Chapter 3
Introductory Example

Abstract The fact that a matrix can be simplified by compressing its submatrices is not new. The panel clustering method (cf. [149], [225, §7]), the multipole method (cf. [115], [225, §7.1.3.2]), mosaic approximation (cf. [238]), and matrix compression techniques by wavelets (cf. [76]) are based on the same concept. However, in none of these cases is it possible to efficiently perform matrix operations other than matrix-vector multiplication. Therefore, in this chapter we want to illustrate how matrix operations are performed and how costly they are. In particular, it will turn out that all matrix operations can be computed with almost linear work (instead of $\mathcal{O}(n^2)$ or $\mathcal{O}(n^3)$ for the full matrix representation). On the other hand, we have to notice that, in general, the results contain approximation errors (these will be analysed later). In the following model example we use a very simple and regularly structured block partition. We remark that in realistic applications the block partition will be adapted individually to the actual problem (cf. Chapter 5).

3.1 The Model Format $\mathcal{H}_p$

We consider the index sets $I = \{1, \ldots, n\}$, where n is a power of two:

$$n = 2^p,$$

and define the matrix format $\mathcal{H}_p$ inductively with respect to p. To indicate that I depends on p, we also write I_p instead of I.

For $p = 0$, the matrix $M \in \mathbb{R}^{I \times I}$ is a scalar (formally a 1×1 matrix represented as a full matrix). Accordingly, we define $\mathcal{H}_0$ as the set of 1×1 matrices in the representation `full_matrix`$(1, 1)$. The representations $\mathcal{H}_p$ for larger p are defined recursively.

Assume that the format of $\mathcal{H}_{p-1}$ for matrices from $\mathbb{R}^{I_{p-1} \times I_{p-1}}$ is known. Then a matrix from $\mathbb{R}^{I_p \times I_p}$ can be represented as the following block matrix:

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$$M = \begin{bmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{bmatrix}, \qquad M_{ij} \in \mathbb{R}^{I_{p-1} \times I_{p-1}}. \tag{3.1a}$$

We restrict the set of all $M \in \mathbb{R}^{I \times I}$ by the conditions

$$M_{11}, M_{22} \in \mathcal{H}_{p-1}, \quad M_{12}, M_{21} \in \mathcal{R}_{p-1}(r), \tag{3.1b}$$

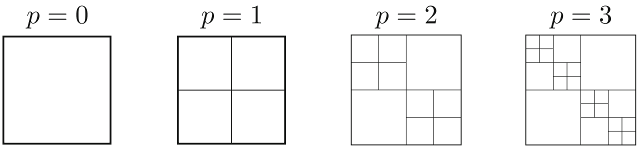
where $\mathcal{R}_{p-1}(r) := \mathcal{R}_{p-1}(r, I_{p-1}, I_{p-1})$ is the rank-r matrix family from Definition 2.5. The set of matrices (3.1a) with (3.1b) forms the set $\mathcal{H}_p$. In principle, the local rank r should be chosen such that a certain accuracy is reached. However, in this chapter the approximation error is irrelevant. We choose

$$r = 1 \tag{3.1c}$$

and abbreviate $\mathcal{R}_{p-1}(1)$ by $\mathcal{R}_{p-1}$. The recursive structure of the format $\mathcal{H}_p$ can be symbolised by

$$\mathcal{H}_p = \begin{bmatrix} \mathcal{H}_{p-1} & \mathcal{R}_{p-1} \\ \mathcal{R}_{p-1} & \mathcal{H}_{p-1} \end{bmatrix}. \tag{3.1d}$$

The following diagrams show the resulting block partitions for $p = 0, 1, 2, 3$:



(3.2)

The left partition in Figure 3.1 shows the case of $n = 2^7 = 128$. By definition of $\mathcal{R}_p(r)$, each block b contains a matrix block $M|_b$ of $\mathrm{rank}(M|_b) \leq r$, where $r = 1$ is chosen according to (3.1c).

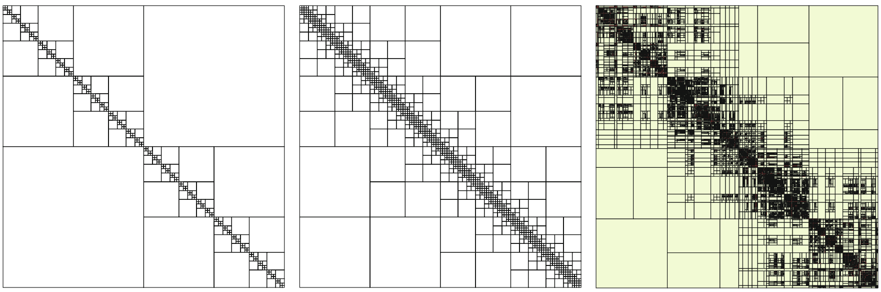


Fig. 3.1 Left: model block partition $\mathcal{H}_7$. Middle: admissible block partition. Right: partition for a real-life application of size 447488.

