Variable projection for affinely structured low-rank approximation in weighted 2-norms

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Abstract

The structured low-rank approximation problem for general affine structures, weighted 2-norms and fixed elements is considered. The variable projection principle is used to reduce the dimensionality of the optimization problem. Algorithms for evaluation of the cost function, the gradient and an approximation of the Hessian are developed. For $m \times n$ mosaic Hankel matrices the algorithms have complexity $O(m^2 n)$.

Keywords: structured low-rank approximation, variable projection, mosaic Hankel matrices, weighted 2-norm, fixed elements, computational complexity

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1. Introduction

An affine matrix structure is an affine map from a structure parameter space $\mathbb{R}^{n_p}$ to a space of matrices $\mathbb{R}^{m \times n}$, defined by

$$\mathcal{S}(p) = S_0 + \sum_{i=1}^{n_p} p_k S_k,$$

where $S_k \in \mathbb{R}^{m \times n}$. Without loss of generality, we can consider only the case $m \leq n$. The structured low-rank approximation is the problem of finding the best low-rank structure-preserving approximation of a given data matrix [1, 2].

Problem 1 (Structured low-rank approximation). Given an affine structure $\mathcal{S}$, data vector $p_D \in \mathbb{R}^{n_p}$, norm $\| \cdot \|$ and natural number $r < \min(m,n)$

$$\minimize_{\tilde{p} \in \mathbb{R}^{n_p}} \| p_D - \tilde{p} \| \quad \text{subject to} \quad \text{rank}(\mathcal{S}(\tilde{p})) \leq r.$$  (SLRA)

In this paper, we consider the case of a weighted 2-norm, given by

$$\| p \|^2_W := p^T W p, \quad W \in \mathbb{R}^{n_p \times n_p},$$

where $W$ is

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• either a symmetric positive definite matrix,
• or a diagonal matrix

\[
W = \text{diag}(w_1, \ldots, w_n), \quad w_i \in (0; \infty),
\]

where \( \infty \cdot 0 = 0 \) by convention. A finiteness constraint \( \| \hat{p}_0 - \tilde{p} \|^2_W < \infty \) is additionally imposed on (SLRA). Problem (SLRA) with the weighted norm \( \| \cdot \|_W \) given by \( \|w \rightarrow W\) is equivalent to (SLRA) with an element-wise weighted 2-norm

\[
\|p\|_w^2 = \sum_{w_i \neq \infty} w_i p_i^2,
\]

and a set of fixed values constraints

\[
(p_0)_i = \tilde{p}_i \text{ for all } i \text{ with } w_i = \infty.
\]

The structured low-rank approximation problem with the weighted 2-norm appears in signal processing, computer algebra, identification of dynamical systems, and other applications. We refer the reader to [1, 2] for an overview. In this paper, we consider general affine structures \( (\mathcal{Z}) \) and, in particular, structures that have the form

\[
\mathcal{Z}(p) = \Phi \mathcal{H}_{m,n}(p),
\]

where \( \Phi \) is a full row rank matrix and \( \mathcal{H}_{m,n} \) is a mosaic Hankel matrix structure.

Many data modeling problems can be reduced to (SLRA) with the structure \( \Phi \mathcal{H}_{m,n} \) and weighted norm, defined by \( \|w \rightarrow W\), see [1, 4]. In data modeling, the number of rows \( m \) usually has the meaning of the model complexity and the number of columns \( n \) is of the same order as the number of data points [2]. Typically, the case \( m \ll n \) is of interest, i.e. approximation of a large amount of data by a low-complexity model.

### 1.1. Mosaic Hankel structure

A mosaic Hankel matrix structure \( \mathcal{H}_{m,n} \) is a map defined by two integer vectors

\[
\mathbf{m} = [m_1 \cdots m_q] \in \mathbb{N}^q \quad \text{and} \quad \mathbf{n} = [n_1 \cdots n_N] \in \mathbb{N}^N \quad (\mathbf{m}, \mathbf{n})
\]
as follows:

\[
\mathcal{H}_{m,n}(p) := \begin{bmatrix}
\mathcal{H}_{m_1,n_1}(p^{(1,1)}) & \cdots & \mathcal{H}_{m_1,n_N}(p^{(1,N)}) \\
\vdots & \ddots & \vdots \\
\mathcal{H}_{m_q,n_1}(p^{(q,1)}) & \cdots & \mathcal{H}_{m_q,n_N}(p^{(q,N)})
\end{bmatrix}, \quad (\mathcal{H}_{m,n})
\]

where

\[
p = \text{col}(p^{(1,1)}, \ldots, p^{(q,1)}, \ldots, p^{(1,N)}, \ldots, p^{(q,N)}), \quad p^{(k,l)} \in \mathbb{R}^{m_k+n_l-1}, \quad (p)
\]
is the partition of the parameter vector, and \( \mathcal{H}_{m,n} : \mathbb{R}^{m+n-1} \rightarrow \mathbb{R}^{m \times n} \) is the Hankel structure

\[
\mathcal{H}_{m,n}(p) := \begin{bmatrix}
p_1 & p_2 & \cdots & p_n \\
p_2 & p_3 & \cdots & p_{n+1} \\
p_3 & \ddots & \ddots & \vdots \\
\vdots & \ddots & \ddots & \ddots \\
p_n & p_{m+1} & \cdots & p_{m+n-2} \\
p_{m+1} & \cdots & p_{m+n-2} & p_{m+n-1}
\end{bmatrix}.
\]
Note that the number of parameters for \( \mathcal{H}_{m,n} \) is equal to
\[
n_p = N \sum_{k=1}^{q} m_k + q \sum_{l=1}^{N} n_l - N q,
\]
the number of columns is equal to \( \sum_{k=1}^{q} m_k \), and the number of rows is \( \sum_{l=1}^{N} n_l \).

The mosaic Hankel structure is a generalization of the block-Hankel structure, which is defined as
\[
\mathcal{H}_{m_1,n_1}(C) := \begin{bmatrix} C_{1,:,} & C_{2,:,} & \cdots & C_{n_1,:,} \\ C_{2,:,} & \ddots & \vdots & \vdots \\ \vdots & \ddots & \ddots & \vdots \\ C_{m_1,:,} & \cdots & C_{m_1+n_1-1,:,} & \cdots & C_{m_1+n_1,:,} \end{bmatrix}, \quad (\mathcal{H}_{m_1,n_1}(C))
\]
where \( C \in \mathbb{R}^{(m_1+n_1-1) \times q \times N} \) is a 3-dimensional tensor. Indeed, consider permutation matrices
\[
\Pi^{(k,l)} := \begin{bmatrix} I_k \otimes e^{(1)} & \cdots & I_k \otimes e^{(l)} \end{bmatrix}^T,
\]
where \( \otimes \) is the Kronecker product. Then the block-Hankel structure \( \mathcal{H}_{m_1,n_1}(C) \) can be transformed to a mosaic Hankel structure \( \mathcal{H}_{m,n} \) by permutation of the rows and columns
\[
\Pi^{(m_1,q)} \mathcal{H}_{m_1,n_1}(C)(\Pi^{(n_1,N)})^T = \mathcal{H}_{m_1 \cdots m_1 \cdots \cdots \cdots n_1 \cdots n_1}(p), \quad (\mathcal{H}_{m_1,n_1}(C) \leftrightarrow \mathcal{H}_{m,n})
\]
where \( p \) is defined as \([\overline{p}]\) with \( p^{(k,l)} := C_{i,k,l} \) (an unfolding of the tensor \( C \)).

1.2. Optimization methods and the variable projection

Problem (SLRA) is non-convex and except for a few special cases (e.g. for unstructured matrices and Frobenius norm, for circulant matrices, and for some classes of square matrices, see [3, 1]) has no closed-form solution.

Different optimization methods have been developed for different structures and approximation criteria, see [1] for a historical overview. Many optimization methods use the fact that the rank constraint \( \mathcal{R}(\hat{p}) \leq r \) is equivalent to existence of a full row rank matrix \( R \in \mathbb{R}^{d \times m} \) satisfying \( R \mathcal{R}(\hat{p}) = 0 \), where \( d := m - r \) is the rank reduction in (SLRA). Problem (SLRA) then can be rewritten (for weighted 2-norm) as
\[
\min_{R \in \mathbb{R}^{d \times m}, p \in \mathbb{R}^r} \| p_R - \hat{p} \|^2_W \quad \text{subject to} \quad \text{rank} R = d \quad \text{and} \quad R \mathcal{R}(\hat{p}) = 0. \quad (\text{SLRA}_R)
\]
Methods for (SLRA) include Riemannian SVD [6], structured total least norm approach [7, 8], and methods based on the variable projection principle. Note that most of the optimization methods mentioned above were developed for the structured total least squares problem, which is the problem (STLS) with an additional constraint
\[
R = [X \ -I_d], \quad X \in \mathbb{R}^{d \times r}. \quad (\text{STLS})
\]
Most of the methods listed above were designed only for special cases of the weighted 2-norm \( \| \cdot \|^2_W \).
The variable projection approach was proposed in [9] for separable nonlinear least squares problems. Variable projection was first applied for some special cases of (SLRA) [10, 11]. In the variable projection approach, (SLRA) is rewritten as

\[
\text{minimize } f(R), \quad \text{where } \begin{cases} 
R \in \mathbb{R}^{d \times m}, \text{rank } R = d \\
f(R) := \left( \min_{\hat{p} \in \mathbb{R}^n} \| p - \hat{p} \|_W^2 \right) \text{ subject to } R \mathcal{S}(\hat{p}) = 0
\end{cases}
\]

The inner minimization problem \( f(R) \) is a least-norm problem [12] and has a closed form solution. Therefore (SLRA) is reduced to optimization of \( f(R) \) on a space of dimension \( dm \), which is typically much smaller than the dimension \( np \) of the eliminated variable \( \hat{p} \).

