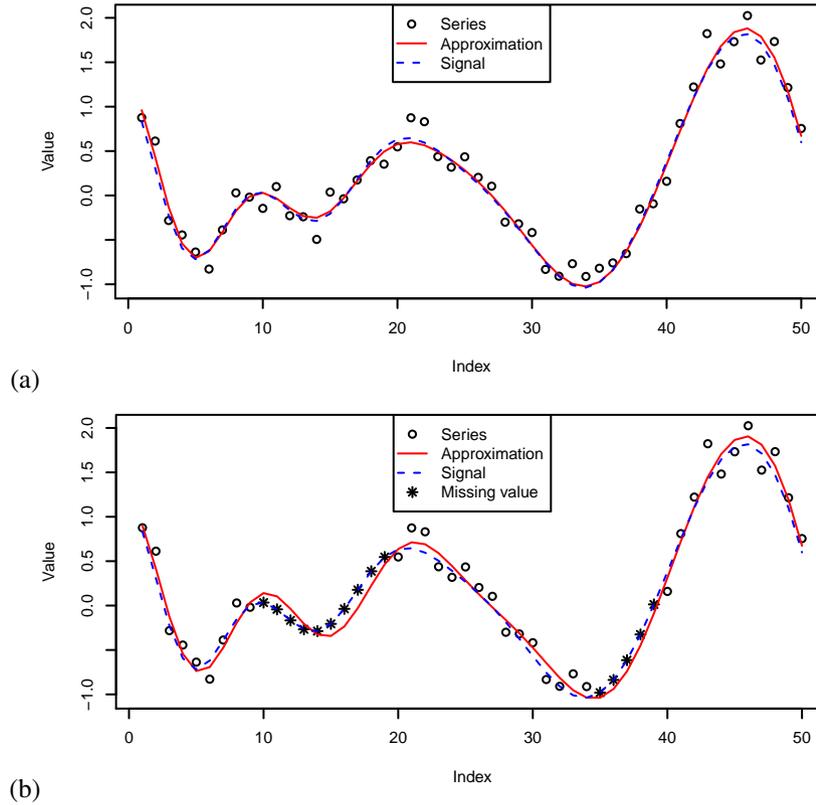


FIGURE 4 Estimates of the signal S_{50} using the MGN algorithm, (a) without gaps (b) with gaps.

Let us consider the same signal (26) corrupted by AR(1) noise with coefficient 0.9 (red noise) instead of white noise. We compare two versions of the MGN-H algorithm, with $\mathbf{W}^{(W)} = \mathbf{I}_N$ and with $\mathbf{W}^{(R)} = \mathbf{\Sigma}^{-1}$, where $\mathbf{\Sigma}$ is the $N \times N$ covariance matrix of the AR process. The latter corresponds to the MLE estimate. To eliminate the influence of the initial GLRR on the comparison, we take it as the minimal GLRR governing the signal.

The estimates of RMSE are obtained by 1000 iterations; in the parentheses we indicate the computational time in seconds. For signal estimation without gaps, we have RMSE equal to 0.075 for $\mathbf{W} = \mathbf{W}^{(W)}$ (80 sec) and 0.066 for $\mathbf{W} = \mathbf{W}^{(R)}$ (75 sec). For gap imputation accuracy in presence of gaps, we have 0.136 for $\mathbf{W}_0 = \mathbf{W}^{(W)}$ (105 sec) and 0.097 for $\mathbf{W}_0 = \mathbf{W}^{(R)}$ (100 sec). The difference between the errors is statistically significant. The computational times are similar and even a bit smaller for the MLE version. This confirms that MGN-H is well working for time series with possible gaps and autoregressive noise.

6 | CONCLUSION

In this paper we presented a new iterative algorithm (MGN, Algorithm 1 with Δ_k calculated by Algorithm 5) for computing the numerical solution to the problem (3) and compared it with a state-of-art algorithm based on the variable projection approach (VPGN, Algorithm 1 with Δ_k calculated by Algorithm 4). We showed that the proposed algorithm MGN allows the implementation, which is more numerically stable especially for the case of multiple unit-modulus roots of the characteristic polynomial (in particular, for polynomial series, where the multiplicity is equal to the polynomial order plus one). This effect can be explained by the inversion of matrices with condition number of order N^t in MGN, where t is the multiplicity, while the direct implementation of VPGN deals with matrices with condition number of order N^{2t} .

The comparison of computational costs in Section 5.2.1 shows that the algorithm MGN has slightly larger costs for the case of banded inverses \mathbf{W}^{-1} of weight matrices. However, in the case of autoregressive noise with covariance matrix $\mathbf{\Sigma}$, the corresponding weight matrix $\mathbf{W} = \mathbf{\Sigma}^{-1}$, which provides the MLE estimate, is banded itself and \mathbf{W}^{-1} is not banded. Then the proposed algorithm MGN has a much lower computational cost in comparison with VPGN.

An important feature of the MGN algorithm is that it can be naturally extended to the case of missing data without increasing the computational cost (see Sections 4.3 and 5.4).

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