3.2 Number of Blocks

As a first quantity we determine the number of blocks in the format $\mathcal{H}_p$. The inductive proof starts with $p = 0$ (i.e., $n = 2^0 = 1$). The 1×1-matrix contains $N_{\text{block}}(0) = 1$ block. Recursion (3.1d) shows that $N_{\text{block}}(p) = 2 + 2N_{\text{block}}(p-1)$ for $p > 0$. This recursive equation has the solution

$$N_{\text{block}}(p) = 3n - 2. \tag{3.3}$$

3.3 Storage Cost

The storage cost of an $\mathcal{R}_p$ matrix ($n = 2^p$) is $S_R(p) = 2^{p+1}$ (cf. Remark 2.6). Let S_p be the storage cost of a matrix from $\mathcal{H}_p$. For $p = 0$, only a 1×1 matrix has to be stored, i.e., $S_0 = 1$. The recursion (3.1d) shows that

$$S_p = 2S_{R1}(p-1) + 2S_{p-1} = 2^{p+1} + 2S_{p-1}\,.$$

Together with $S_0 = 1$, one verifies that $S_p = (2p+1)\,n$ is the solution. This proves the next lemma.

Lemma 3.1. *The storage cost of a matrix from* $\mathcal{H}_p$ $(n = 2^p)$ *is*

$$S_p = n + 2n \log_2 n\,. \tag{3.4}$$

3.4 Matrix-Vector Multiplication

Let $M \in \mathcal{H}_p$ and $x \in \mathbb{R}^{I_p}$ with $n = 2^p$. We denote the cost of $M \cdot x$ by $N_{\text{MV}}(p)$. For $p \geq 1$ decompose M as in (3.1a): $M = \begin{bmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{bmatrix}$. Accordingly, x becomes $x = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$ with $x_1, x_2 \in \mathbb{R}^{I_{p-1}}$. Multiplying $M \cdot x$ requires computing the products $y_{11} := M_{11}x_1$, $y_{12} := M_{12}x_2$, $y_{21} := M_{21}x_1$, $y_{22} := M_{22}x_2$ and the sums $y_{11} + y_{12}$ and $y_{21} + y_{22}$. By Remark 2.9a, $M_{12}x_2$ and $M_{21}x_1$ require $3\frac{n}{2} - 1$ operations each, whereas addition takes $n/2$ operations. This leads to the recursion

$$N_{\text{MV}}(p) = 2N_{\text{MV}}(p-1) + 4n - 2$$

with the starting value $N_{\text{MV}}(0) = 1$. Its solution is $N_{\text{MV}}(p) = 4np - n + 2$.

Lemma 3.2. *Let* $n = 2^p$. *Matrix-vector multiplication of* $M \in \mathcal{H}_p$ *and* $x \in \mathbb{R}^{I_p}$ *requires the work*

$$N_{\text{MV}}(p) = 4n \log_2 n - n + 2\,.$$

Different from the following operations, matrix-vector multiplication yields an *exact* result.

3.5 Matrix Addition

We distinguish between three types of additions:

(1) $A \oplus_1 B \in \mathcal{R}_p$ for $A, B \in \mathcal{R}_p$ with $I = \{1, \ldots, n\}$ and cost $N_{R+R}(p)$.
(2) $A \oplus_1 B \in \mathcal{H}_p$ for $A, B \in \mathcal{H}_p$ with the cost $N_{H+H}(p)$.
(3) $A \oplus_1 B \in \mathcal{H}_p$ for $A \in \mathcal{H}_p$ and $B \in \mathcal{R}_p$ with the cost $N_{H+R}(p)$.