The cost function \( f(R) \) depends only on the subspace spanned by the rows of the argument \( R \), i.e. \( f(R_1) = f(R_2) \) if \( \text{rowspan } R_1 = \text{rowspan } R_2 \). Therefore, \( f(R) \) can be considered as a function defined on the Grassmann manifold [13] of all \( d \)-dimensional subspaces of \( \mathbb{R}^n \), and the problem (OUTER) is optimization on a Grassmann manifold. The optimization problem on a Grassmann manifold can be either transformed to an optimization problem on an Euclidean space (see [14]), or solved by iterations in tangent spaces (see, for example, [10, 13]). Therefore, standard optimization routines can be used to minimize (OUTER).

The computation of the cost function has complexity \( O(n^3) \) if the inner minimization problem \( f(R) \) is solved by general-purpose methods (e.g. the QR decomposition [15]). For analytic computation of derivatives of \( f(R) \), which can speed up the convergence of local optimization methods, only algorithms with complexity \( O(n^3) \) were proposed in the case of general affine structure [16].

In [11, 17] it was shown that for a class of structures the cost function \( f(R) \) and its gradient can be evaluated in \( O(mn) \) flops, which leads to efficient local optimization methods for (SLRA). The structures considered in [11, 17] are of the form \( [\mathcal{S}(1) \cdots \mathcal{S}(q)]^\top \), where each block \( \mathcal{S}(l) \) is block-Toeplitz, block-Hankel or unstructured, and only whole blocks can be fixed. Only the 2-norm approximation criterion was considered and the constraint (STLS) on \( R \) was required.

1.3. Main results and composition of the paper

In this paper we show that the cost function \( f(R) \), its gradient and an approximation of its Hessian can be evaluated in \( O(m^2 n) \) operations for structure \( [\mathcal{S}] \in \mathbb{R}^{m \times n} \) and element-wise weighted 2-norm (that allows fixed values constraints). If the weights are block-wise (or only whole blocks are fixed), the cost function and the gradient can be evaluated in \( O(mn) \) operations, as in [18].

We develop algorithms for evaluation of \( f(R) \) and its gradient for general affine structure and arbitrary weighted 2-norm. The structure of \( f(R) \) is derived in a similar way to [11], but in contrast to [11, 17] we do not use a probabilistic interpretation of (SLRA). Instead, we show how the matrix structure \( [Z] \) is mapped to the structure of the cost function. In addition, our definition of the weighted 2-norm incorporates fixed values constraints, which also simplifies the derivation of the cost function structure in this case.

We provide an explicit derivation of Gauss-Newton approximations of the Hessian of \( f(R) \), for the general affine structure and weighted 2-norm. This derivation was omitted in [17] and other papers, but was used in the computational routines in [18]. We provide two variants of the approximation of the Hessian, based on two different representations of \( f(R) \) as a sum of squares.
The paper is organized as follows. In Section 2, we review some basic properties of affine structures and (SLRA) in the weighted 2-norm. Section 3 covers the derivation of \( f(R) \) for the general affine structure and weighted 2-norm. For block structures, the cost function is expressed via cost functions for the blocks. Based on results of Section 3, we develop general-purpose algorithms for evaluation of the cost function and its derivatives in Section 4. Finally, in Section 5, we specialize the algorithms from Section 4 for mosaic Hankel structures and derive their computational complexity. In Section 6, we discuss the conditions on \( S \) and \( r \) under which the algorithms in the paper are applicable; we also discuss accuracy of the computations.

1.4. Notation

We use lowercase letters for vectors and uppercase letters for matrices (square matrices are denoted by upright letters). By convention, blank elements in matrices denote zeros. Some of the notation used in the paper is summarized in Table 1.

| \( a_i, A_{i,j} \) | elements of vectors and matrices. |
| \( k : l \) | the integer vector \([k \cdots l]\); we also frequently use convention \( i \in k : l \) to denote that an integer \( i \) satisfies \( k \leq i \leq l \). |
| \( a_{I,I,J} \) | sub-vectors and sub-matrices indexed by integer vectors; a single colon stands for selecting all indices, e.g. \( A_{:2} \) is the second column of the matrix \( A \). |
| \( 0_{m \times n} \) | \( m \times n \) matrix of zeros. |
| \( 1_{m \times n} \) | \( m \times n \) matrix of ones. |
| \( I_m \) | \( m \times m \) identity matrix. |
| \( J_m \) | \( m \times m \) shift matrix, i.e. \( J_m := \begin{bmatrix} 0_{(m-1) \times 1} & 1_{1 \times (m-1)} \end{bmatrix} \). |
| \( e^{(i)} \) | \( i \)-th unit vector. |
| \( \text{col}(v^{(1)}, \ldots, v^{(N)}) \) | concatenation of vectors \( v^{(1)}, \ldots, v^{(N)} \). |
| \( \text{blkdiag}(A_1, \ldots, A_N) \) | block-diagonal matrix composed of matrices \( A_1, \ldots, A_N \). |
| \( \text{vec}A \) | the column-wise vectorization of a matrix. |
| \( W^{-1} \) | either the inverse of \( W \) if \( W \) is nonsingular, or \( \text{diag}(w_1^{-1}, \ldots, w_n^{-1}) \) if \( W = \text{diag}(w_1, \ldots, w_n) \) and \( w_k \in (0; \infty) \) (with the convention \( \infty^{-1} = 0 \)). |
| \( W^{-\top} \) | the transpose of the inverse (i.e. \( (W^{-1})^\top \)). |
| \( L_W \) | either the right Cholesky factor of \( W \) if \( W \) is positive definite, or \( \text{diag}(\sqrt{w_1}, \ldots, \sqrt{w_n}) \) if \( W = \text{diag}(w_1, \ldots, w_n) \) and \( w_k \in (0; \infty) \) (with the convention \( \sqrt{\infty} = \infty \)). |

Table 1: Notation

2. Affine structures and weighted 2-norms

2.1. Basic properties

Affine structures can be defined in an equivalent to (2) vector form

\[
\text{vec} \mathcal{S}(p) = \text{vec} \, S_0 + S_{\mathcal{S}} \, p,
\]

5
where $S_{\mathcal{A}}$ is the matrix representation of the linear part of $\mathcal{A}$ in the basis $\{e^{(i)}(e^{(j)})^\top\}_{i,j=1}^{m,n}$:

\[
S_{\mathcal{A}} := [\text{vec } S_1 \cdots \text{vec } S_{n_p}] .
\]

**Example 1.** $2 \times 3$ Hankel matrices $\mathcal{H}_{2,3}(p)$ can be represented as $\mathcal{A}$ with

\[
\begin{align*}
S_0 &= 0_{2 \times 3}, \quad S_1 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \quad S_2 = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \end{bmatrix}, \quad S_3 = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}, \quad S_4 = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} .
\end{align*}
\]

In this case,

\[
S_{\mathcal{A}} = \begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{bmatrix} .
\]

Using $\text{vec } \mathcal{A}$, it is easy to show that the Frobenius norm is a weighted 2-norm.

**Note 1.** Let $\mathcal{A}$ be an injective map (which corresponds to linearly independent $\{S_k\}_{k=1}^{n_p}$ or $(S_{\mathcal{A}})$ with full column rank). Then

\[
\| \mathcal{A}(\tilde{p}) - \mathcal{A}(p_0) \|_F^2 = \| S_{\mathcal{A}} (\tilde{p} - p_0) \|_2^2 = \| \tilde{p} - p_0 \|_{W_1}^2 ,
\]

where $W_1 = S_{\mathcal{A}}^T S_{\mathcal{A}}$ is the Gramian of the system of matrices $\{S_k\}_{k=1}^{n_p}$.

**Example 2.** In Example 1, the Gramian $S_{\mathcal{A}}^T S_{\mathcal{A}}$ is diagonal, and the weighted norm corresponding to the Frobenius norm is given by $(W \rightarrow W)$ with $w = \text{col}(1, 2, 2, 1)$.

It is not difficult to show that the Frobenius norm in Note 1 can be replaced by any weighted Frobenius norm (a weighted 2-norm of vec $(\mathcal{A}(\tilde{p}) - \mathcal{A}(p_0)))$.

### 2.2. From weighted 2-norm to 2-norm

Any (SLRA) problem with weighted 2-norm can be reduced to an unweighted (SLRA) problem. Consider the following change of parameters

\[
\tilde{p} = p_0 - L_W^{-1} \Delta p .
\]

We define the transformed structure in the vector form $\text{vec } \mathcal{A}$:

\[
\text{vec } \mathcal{A}(\Delta p) := \text{vec } \mathcal{A}(p_0) - S_{\mathcal{A}} L_W^{-1} \Delta p ,
\]

$\mathcal{A}(\Delta p)$ satisfies

\[
\mathcal{A}(\Delta p) = \mathcal{A}(\tilde{p})
\]

for any $\Delta p$. If $W$ in $\| \cdot \|_W$ is positive definite, then by $W = L_W L_W^T$ we have that

\[
\| \tilde{p} - p_0 \|_W^2 = \Delta p^T L_W^{-1} W L_W^{-1} \Delta p = \| \Delta p \|_2^2 .
\]

Note that $\| \cdot \|_W = \| \cdot \|_2$ does not hold for $(W \rightarrow W)$. Nevertheless, the following result holds.