The symbol $\oplus_1$ indicates that instead of exact addition we use a blockwise truncation to rank-1 matrices. According to Corollary 2.19b, we have $N_{R+R}(p) = 17n + 19$ (later used in the form of $N_{R+R}(p-1) = \frac{17}{2}n + 19$). In the case of $A, B \in \mathcal{H}_p$, we use the block structure (3.1d). The sum is of the structural form

$$\begin{bmatrix} \mathcal{H}_{p-1} & \mathcal{R}_{p-1} \\ \mathcal{R}_{p-1} & \mathcal{H}_{p-1} \end{bmatrix} + \begin{bmatrix} \mathcal{H}_{p-1} & \mathcal{R}_{p-1} \\ \mathcal{R}_{p-1} & \mathcal{H}_{p-1} \end{bmatrix} = \begin{bmatrix} \mathcal{H}_{p-1} + \mathcal{H}_{p-1} & \mathcal{R}_{p-1} + \mathcal{R}_{p-1} \\ \mathcal{R}_{p-1} + \mathcal{R}_{p-1} & \mathcal{H}_{p-1} + \mathcal{H}_{p-1} \end{bmatrix}.$$

The exact definition of the operation $\oplus_1 : \mathcal{H}_p \times \mathcal{H}_p \to \mathcal{H}_p$ is as follows. For $p=0$, $\oplus_1 = +$ is the exact addition. Otherwise, use the recursion

$$M' \oplus_1 M'' := \begin{bmatrix} M'_{11} \oplus_1 M''_{11} & M'_{12} \oplus_1 M''_{12} \\ M'_{21} \oplus_1 M''_{21} & M'_{22} \oplus_1 M''_{22} \end{bmatrix}. \tag{3.5}$$

$\oplus_1 : \mathcal{R}_{p-1} \times \mathcal{R}_{p-1} \to \mathcal{R}_{p-1}$ is already defined in the off-diagonal blocks by the formatted addition of $\mathcal{R}_{p-1}$ matrices (cf. (2.11)), whereas in the block diagonals the operation $\oplus_1 : \mathcal{H}_{p-1} \times \mathcal{H}_{p-1} \to \mathcal{H}_{p-1}$ of level $p-1$ appears. According to (3.5), we obtain the recursion

$$N_{H+H}(p) = 2N_{H+H}(p-1) + 2N_{R+R}(p-1) = 2N_{H+H}(p-1) + 17n + 38$$

for the number of arithmetic operations. Together with $N_{H+H}(0) = 1$, it follows that $N_{H+H}(p) = 17n \log_2 n + 39n - 38$.

In the third case, B can be written as $\begin{bmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{bmatrix}$ with $B_{ij} \in \mathcal{R}_{p-1}$ symbolised by $B = \begin{bmatrix} \mathcal{R}_{p-1} & \mathcal{R}_{p-1} \\ \mathcal{R}_{p-1} & \mathcal{R}_{p-1} \end{bmatrix}$ (cf. Remark 2.7). The sum

$$A + B = \begin{bmatrix} \mathcal{H}_{p-1} + \mathcal{R}_{p-1} & \mathcal{R}_{p-1} + \mathcal{R}_{p-1} \\ \mathcal{R}_{p-1} + \mathcal{R}_{p-1} & \mathcal{H}_{p-1} + \mathcal{R}_{p-1} \end{bmatrix}$$

leads to the recursion $N_{H+R}(p) = 2N_{H+R}(p-1) + 2N_{R+R}(p-1)$. Since this inequality and the starting value $N_{H+R}(0) = 1$ are identical to those for $N_{H+H}(p)$, we obtain again the solution $N_{H+R}(p) = 17n \log_2 n + 39n - 38$.

Lemma 3.3. *Let $n = 2^p$. The formatted addition $\oplus_1$ of two matrices from $\mathcal{H}_p$ as well as the $\mathcal{R}_1$ addition $\oplus_1$ of an $\mathcal{H}_p$-matrix and an $\mathcal{R}_p$-matrix require*

$$17n \log_2 n + 39n - 38$$

operations.

3.6 Matrix-Matrix Multiplication

Let $n = 2^p$. We distinguish between three kinds of matrix-matrix multiplications:

(1)	$A \cdot B \in \mathcal{R}_p$	for $A, B \in \mathcal{R}_p$	with the cost $N_{R \cdot R}(p)$.
(2a)	$A \cdot B \in \mathcal{R}_p$	for $A \in \mathcal{R}_p$ and $B \in \mathcal{H}_p$	with the cost $N_{R \cdot H}(p)$.
(2b)	$A \cdot B \in \mathcal{R}_p$	for $A \in \mathcal{H}_p$ and $B \in \mathcal{R}_p$	with the cost $N_{H \cdot R}(p)$.
(3)	$A \odot B \in \mathcal{H}_p$	for $A, B \in \mathcal{H}_p$	with the cost $N_{H \cdot H}(p)$.