**Proposition 1.** Any problem (SLRA) with $\| \cdot \|_W$ is equivalent to

\[
\begin{align*}
\text{minimize} & \quad \| \Delta p \|_2^2 \\
\text{subject to} & \quad \text{rank } \mathcal{A}(\Delta p) \leq r .
\end{align*}
\]

$\mathcal{A}$

**Proof.** The proof is given in Appendix A.
3. Variable projection

3.1. Variable projection for the weighted 2-norm

In this subsection, we derive an explicit expression for the cost function \( f(R) \) for the general affine structure \( \mathbb{Z} \) and weighted 2-norm \( \| \cdot \|_W^2 \). Consider the change of variables \( \Delta p \rightarrow \hat{p} \).

By Proposition [1] and \( \mathbb{Z} \leftrightarrow \mathbb{S} \), the optimization problem in \( f(R) \) is equivalent to

\[
\begin{align*}
\text{minimize} & \quad \| \Delta p \|_2^2 \\
\text{subject to} & \quad R^T \mathbb{S} \Delta p = 0,
\end{align*}
\]

By \( \mathbb{S} \) and properties of the vectorization operator, \( \mathbb{S} \mathbb{V} \) can be rewritten as

\[
\begin{align*}
\text{minimize} & \quad \| \Delta p \|_2^2 \\
\text{subject to} & \quad G(R) \Delta p = s(R),
\end{align*}
\]

where \( s(R) \in \mathbb{R}^{dn} \) and \( G(R) \in \mathbb{R}^{dn \times np} \) are defined as

\[
\begin{align*}
s(R) & := \text{vec}(R \mathbb{S}(p_0)) = (I_n \otimes R) \text{vec}(p_0), \quad (s(R)) \\
G(R) & := (I_n \otimes R) \mathbb{S} \mathbb{L}^{-1}_W = \left[ \text{vec}(RS_1) \cdots \text{vec}(RS_{np}) \right] \mathbb{L}^{-1}_W. \quad (G(R))
\end{align*}
\]

Problem \( \mathbb{L} \) is a linear least-norm problem in a standard form [12, Ch. 6], and has a closed-form solution. If \( G(R) \) is of full row rank, the solution of \( \mathbb{L} \) exists and is given by

\[
\Delta p^*(R) = G^T(R) \Gamma^{-1}(R) s(R), \quad (\Delta p^*(R))
\]

\[
f(R) := \| \Delta p^*(R) \|_2^2 = s^T(R) \Gamma^{-1}(R) s(R), \quad (s^T \Gamma^{-1} s)
\]

where

\[
\Gamma = \Gamma(R) := G(R) G^T(R) \in \mathbb{R}^{dn \times dn}. \quad (\Gamma(R))
\]

**Note 2.** If \( G(R) \) is not of full row rank but the problem \( \mathbb{L} \) is feasible, the solution of \( \mathbb{L} \) is given by replacing the inverse of \( \Gamma \) with its pseudoinverse in \( \Delta p^*(R) \) and \( s^T \Gamma^{-1} s \).

In what follows, we assume that \( G(R) \) is of full row rank, which is equivalent to \( \Gamma(R) \) being invertible. A necessary condition for this is

\[ np \geq nd, \quad (\text{NC}) \]

i.e. the number of rows of \( G(R) \) should not exceed the number of its columns. We discuss the invertibility conditions of \( \Gamma \) for mosaic Hankel matrices in Section [4].

**Note 3.** Since \( \Gamma \) is a polynomial matrix (in the entries of \( R \)), it can be inverted symbolically if it is nonsingular at least for one \( R \). In this case, \( \Gamma \) is infinitely differentiable for all \( R \) such that \( \Gamma(R) \) is nonsingular [14].
3.2. Block partitioning of $\Gamma(R)$

Next, we show how the computation of $\Gamma$ can be simplified. Let us define

$$V = V_{S,W} := S W^{-1} S^T \in \mathbb{R}^{m\times m}.$$  \hspace{1cm} (V)

Consider the following block partitioning of $\Gamma$ and $V$:

$$\Gamma(R) = \begin{bmatrix} \Gamma_{#11}(R) & \cdots & \Gamma_{#1n}(R) \\ \vdots & \ddots & \vdots \\ \Gamma_{#n1}(R) & \cdots & \Gamma_{#nn}(R) \end{bmatrix}, \quad V = \begin{bmatrix} V_{#11} & \cdots & V_{#1n} \\ \vdots & \ddots & \vdots \\ V_{#n1} & \cdots & V_{#nn} \end{bmatrix},$$

where $\Gamma_{#ij}(R) \in \mathbb{R}^{d \times d}$ and $V_{#ij} \in \mathbb{R}^{m \times m}$. Then, $\Gamma_{#ij}(R)$ and $V_{#ij}$ are related by

$$\Gamma_{#ij}(R) := RV_{#ij} R^T. \hspace{1cm} (\Gamma_{#ij})$$

Indeed, from $[\Gamma(R)]$ and $[G(R)]$ and the fact that $L_W^{-1} L_W^{-\top} = W^{-1}$ we have that

$$\Gamma(R) = (I_n \otimes R) V (I_n \otimes R^T) = \text{blkdiag}(R, \ldots, R)V \text{blkdiag}(R^T, \ldots, R^T),$$

which proves $[\Gamma_{#ij}]$.

**Note 4.** The structure of $\Gamma$ is determined by the structure of $V$. For example, if $V$ is block-sparse, block-banded or block-Toeplitz, then $\Gamma$ has the same structural property. The structural properties of $V$ depend on the matrix structure $S$ and the weight matrix $W$.

A partition of type $[\Gamma_{#ij}]$ was derived in [11, 17] from statistical considerations for a class of structures. Here we have derived it for general $S$ and $W$ via a series of algebraic transformations.

**Example 3.** In Example 2, $G(R)$ has the form

$$G(R) = \begin{bmatrix} R_{1,1} & R_{1,2} \\ R_{2,1} & R_{1,2} \\ R_{1,1} & R_{1,2} \end{bmatrix} \text{diag}(1, \sqrt{2}, \sqrt{2}, 1)$$

for $R \in \mathbb{R}^{1\times 2}$. In addition, $V$ has the form

$$V_{S,W} = \begin{bmatrix} 1 \\ 2 & 2 \\ 2 & 2 \\ 2 & 2 \\ 2 & 2 \end{bmatrix}$$

Examples 1 and 3 will be generalized in Section 5.1 to $\mathcal{H}_{m,n}$ with arbitrary $m$ and $n$.

3.3. Variable projection for block matrices

In this subsection, we consider basic transformations of structures and derive the form of $[f(R)]$ for these transformed structures. First, we consider striped and layered block matrices.
Lemma 1 (Striped structure). Let \( p = \text{col}(p^{(1)}, \ldots, p^{(N)}) \), with \( p^{(l)} \in \mathbb{R}^{n_l} \) and
\[
\mathcal{S}(p) = \left[ \mathcal{S}^{(1)}(p^{(1)}) \quad \cdots \quad \mathcal{S}^{(N)}(p^{(N)}) \right],
\]
be the striped structure, \( \mathcal{S}^{(l)} : \mathbb{R}^{n_l} \rightarrow \mathbb{R}^m \). Then for \( \mathcal{S} \) and \( W = \text{blkdiag}(W^{(1)}, \ldots, W^{(N)}) \), \( W^{(l)} \in \mathbb{R}^{n_l \times n_l} \), we have that:

1. the cost function \( f(R) \) is equal to the sum
\[
f(R) = \sum_{l=1}^{N} f^{(l)}(R),
\]
where \( f^{(l)} \) is the cost function \( f(R) \) for the structure \( \mathcal{S}^{(l)} \) and the weight matrix \( W^{(l)} \);
2. the optimal correction \( \Delta p^*(R) \) is the concatenation
\[
\Delta p^*(R) = \text{col}\left( \Delta p^{(1)*}(R), \ldots, \Delta p^{(N)*}(R) \right)
\]
of the corrections \( \Delta p^{(l)*}(R) \) for the structures \( \mathcal{S}^{(l)} \) and weight matrices \( W^{(l)} \).

Proof. The inner minimization problem \( \text{LN}_\Delta \) can be expressed as
\[
\min_{\Delta p^{(l)} \in \mathbb{R}^{n_l}} \sum_{l=1}^{N} \| \Delta p^{(l)} \|^2 \quad \text{subject to} \quad R \mathcal{S}^{(l)}(\Delta p^{(l)}) = 0, \quad \text{for} \quad l \in 1 : N.
\]
This sum of squares is minimized by \( \text{striped } \Delta p^* \), and its norm is given by \( \text{striped } f \). \( \square \)

Lemma 2 (Layered structure). Let \( p = \text{col}(p^{(1)}, \ldots, p^{(q)}) \), with \( p^{(k)} \in \mathbb{R}^{n_k} \) and
\[
\mathcal{S}(p) = \left[ \begin{array}{c} \mathcal{S}^{(1)}(p^{(1)}) \\ \vdots \\ \mathcal{S}^{(q)}(p^{(q)}) \end{array} \right],
\]
be a layered structure, \( \mathcal{S}^{(k)} : \mathbb{R}^{n_k} \rightarrow \mathbb{R}^m \). Then for \( \mathcal{S} \) and \( W = \text{blkdiag}(W^{(1)}, \ldots, W^{(q)}) \), \( W^{(k)} \in \mathbb{R}^{n_k \times n_k} \) we have that:

1. the \( G \) matrix is
\[
G(R) = \left[ G^{(1)}(R^{(1)}) \quad \cdots \quad G^{(q)}(R^{(q)}) \right],
\]
where
\[
R = \left[ R^{(1)} \quad \cdots \quad R^{(q)} \right] \quad (R^{(k)})
\]
is the partition of \( R \) into \( R^{(k)} \in \mathbb{R}^{d \times m_k} \);
2. the \( \Gamma \) matrix is equal to the sum
\[
\Gamma(R) = \sum_{k=1}^{q} \Gamma^{(k)}(R^{(k)})
\]
of the matrices \( \Gamma^{(k)}(R^{(k)}) \) corresponding to \( \text{SLRA} \) with \( \mathcal{S}^{(k)} \) and \( W^{(k)} \).
3. the matrix $\mathbf{V}$ for $\mathcal{S}$ and $\mathbf{W}$ is composed of the blocks

$$V_{#ij} = \text{blkdiag}(V^{(1)}_{#ij}, \ldots, V^{(q)}_{#ij}),$$

where $V^{(k)}$ is the matrix $\mathbf{V}$ for the structure $\mathcal{S}^{(k)}$ and the weight matrix $W^{(k)}$;

4. the optimal correction $\Delta p^*(R)$ can be expressed as

$$\Delta p^*(R) = \text{col} (\Delta p^{(1)*}(R), \ldots, \Delta p^{(N)*}(R)),$$

where $\Delta p^{(k)*}(R) := (G^{(k)}(R^{(k)}))^\top \Gamma^{-1}(R)s(R)$.

Proof. It is sufficient to prove statement 1, which follows from

$$\text{vec}(R\mathcal{S}(\Delta p)) = \sum_{k=1}^{q} \text{vec}(R^{(k)}\mathcal{S}^{(k)}(\Delta p^{(k)}))$$

$$= \sum_{k=1}^{q} \left( \text{vec}(R^{(k)}\mathcal{S}^{(k)}(p^{(k)}_0)) - G^{(k)}(R^{(k)})\Delta p^{(k)} \right)$$

$$= \text{vec}(R\mathcal{S}(p_0)) - \left[ G^{(1)}(R^{(1)}) \ldots G^{(q)}(R^{(q)}) \right] \Delta p.$$

The other statements follow from $[\Gamma(R)]$ and $[\mathbf{V}]$.

Next we examine the effect of left multiplication of the structure by a matrix of full row rank.

Lemma 3 (Multiplication by $\Phi$). Let $\mathcal{S}$ be defined as

$$\mathcal{S}(p) = \Phi \mathcal{S}'(p),$$

where $\mathcal{S}' : \mathbb{R}^n_r \to \mathbb{R}^{m' \times n'}$ and $\Phi \in \mathbb{R}^{m \times m'}$ is such that rank $\Phi = m \leq m'$. Then,

$$f_{\mathcal{S}}(R) = f_{\mathcal{S}'}(R\Phi).$$

Proof. This property is easily verified by rewriting the constraint in $f(R)$ as

$$R\mathcal{S}(\hat{p}) = R\Phi \mathcal{S}'(\hat{p}) = 0,$$

where rank $R\Phi = m$.

4. Cost function and derivatives evaluation

In this section, we develop algorithms for computing the cost function $f(R)$, optimal correction $\Delta p^*(R)$ and their derivatives, for the general affine structure $\mathcal{S}$. The algorithms can be specialized for a specific class of structures by deriving the form of $V_{#ij}$, as it will be done in Section 5 for the mosaic Hankel structure.

In Section 4.1 we provide algorithms for evaluation of $f(R)$, computation of the optimal correction $\Delta p^*(R)$, and computation of the gradient of $f(R)$. In Sections 4.2 and 4.3 we consider the following approximation of the Hessian of $f(R)$. Let $f(R) = \|g(R)\|_2^2$, where $g(R) \in \mathbb{R}^{n_s}$ with $n_s \geq dm$, and $J_g$ be the Jacobian of $g$. Then, $2J_g^\top J_g$ is an approximation of the Hessian of $f(R)$. Substituting this approximation in the Newton method is equivalent
to performing Gauss-Newton iterations, and we will call it a Gauss-Newton approximation of the Hessian. The Gauss-Newton approximation is frequently used in trust-region methods for solving nonlinear least-squares problems, e.g. in the Levenberg-Marquardt algorithm [19]. In Section 4.2, we consider the Jacobian of \( g(\cdot) = \Delta p^*(\cdot) \), where \( \Delta p^*(\cdot) \) is defined in \( \Delta p^*(R) \). In Section 4.3, we consider \( g(\cdot) = L^{-\top}s(\cdot) \), where \( L \) is the right Cholesky factor of \( \Gamma \).

We will frequently use the following notation for the solution of the system \( \Gamma y = s(R) \):

\[
y = y(R) := \Gamma^{-1}s(R),
\]

4.1. Cost function, correction and gradient

From \( y(R) \) and \( s^\top \Gamma^{-1}s \), the cost function \( f(R) \) can be represented as

\[
f(R) = y^\top(R) s(R) = s(R)^\top y(R),
\]

and can be computed by Algorithm 1.

**Algorithm 1** (Cost function evaluation).

**Input:** \( S, W, \Gamma_{\#ij}, p, R \)

1: Compute \( s(R) \).
2: Compute \( \Gamma_{\#ij} \) using \( \Gamma_{\#ij} \).
3: Compute \( y(R) \).
4: Compute the cost function \( f(R) \) as \( \{y^\top s\} \).

**Output:** \( f(R) \)

The term \( \Delta p^*(R) \) in \( \Delta p^*(R) \) can be evaluated by Algorithm 2.

**Algorithm 2** (Correction computation).

**Input:** \( S, W, \Gamma_{\#ij}, p, R \)

1: Perform steps 1–3 of Algorithm 1.
2: Set \( \Delta p^*(R) = G^{-\top}(R)y \).

**Output:** \( \Delta p^*(R) \)

**Note 5.** The optimal \( \hat{p} \) in \( \Delta p^*(R) \) can be computed by combining Algorithm 3 and \( \Delta p \rightarrow \hat{p} \).

Instead of the gradient \( \nabla f \), for convenience, we use the matrix gradient \( \nabla_{d \times m} f \in \mathbb{R}^{d \times m} \), defined as

\[
\text{vec}(\nabla_{d \times m} f) := \nabla f.
\]

**Proposition 2.** Let \( Y \in \mathbb{R}^{d \times n} \) be the matrix constructed from the \( \hat{p} \) as follows:

\[
y = \text{vec} Y.
\]

Then the matrix gradient is given by

\[
\nabla_{d \times m}(f) = 2Y \mathcal{J}^\top(p) - 2 \sum_{i,j=1}^{m} Y_{i,j} V_{i,j} R \Gamma_{\#ij}.
\]

**Proof.** The proof is given in Appendix A.

From Proposition 2, the gradient can be computed by Algorithm 3.11
Algorithm 3 (Gradient evaluation).

**Input:** $\mathcal{A}$, $W$, $V_{\#ij}$, $p_D$, $R$

1: Perform steps 1–3 of Algorithm 7
2: Compute the first term $2Y^\top \mathcal{A} (p_D)$ of the gradient $(\nabla_{d \times m})$
3: Compute the second term of the gradient $(\nabla_{d \times m})$

**Output:** $\nabla_{d \times m} f (R)$

4.2. Approximation of the Hessian: Jacobian of $\Delta p^*$

The following proposition gives an expression to compute the Jacobian of $(\Delta p^* (R))$.

**Proposition 3.**

- The Jacobian of $(\Delta p^* (R))$ is given by
  \[
  \frac{\partial \Delta p^*}{\partial R_{ij}} = G^\top (R) \Gamma^{-1} z_{ij} + \frac{\partial G^\top}{\partial R_{ij}} y,
  \]
  \[
  (\partial \Delta p^*/R_{ij})
  \]
  where
  \[
  z_{ij} := \frac{\partial s}{\partial R_{ij}} - \frac{\partial \Gamma}{\partial R_{ij}} y.
  \]

- The vector $z_{ij}$ can be expressed as
  \[
  z_{ij} = (\mathcal{A}^\top (p_D))_{i,j} \otimes e^{(i)} - \left( (z_{ij}^{(1)}) \otimes e^{(i)} + z_{ij}^{(2)} \right),
  \]
  where
  \[
  z_{ij}^{(1)} := \sum_{k=1}^{n} \text{col} \left( (e^{(j)})^\top V_{\#1k} R^\top Y_{i,k} \ldots , (e^{(j)})^\top V_{\#nk} R^\top Y_{i,k} \right),
  \]
  \[
  z_{ij}^{(2)} := \sum_{k=1}^{n} Y_{i,k} \text{col} \left( RV_{\#1k} e^{(j)} , \ldots , RV_{\#nk} e^{(j)} \right).
  \]

**Proof.** The proof is given in Appendix A.

**Proposition 4** leads to the following algorithm.

Algorithm 4 (Jacobian evaluation).

**Input:** $\mathcal{A}$, $W$, $V_{\#ij}$, $p_D$, $R$

1: Perform steps 1–3 of Algorithm 7
2: for $j \in 1 : m$ do
3:   Compute $(z_{ij}^{(1)})$,
4:   for $i \in 1 : d$ do
5:     Compute $(z_{ij}^{(2)})$ and $(z_{ij})$.
6:     Set $x \leftarrow G^\top \Gamma^{-1} z_{ij}$.
7:   Set $\frac{\partial \Delta p^*}{\partial R_{ij}} \leftarrow x + \frac{\partial G^\top}{\partial R_{ij}} y$.
8: end for
9: end for

**Output:** Jacobian of $\Delta p^* (R)$
4.3. Using Cholesky factorization

In this section, we show that the cost function and an approximation of the Hessian can be computed using the Cholesky factorization of $\Gamma$

$$\Gamma = L_\Gamma^T L_\Gamma.$$ 

The Cholesky factorization yields a numerically reliable way [15, Ch. 4] to solve the system of equations $\Gamma u = v$, by using the following identity

$$\Gamma^{-1} = L_\Gamma^{-1} L_\Gamma^{-T}.$$ 

Algorithm 5 (Solve system $\Gamma u = v$).

**Input:** $\Gamma$, $v$

1: Compute the Cholesky factor $L_\Gamma$ of $\Gamma$.

2: Solve $L_\Gamma^T g = v$ and $L_\Gamma u = g$ by backward substitution.

**Output:** $u$

Moreover, the cost function can be represented as

$$f(R) = \|L_\Gamma^{-T} s(R)\|_2^2,$$

which leads to a more efficient algorithm for the cost function evaluation than Algorithm 1.

Algorithm 6 (Cost function evaluation using Cholesky factorization).

**Input:** $S$, $W$, $V^{\#}_{ij}$, $pD$, $R$

1: Compute $s(R)$.

2: Compute $\Gamma^{\#}_{ij}$ using $V^{\#}_{ij}$.

3: Compute the Cholesky factor $L_\Gamma$.

4: Solve $L_\Gamma^T g_s(R) = s(R)$.

5: Compute $f(R) = \|g_s(R)\|_2^2$.

**Output:** $f(R)$

In addition, equation $\|L_\Gamma^{-T} s\|_2^2$ defines a representation of the cost function as a sum of squares, which is more compact and easier to compute than $s^\top \Gamma^{-1} s$. Indeed, $\Delta p^*(R) \in \mathbb{R}^{n_p}$, but $g_s(R) \in \mathbb{R}^{nd}$. However, the elements of the Jacobian of $g_s$

$$\frac{\partial g_s}{\partial R_{ij}} = L_\Gamma^{-T} \frac{\partial s(R)}{\partial R_{ij}} + \frac{\partial L_\Gamma^{-T}}{\partial R_{ij}} s(R),$$

cannot be computed analytically due to the need of differentiation of $L_\Gamma^{-T}$. For this purpose the pseudo-Jacobian, proposed in [20], can be used

$$\frac{\partial(p) g_s}{\partial R_{ij}} := \left(L_\Gamma^{-T} \frac{\partial s(R)}{\partial R_{ij}} - \frac{1}{2} L_\Gamma^{-T} \frac{\partial \Gamma}{\partial R_{ij}} \Gamma^{-1} s(R) \right).$$

**Note 6.** In [20] it was shown that for functions of the form $s^\top \Gamma^{-1} s$, the pseudo-Jacobian $J_y^{(p)}$ yields the same stationary points of $f(R)$ (i.e., $\nabla f = 2(J_y^{(p)})^\top g$) and provides an approximation of the Hessian of $f(R)$. 

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It is easy to see that \( \frac{\partial (p) g_s}{\partial R_{ij}} \) and \( z_{ij}^{(p)} \) differ only by a constant factor in one summand. Therefore,

\[
\frac{\partial (p) g_s}{\partial R_{ij}} = L^T \Gamma(R) z_{ij}^{(p)}; \\
z_{ij}^{(p)} := (\mathcal{S}^T (p)_{i,j} \otimes e_i) - \frac{1}{2} (z_{ij}^{(1)}) \otimes e_i + z_{ij}^{(2)}.
\]

The resulting algorithm is Algorithm 7.

**Algorithm 7** (Pseudo-Jacobian evaluation).

**Input:** \( \mathcal{S}, W, V_{ij}, pD, R \)

1: Compute steps 1–2 of Algorithm 3 using Algorithm 5.
2: for \( j \in 1:m \) do
3: Compute \( z_{ij}^{(1)} \).
4: for \( i \in 1:d \) do
5: Compute \( z_{ij}^{(2)} \) and \( z_{ij}^{(p)} \).
6: Solve \( L^T \Gamma(R) \frac{\partial (p) g_s}{\partial R_{ij}} = z_{ij}^{(p)} \).
7: end for
8: end for

**Output:** The pseudo-Jacobian \( J^{(p)}_{ij} \).

5. Weighted mosaic Hankel structured low-rank approximation problem

In this section, we establish the form of \( \Gamma(R), V_{ij} \) and \( f(R) \) for the structure \( \Phi_{m,n} \)

and weight matrix

\[
W = \text{blkdiag}(W^{(1), \ldots, W^{(q,N)}}).
\]

In view of Lemma 13, we can consider only the scalar Hankel structure.

5.1. Scalar Hankel matrices

**Lemma 4.** For the scalar Hankel structure, the matrix \( S_{\mathcal{S}} \) has the following form

\[
S_{\mathcal{S}_{m,n}} := \begin{bmatrix}
I_m & 0_{m \times (n_p - m)} & J_0^{n_p} \\
I_m & 0_{m \times (n_p - m)} & J_1^{n_p} \\
\vdots & & \vdots \\
I_m & 0_{m \times (n_p - m)} & J_{n_p - 1}^{n_p}
\end{bmatrix}.
\]

**Proof.** Indeed, for a vector \( p = [p_1, \ldots, p_{n_p}]^T \), we have

\[
[I_m \ 0_{(n_p - m) \times m}] J_{n_p}^k p = p_{k+1:k+m}.
\]

Therefore, \( \text{vec} \mathcal{S} \) holds with \( S_{\mathcal{S}_{m,n}} \) and \( S_0 = 0_{m \times n} \).
Corollary 1. The matrix $G_{m,n}$ for $W = I_{m+n-1}$ and $R \in \mathbb{R}^{m \times d}$ has the form

$$G_{m,n}(R) = \begin{bmatrix} R_{1,1} & R_{1,2} & \cdots & R_{1,m} \\ R_{2,1} & R_{2,2} & \cdots & R_{2,m} \\ \vdots & \vdots & \ddots & \vdots \\ R_{m,1} & R_{m,2} & \cdots & R_{m,m} \end{bmatrix} \in \mathbb{R}^{nd \times (m+n-1)}. \quad (G_{m,n})$$

We next consider the case of Hankel low-rank approximation with weighted 2-norm.

Proposition 4. For the scalar Hankel structure and weight matrix $W$, the blocks of $V$ are equal to

$$V_{#ij} = (W^{-1})_{1:i+1+m-1, j:j+m-1}.$$

Proof. From $(W)$ and $(S_{m,n})$, we have that

$$V_{#ij} = [I_m \ 0_m \times (n_p - m)] (J_m 1_{n_p})^{j} W^{-1} (J_m 1_{n_p})^{j-1} [I_m \ 0_{(n_p - m) \times m}]. \quad (V_{#ij}(H_{m,n}))$$

From $[1 \ 0]J^k$ one can verify that $(V_{#ij}(H_{m,n}))$ corresponds an $m \times m$ submatrix of $W^{-1}$. \qed

We will call a symmetric matrix $b$-banded ($b$-block-banded) if all upper diagonals (resp. upper block diagonals) starting from $b$-th are zero. (By convention, the main (block) diagonal is the 0-th upper (block) diagonal.)

Corollary 2. 1. If $W^{-1}$ is $b$-banded then $V$ and $\Gamma$ are $(m + b - 1)$-block-banded.

2. If $W^{-1}$ is Toeplitz then $V$ and $\Gamma$ are block-Toeplitz.

3. For the case $W \rightarrow W$ $V$ and $\Gamma$ are $m$-block-banded. In particular,

(a) For $W = I_{n_p}$, $V_{#ij} = V_{j:i}$, where $V_k := (J_m 1_{m})^k$ for $k \geq 0$, and $V_{-k} = V_k^\top$. (In this case, $\Gamma$ and $V$ are block-Toeplitz.)

(b) For $W = \text{diag}(w_1, \ldots, w_{n_p})$ (element-wise weights and fixed values),

$$V_{#ij} = \begin{cases} \text{diag}(\gamma_{i+m-1}) (J_m^\top)^{j-i}, & \text{for } j \geq i, \\ (V_{#ji})^\top, & \text{for } j < i, \end{cases}$$

where $\gamma_i := w_i^{-1}$.

5.2. The main theorem

By Lemma 1 we can consider only the layered Hankel structure

$$H_{m,n}(p) = \begin{bmatrix} H_{m_1,n}(p^{(1)}) \\ \vdots \\ H_{m_q,n}(p^{(q)}) \end{bmatrix}, \quad \text{where } m = [m_1 \cdots m_q]. \quad (H_{m,n})$$

Theorem 1. For the structure $(H_{m,n})$ and $W = \text{blkdiag}(W^{(1)}, \ldots, W^{(q)})$, with $(W^{(k)})^{-1}$ being $b^{(k)}$-banded, the following statements hold true:

1. the matrix $\Gamma$ is $\mu$-block banded with $d \times d$ blocks, with $\mu := \max_k \{m_k + b^{(k)} - 1\}$;
2. If \( W^{(k)} \) are all Toeplitz, then \( \Gamma \) is block-Toeplitz.

3. For the case \( \mathbf{w} \rightarrow \mathbf{W} \) and \( W^{(k)} = \text{diag} \ w^{(k)} \), \( w^{(k)} \in \mathbb{R}^{n_k} \), the matrices \( V_{\mathcal{K}_{m,n}} \) and \( \Gamma_{\mathcal{K}_{m,n}}(R) \) are block-banded with block bandwidth

\[ \mu := \max\{m_l\}_{l=1}^q, \]

in particular,

(a) the matrices \( V_{\#ij} \) for \( j \geq i \) can be expressed as

\[ V_{\#ij} = \text{diag} \left( \text{col} \left( \gamma_{\mathbf{1}}, \ldots, \gamma_{\mathbf{q}} \right) \right) \begin{pmatrix} J_m \end{pmatrix}_{j-i} \]

where \( \gamma^{(k)} = (w^{(k)})^{-1} \) and \( J_m = \text{blkdiag} \begin{pmatrix} J_{m_1}, \ldots, J_{m_q} \end{pmatrix} \);

(b) if the weights are constant for the blocks of \( \mathcal{K}_{m,n} \), i.e., \( w^{(l)} \equiv \omega_l \), where \( \omega_l \in \mathbb{R} \), (block-wise \( \mathbf{w} \))

then \( V \) is block-Toeplitz, i.e., \( V_{\#ij} = V_{j-i} \), and

\[ \Gamma_{\#ij}(R) = \Gamma_{j-i}, \quad \Gamma_k = RV_kR^\top, \]

\[ V_k = \text{blkdiag} \begin{pmatrix} \gamma_1 I_{m_1}, \ldots, \gamma_q I_{m_q} \end{pmatrix} \begin{pmatrix} J_m \end{pmatrix}_k \]

and \( \gamma_l := \omega_l^{-1} \).

**Proof.** Theorem 1 follows from Lemma 2 and Corollary 2.

---

5.3. Computational complexity of the algorithms for layered and mosaic Hankel structures

In this section, we assume that \( \mathbf{W} \) is given by \( \mathbf{w} \rightarrow \mathbf{W} \), and therefore \( \Gamma \) matrix is \( \mu \)-block-banded with \( \mu = \max_k \{m_k\} \). This case is implemented in the C++ solver of [4]. In our complexity analysis, we count only the number of multiplications, since the number of additions is typically less than the number of multiplications.

**Lemma 5.** For \( \mathcal{K}_{m,n} \), the complexity of the steps in the Algorithm 5 is given by \( O(d^3 \mu^2 n) \) for step 1 and \( O(d^2 \mu n) \) for step 2.

**Proof.** \( \Gamma \in \mathbb{R}^{nd \times nd} \) is \( \mu d \)-banded, and the complexity of both steps is given in [15, Ch. 4].

**Theorem 2.** For \( \mathcal{K}_{m,n} \), the complexity of the cost function evaluation using Algorithm 6 and gradient evaluation using Algorithm 3 is \( O(d^3 \mu mn) \).

**Proof.** The proof is given in Appendix A.

**Note 7.** By Lemma 8 for the mosaic Hankel structure \( \mathcal{K}_{m,n} \) the complexity of the cost function and gradient evaluation is also \( O(d^3 \mu mn) \).

**Note 8.** The computation on the step 2 in the Algorithm 2 has complexity \( O(dmn) \).

**Theorem 3.** The computational complexity of Algorithm 7 for the Jacobian is \( O(d^3 m^2 n) \). The computational complexity of Algorithm 7 (for the pseudo-Jacobian) is \( O(d^3 \mu mn) \).

**Proof.** The proof is given in Appendix A.
Next, we show that the complexity is linear in \( m \) (for fixed \( d \) and \( n \)) for the cost function and the gradient in the case (block-wise \( w \)). In the cost function evaluation, the most expensive step is the Cholesky factorization, which can be performed in linear in \( m \) number of operations in this case [21]. The computation of the gradient can be also simplified due to block-Toeplitz structure of \( \Gamma \).

**Proposition 5.** Let \( y, Y \) be defined as in (\( y \)), \( (Y) \), and weights satisfy (block-wise \( w \)). Then the gradient \( \nabla_{d \times m}(f) \) can be simplified to

\[
\nabla_{d \times m}(f) = 2Y \mathcal{S}^T(p_0) - 2 \left( N_0 RV_0 + \sum_{0 < k \leq \min(n, \mu)} (N_k RV_k + N_k^T RV_k^T) \right),
\]

where \( N_k := Y (J_n^T)^k (Y)^T \).

**Proof.** The proof is given in Appendix A. \( \square \)

Using Proposition 5, the following theorem can be proved.

**Theorem 4.** For the case (block-wise \( w \)), the complexity of the cost function and gradient evaluation is equal to \( O(d^3 mn) \).

**Proof.** The proof is given in Appendix A. \( \square \)

**Note 9.** The computations can be further simplified for mosaic Hankel matrices \( H_{m,n} \) and block-wise weights, which are constant along the block rows of the mosaic Hankel matrix, i.e.

\[
w = \text{col} \left( w^{(1,1)}, \ldots, w^{(q,1)}, \ldots, w^{(1,N)}, \ldots, w^{(q,N)} \right), \text{ where } w^{(l,k)} \equiv \omega_l, \omega_l \in \mathbb{R}.
\]

Let the \( \Gamma^{(l)} \) be the \( \Gamma \) matrix for the structure \( H_{m,n} \), as in Lemma 1. Then all \( \Gamma^{(l)} \) are submatrices of \( \Gamma^{(l_{\text{max}})} \), where \( n_{l_{\text{max}}} \geq n_l \) for all \( l \). Therefore, only the Cholesky factorization of \( \Gamma^{(l_{\text{max}})} \) needs to be computed.

**Note 10.** We have considered only the case when \( W \) is diagonal. However, by Theorem 7 \( \Gamma \) is block-banded/block-Toeplitz if \( W^{-1} \) is b-banded. In this case the algorithms will have complexity similar to that in Theorems 2–4, with an additional factor \( b \).

Note 10 generalizes the results of [22], where this type of weights was first considered.

### 5.4. Numerical experiments

First, we consider a family of \( 2 \times 2 \) mosaic Hankel matrices

\[
H_{[m_1, m_2], [n_1, n_2]}, m_1 = 20, m_2 = 22, [n_1, n_2] = [250, 255] + 250k. \quad (\text{EX1})
\]

In the case of 2-norm (\( W = I_{n_1} \)) we compute the cost function and its derivatives using the SLRA package [4]. Hereafter, we use the term “element-wise variant” for the algorithms that treat weights as different values (implemented in the \( \text{WLayeredHankelStructure C++} \) class). We use the term “block-wise variant” for the algorithms that utilize Theorem 5 (block-Toeplitz structure of \( \Gamma \)), and is implemented in the \( \text{LayeredHankelStructure C++} \) class. In these examples, we consider only the rank reduction \( d = 1 \) (\( r = m - 1 \)).
Fig. 1 shows the time needed for computation of the cost function, gradient and pseudo-Jacobian for (EX1), with \( k \in 0 : 10 \). The computation time is plotted in logarithmic scale. In all cases the computation time is bounded by a linear function in \( n \). This empirical observation is in agreement with Theorem 2 and Theorem 4.

Next, we show the computation time for varying \( m \), for scalar Hankel matrices. In Fig. 2 the computational time is plotted for element-wise and block-wise variants, as explained above.

Fig. 2 shows that the computational time for the cost function and the gradient is growing faster than linearly in \( m \) (in contrast to Theorems 2 and 3). The computation of the pseudo-Jacobian is also growing faster than quadratically in \( m \) (in contrast to Theorem 3). These effects
can be expected because in the current version of the software [4] (7 March 2013) products by $V_{#ij}$ matrices are implemented as products by precomputed matrices, and not as element-wise products.

The examples in this section are reproducible and can be found in the directory

```
/test_c/test_speed
```

of the publicly available software package [4]. The results in this section were obtained on a 2.6GHz Intel Core i5 CPU with 4GB RAM, running under 64-bit Linux Mint Debian Edition.

6. Conditioning of $\Gamma$, solvability conditions, and accuracy of computations

It is important to know the condition number $\kappa_2(\Gamma)$ in order to use the methods of the paper. Indeed, $\kappa_2(\Gamma)$ should be finite in order to apply the efficient algorithms of the paper ($\Gamma$ should be invertible). If $\Gamma$ is invertible, then $\kappa_2(\Gamma)$ determines the accuracy of the computational process.

Next, we discuss the invertibility of $\Gamma$ and the behavior of $\kappa_2(\Gamma)$ for mosaic Hankel matrices.

6.1. Invertibility of $\Gamma$

In this subsection, we investigate the conditions of invertibility of $\Gamma$ for mosaic Hankel matrices ($H_{m,n}$). By Lemma 1 it is necessary that $G(R)$ is of full row rank for each $H_{m,n,k}$. By simple calculation of dimensions we have that the necessary condition (NC) is equivalent to

$$\sum_{l=1}^{q} (m_l + n_k - 1) \geq n_k d \iff (q - d)n_k \geq q - m,$$

which is satisfied if $d \leq q$ (and is equivalent to $d \leq q$ if $m < n_k - q$ for all $k$).

As it was noted in [4], the condition $d \leq q$ can always be satisfied in applications of mosaic Hankel (SLRA) to approximate realization, system identification and model reduction. In particular, any Hankel (SLRA) can be reduced to an equivalent problem with $d = 1$.

**Proposition 6.** For the Hankel structure $H_{m,n,p-m+1}$, $r < \min(m, n_p - m + 1)$ and $p_n \in \mathbb{R}^{n_p}$, problem (SLRA) is equivalent to (SLRA) for the structure $H_{r+1,n_p-r}$, rank $r$ and $p_n$.

**Proof.** It is sufficient to show that if $r < \min(m, n_p - m + 1)$

$$\text{rank } H_{m,n,p-m+1}(p) \leq r \iff \text{rank } H_{r+1,n_p-r}(p) \leq r,$$

which is a corollary of [23, Prop. 5.4].

The next proposition shows that for the general mosaic Hankel structure, if $d \leq q$ then $\Gamma$ is nonsingular for almost all $R$ (is singular on a submanifold of smaller dimension).

**Proposition 7.** Let $d \leq q$, and $W$ be positive definite.

- If $d = 1$ then $\Gamma(R)$ is nonsingular for all $R \in \mathbb{R}^{1 \times m} \setminus \{0_{1 \times m}\}$.
- If $d > 1$, there exists a permutation matrix $\Pi \in \mathbb{R}^{m \times m}$ such that $\Gamma(R)$ is nonsingular at $R = [X \hspace{1cm} 1_d] \Pi$ for any $X \in \mathbb{R}^{d \times (m-d)}$.

**Proof.** The proof is given in Appendix A.

Proposition 7 is an extended to the mosaic Hankel matrices Corollary 4.11 from [17].
6.2. Accuracy of the computational process

The key computational procedure in evaluation of the cost function and its derivatives is the solution of a system of equations $\Gamma u = v$ using Cholesky factorization. The accuracy of this step depends on the condition number of $\Gamma$ [13]. In what follows, we review some results concerning conditioning of symmetric block-Toeplitz $\mu$-block-banded $\Gamma$ (the case of layered Hankel structures with block-wise weights, see Theorem [1]). For convenience, we denote by $\Gamma^{(n)}$ the $nd \times nd$ $\Gamma$ matrix.

Since $\Gamma^{(n)}$ is symmetric positive-semidefinite, $\kappa_2(\Gamma^{(n)})$ (the condition number for 2-norm) is equal to the ratio of its extreme eigenvalues $\lambda_{\text{min}}(\Gamma^{(n)})$ and $\lambda_{\text{max}}(\Gamma^{(n)})$. The properties of the eigenvalues of the matrices $\Gamma^{(n)}$ are determined by their generating function $F : \mathbb{C} \rightarrow \mathbb{C}^{m \times m}$, defined as

$$F(z) = \sum_{k=-\mu}^{\mu} \Gamma_k z^k.$$

Since $F(z)$ is Hermitian for all $z$ and $F$ is continuous on the unit circle $T$, we can define

$$a_F := \min_{\mathbb{T}} \lambda_{\text{min}}(F(z)) \geq 0, \quad b_F := \max_{\mathbb{T}} \lambda_{\text{max}}(F(z)) < \infty.$$

The results of [24] imply that $\lambda_{\text{min}}(\Gamma^{(n)}) \not\leq a_F$, and $\lambda_{\text{max}}(\Gamma^{(n)}) \not\geq b_F$, i.e. the eigenvalues are in $[a_F; b_F]$ and converge to the endpoints as $n \rightarrow \infty$. Therefore,

$$\kappa_2(\Gamma^{(n)}) \geq \frac{b_F}{a_F}.$$

If $F(z)$ is positive definite on $T$, then $\kappa_2(\Gamma^{(n)}) \leq b_F/a_F < \infty$. Otherwise, $\kappa_2(\Gamma^{(n)}) \rightarrow \infty$.

For simplicity, in what follows we consider the case $d = 1$. For Hankel structures we have

$$F(z) = R(z)\overline{R(z)} = |R(z)|^2 \quad \text{for} \quad z \in T,$$

where $R(z) = R_{1,1} + R_{1,2}z + \ldots + R_{1,m}z^{m-1}$ is the characteristic polynomial of the difference equation defined by $R \in \mathbb{R}^{1 \times m}$. By Lemma [2], in the general case of mosaic Hankel matrices with block-wise weights $w_l$, the function $F$ is expressed as

$$F(z) = \sum_{k=1}^{q} w_l^{-1} |R^{(l)}(z)|^2 \quad \text{for} \quad z \in T.$$

For Hankel structures, the condition number of $\Gamma^{(n)}$ tends to infinity if and only if $R(z)$ has roots on $T$. The growth rate is $n^{2\alpha}$ [26], where $\alpha$ is the maximal root multiplicity on $T$. In Fig [3] we plot the dependence of $\kappa_2$ on $n \in 100 : 1000$ for $K = 50$ random instances of

$$R(z) = \prod_{k=1}^{4} (z - \lambda_k)(z - \overline{\lambda_k}).$$

The roots $\lambda_k$ are generated uniformly on the upper half of the unit circle, and the condition number was computed by the function $\text{cond}$ of Matlab. Fig [4] shows that the matrices can be very ill-conditioned. In most cases, we have $\kappa_n$ grows as $n^\alpha$. In a few cases, the condition number growth is similar to $n^4$, which can be explained by the neighboring roots behaving as multiple roots.
In the mosaic Hankel case, $\kappa_2(\Gamma^{(n)})$ is unbounded if and only if $(F_{m,n})$ has zeros on $\mathbb{T}$. If only one block has a nonzero weight, then the function $(F_{m,n})$ is of form $(F_{m,n})$ and $\Gamma^{(n)}$ has the same conditioning properties as that for the scalar Hankel structure. Otherwise, if at least two blocks have weights $w_l < \infty$ (are not fixed), then all corresponding polynomials in $(F_{m,n})$ need to have common zeros on $\mathbb{T}$ in order for $F$ to have a zero on $\mathbb{T}$.

In system identification—one of the main applications of (SLRA) [1]—the former case corresponds to output-error identification. The latter case corresponds to errors-in-variables system identification. For several polynomials, it is less common (compared to a single polynomial) to have approximately common zeros on or close to the unit circle. Therefore, errors-in-variables identification with (SLRA) is typically better conditioned than output-error identification.

7. Conclusions

In this paper we considered the structured low-rank approximation problem for general affine structures, weighted 2-norms and fixed values constraints. We used the variable projection principle, which has many advantages when applied to (SLRA). The $\Gamma$ matrix in $(s^\top \Gamma^{-1} s)$ is structured and its structure is determined by the original matrix structure. For the mosaic Hankel structure $(\mathcal{H}_{m,n})$, the $\Gamma$ matrix is block-banded/block-Toeplitz, depending on the structure of the weight matrix. This allows us to evaluate the cost function $f(R)$ and its derivatives in $O(m^2n)$ flops ($O(mn)$ for the cost function and the gradient if $\Gamma$ is block-Toeplitz). The approach in this paper can be applied to other matrix structures $\mathcal{S}$, where the structure of $\Gamma$ (e.g. sparseness) can be exploited for efficient computations.

Whenever possible, we considered the most general cases (structures, weights) and developed the algorithms for the general affine structure. We showed how the cost functions for the blocked structures (layered, striped) can be expressed through the cost functions of the blocks. This allowed us to reduce the mosaic Hankel case to the scalar Hankel case and helped to simplify the derivations of the algorithms and their complexities (compared to [11, 17]). We also considered fixed values as a special case of the weighted norm, which also simplified treatment of this case.

The developed algorithms require invertibility of the $\Gamma$ matrix. For affine structures, a necessary condition of invertibility is $n_p \geq nd$, which for mosaic Hankel matrices is satisfied if the rank reduction $d$ does not exceed the number of block rows $q$ in $(\mathcal{H}_{m,n})$. If the condition $d \leq q$ is satisfied, the $\Gamma$ matrix is nonsingular for a generic $R$.

The accuracy of the computations mainly depends on the conditioning of $\Gamma$. If $\Gamma$ is block-Toeplitz, the properties of its condition number can be expressed through its generating function. Deeper investigation of properties of $\Gamma$, such as invertibility and conditioning, is a direction of future research.
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Appendix A. Proofs

Proof of Proposition 1. If $W$ is positive definite, then $(\Delta p \rightarrow \hat{p})$ is an invertible transformation and problems $\text{SLRA}_{\Delta}$ and $\text{SLRA}$ are equivalent by $(\mathcal{Z}_{\Delta} \leftrightarrow \mathcal{Z})$ and $\| \cdot \|_W = \| \cdot \|_2$.

Now consider the case when $W$ is given by $(w \rightarrow W)$. We have that

$$L_W^{-1} = \text{diag}(\sqrt{w_1^{-1}}, \ldots, \sqrt{w_{n_x}^{-1}}),$$

where $\sqrt{\infty} = 0$. Therefore, the parametrization $(\Delta p \rightarrow \hat{p})$ keeps $\hat{p}_k = (p_0)_k$ for fixed values (k such that $w_k = \infty$) and runs over all possible $\hat{p}_k$ for other $k$. Therefore, all admissible $\hat{p}$ for $(\text{SLRA})$ (with fixed values constraints) can be parametrized as $(\Delta p \rightarrow \hat{p})$.

Instead of $\| \cdot \|_W = \| \cdot \|_2$, in the case $(w \rightarrow W)$ we have that

$$\| \Delta p \|_2^2 = \| \hat{p} - p_0 \|_W^2 + \sum_{k: w_k = \infty} (\Delta p_k)^2,$$  (A.1)

and by $(\mathcal{Z}_{\Delta} \leftrightarrow \mathcal{Z})$ and (A.1), $(\text{SLRA}_{\Delta})$ is equivalent to

$$\min_{\Delta p \in \mathbb{R}^{p}} \| \Delta p \|_2^2 \text{ subject to } \text{rank } \mathcal{Z}(\Delta p) \leq r. \quad (A.2)$$

It is straightforward that $\mathcal{Z}(\Delta p)$ does not depend on $\Delta p_k$ corresponding to the fixed values. From the first-order optimality conditions of (A.2), all local minima of (A.2) must satisfy $\Delta p_k = 0$ for $w_k = \infty$. Hence, the local minima of $(\text{SLRA}_{\Delta})$ coincide with the local minima of (A.2). \hfill \Box

Proof of Proposition 2. First, note that if the differential of $f$ is represented as

$$df(R, H) = \text{tr}(AH^T),$$

where $\text{tr}$ is the trace operator, then $\nabla_{d \times m}(f) = A$. From $[\mathcal{Z} \leftrightarrow S]$, the differential of $f$ is given by

$$df(R, H) = 2y^Tds(R, H) - y^T\nabla(R, H)y.$$  (df(R, H))

By $(\mathcal{Z}(H) \leftrightarrow V)$, the first term in $(df(R, H))$ is equal to

$$2y^Tds(R, H) = \text{tr} \left( 2Y(H, \mathcal{Z}(p_0)) \right) = \text{tr} \left( 2YH^T(p_0)H^T \right).$$

By $(\mathcal{Z} \leftrightarrow S)$, the second term in $(df(R, H))$ is equal to

$$y^T\nabla(R, H)y = \sum_{i,j=1}^n Y^T_{i,j}d\mathcal{Z}_{ik}(R, H)Y_{i,j}$$

$$= \sum_{i,j=1}^n Y^T_{i,j}(HN_{\#ij}R^T + RV_{\#ij}H^T)Y_{i,j}$$

$$= \sum_{i,j=1}^n \text{tr} \left( (Y_{i,j}Y^T_{i,j}RV_{\#ij} + Y_{i,j}Y^T_{i,j}RV_{\#ij})H^T \right),$$

which in combination with $V_{\#ij} = \mathcal{V}_{\#ij}$ yields $\nabla_{d \times m}$. \hfill \Box
Proof of Proposition 3. The equation \( \partial \Delta p^*/R_{ij} \) can be obtained by differentiation of \( \Delta p^*(R) \). The first summand in \( z_{ij} \) can be expressed as

\[
\frac{\partial s}{\partial R_{ij}} = \text{vec} \left( e^{(i)} (e^{(j)})^T \mathcal{F}(p_b) \right) = \left( \mathcal{F}^T(p_b) \right)_{i,j} \otimes e^{(i)}.
\]

The second summand is

\[
\frac{\partial \Gamma}{\partial R_{ij}} y = \text{col}(a_1, \ldots, a_n), \quad a_l \in \mathbb{R}^d,
\]

where

\[
a_l = \sum_{k=1}^{n} \frac{\partial V_{lk}}{\partial R_{ij}} Y_{c,k} = \sum_{k=1}^{n} \left( e^{(i)} (e^{(j)})^T V_{l1k} R^T + RV_{l1k} e^{(j)} (e^{(i)})^T \right) Y_{c,k}
\]

\[
= \left( \sum_{k=1}^{n} (e^{(j)})^T V_{l1k} R^T Y_{c,k} \right) e^{(i)} + \sum_{k=1}^{n} Y_{l1,k} RV_{l1k} e^{(j)}.
\]

Proof of Theorem 2. The complexities for each individual step of Algorithm 6 are given in Table A.2. The complexities of the steps for Algorithm 3 are given in Table A.3.

1. Compute \( s(R) \) — \( O(dmn) \), see Table A.2.
2. Compute \( \Gamma_{ijkl} \) — \( O(d^2 \mu mn) \). We need to compute \( \mu n \) matrices \( \Gamma_{ijkl} \). By Theorem 1 each \( V_{ijkl} \) has \( \leq m \) nonzero elements, and each \( \Gamma_{ijkl} \) needs \( d^2 m \) multiplications.
3. Compute \( L_{\Gamma} \) — \( O(d^3 \mu n^2) \), by Lemma 5.
4. Solve \( L_{\Gamma}^T g_s(R) = s(R) \) — \( O(d^2 \mu n) \), by Lemma 5.
5. Compute \( \|g_s(R)\|_2^2 \) — \( O(nd) \).

Table A.2: Complexity of the steps of Algorithm 6.

1. Steps 1–3 of Algorithm 6 — \( O(d^3 \mu^2 n) \), see Table A.2.
2. Compute \( 2Y^T \mathcal{F}^T(p_b) \) — \( O(nmd) \), since it is multiplication of a \( d \times m \) matrix by \( n \times m \) matrix.
3. Compute the second term — \( O(d^2 \mu mn) \). We need to compute \( 2 \mu n \) products \( Y_{c,j} Y_{c,i}^T RV_{ijkl} \). By Theorem 1 \( V_{ijkl} \) has only one nonzero diagonal and \( u := Y_{c,i}^T RV_{ijkl} \) can be computed in \( dm \) flops. The product \( Y_{c,j} u \) takes \( dm \) flops.

Table A.3: Complexity of the steps of Algorithm 3.

Proof of Theorem 3. For each \( e^{(j)} \), due to block-bandedness of \( V \), we need to compute \( 2 \mu n \) products of the form \( a_{j,k,l}^T Y_{c,k} \), where

\[
a_{j,k,l}^T := (e^{(j)})^T V_{l1k} R^T.
\]
By Theorem 1, each \((e^{(i)})^\top V_{\#ik}\) has at most one nonzero element, and computing \(a_{j,k,l}^\top\) takes \(d\) multiplications. Another \(d\) multiplications are needed to compute the inner product of \(a_{j,k,l}\) and \(Y_{i,k}\). The computation of \(z_{ij}^{(2)}\) is repeated \(m\) times, which leads to \(O(d^2mn)\) complexity.

For each \(z_{ij}^{(2)}\), we need to compute \(2\mu n\) products of the form \(Y_{i,k}RV_{\#ik}e^{(j)}\), where each product has complexity \(d\), as in the previous step. The computation of \(z_{ij}^{(2)}\) is repeated \(md\) times, which leads to \(O(d^3mn)\) complexity.

For pseudo-Jacobian, we need to solve \(\sum_{j} z_{ij}^{(2)}\) times the banded system with the Cholesky factor \(L_R^\top\) and \(z_{ij}\), which has complexity \(O(d^3mn)\). For Jacobian, we also need to multiply each \(\Gamma^{-1}z_{ij}\) from the left by \(G^\top(R)\), which has complexity \(d^2m\) by Note 8. Therefore, this step has additional complexity \(O(d^2m^2n)\).

**Proof of Proposition 5** The second term in \(\nabla_{d\times m}\) can be represented as

\[
\sum_{k=-\mu}^{\mu} \min(n-k,n) Y_{i,i+k} Y_{i,i+k}^\top RV_k = \sum_{k=0}^{\mu} \sum_{i=1}^{n-k} Y_{i,i+k} Y_{i,i+k}^\top RV_k + \sum_{k=1}^{\mu} \sum_{i=1}^{n-k} Y_{i,i+k} Y_{i,i+k}^\top RV_k.
\]

It is easy to see that for \(k \geq 0\)

\[
\sum_{i=1}^{n-k} Y_{i,i+k} Y_{i,i+k}^\top = Y(J_m^\top)^k(Y)^\top = N_k.
\]
where \( Q = [Q^{(1)} \quad Q^{(2)} \quad \ldots \quad Q^{(m_1)}] \) is the partition of \( Q \) into \( Q^{(k)} \in \mathbb{R}^{d \times q} \).

If \( d = 1 \), then the matrix \( G_{H_{m,n}}(R)\Pi^{(m_1+n-1,q)} \) is of full row rank for all nonzero \( Q \).

For \( d \geq 1 \), consider \( Q = [X \quad 1_d] \). Since \( d \leq q \), \( Q^{(m_1)} \) has the form \( Q^{(m_1)} = \left[ \ast \quad 1_d \right] \) and \( G_{H_{m,n}}(R)\Pi^{(m_1+n-1,q)} \) is of full row rank due to its row echelon form.

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