In the cases of (1) and (2a,b), the results are exact. In the last case (3), the product in $\mathcal{H}_p$ is determined approximately.

In the first case, the solution is $N_{R \cdot R}(p) = 3n - 1$ (cf. Remark 2.9c).

In the case of $A \in \mathcal{H}_p$ and $B \in \mathcal{R}_p$, we use $A \cdot ab^\mathsf{T} = (Aa) \cdot b^\mathsf{T}$; i.e., the result is $a'b^\mathsf{T} \in \mathcal{R}_p$ with $a' := Aa$. This requires one matrix-vector multiplication $A \cdot a$. According to Lemma 3.2, the cost amounts to $N_{H \cdot R}(p) = 4n \log_2 n - n + 2$.

Similarly, for $B \in \mathcal{R}_p$ and $A \in \mathcal{H}_p$ we perform $BA = ab^\mathsf{T} \cdot A = a \cdot (A^\mathsf{T})^\mathsf{T}$ so that $N_{R \cdot H}(p) = N_{H \cdot R}(p)$.

In the third case of $A, B \in \mathcal{H}_p$, the product AB is of the form

$$\begin{bmatrix} \mathcal{H}_{p-1} & \mathcal{R}_{p-1} \\ \mathcal{R}_{p-1} & \mathcal{H}_{p-1} \end{bmatrix} \cdot \begin{bmatrix} \mathcal{H}_{p-1} & \mathcal{R}_{p-1} \\ \mathcal{R}_{p-1} & \mathcal{H}_{p-1} \end{bmatrix}$$
$$= \begin{bmatrix} \mathcal{H}_{p-1} \cdot \mathcal{H}_{p-1} + \mathcal{R}_{p-1} \cdot \mathcal{R}_{p-1} & \mathcal{H}_{p-1} \cdot \mathcal{R}_{p-1} + \mathcal{R}_{p-1} \cdot \mathcal{H}_{p-1} \\ \mathcal{R}_{p-1} \cdot \mathcal{H}_{p-1} + \mathcal{H}_{p-1} \cdot \mathcal{R}_{p-1} & \mathcal{R}_{p-1} \cdot \mathcal{R}_{p-1} + \mathcal{H}_{p-1} \cdot \mathcal{H}_{p-1} \end{bmatrix}.$$

On level $p - 1$ all three types of multiplications appear. The third multiplication type $\mathcal{H}_{p-1} \cdot \mathcal{H}_{p-1}$ requires an approximation by $\odot$. Finally, addition via $\oplus_1$ has to be performed. Counting the operations, we derive the recursion

$$\begin{aligned} N_{H \cdot H}(p) = {} & 2N_{H \cdot H}(p-1) + 2N_{R \cdot R}(p-1)) + 2N_{H \cdot R}(p-1) \\ & + 2N_{R \cdot H}(p-1) + 2N_{H+R}(p-1) + 2N_{R+R}(p-1) \ . \end{aligned}$$

Inserting the known quantities

$$\begin{aligned} N_{R \cdot R}(p-1) &= \frac{3}{2}n - 1, \qquad (3.6) \\ N_{H \cdot R}(p-1) &= N_{R \cdot H}(p-1) = 4\frac{n}{2}\log_2 \frac{n}{2} - \frac{n}{2} + 2 = 2n \log_2 n - \frac{5}{2}n + 2, \\ N_{H+R}(p-1) &= 17\frac{n}{2}\log_2 \frac{n}{2} + 39\frac{n}{2} - 38 \;=\; \frac{17}{2}n \log_2 n + 11n - 38, \\ N_{R+R}(p-1) &= \frac{17}{2}n + 19, \end{aligned}$$

we obtain $N_{H \cdot H}(p) = 2N_{H \cdot H}(p-1) + 25pn + 32n - 32$. One verifies that $N_{H \cdot H}(p) = \frac{25}{2}np^2 + \frac{89}{2}np - 31n + 32$ solves this recursion with the starting value $N_{H \cdot H}(0) = 1$.

Lemma 3.4. *The multiplication of two $\mathcal{H}_p$-matrices costs*

$$N_{H\cdot H}(p) = \frac{25}{2}np^2 + \frac{89}{2}np - 31n + 32 \text{ operations.}$$

The product between $\mathcal{H}_p$ and $\mathcal{R}_p$ requires

$$N_{H\cdot R}(p) = N_{R\cdot H}(p) = 4n\log_2 n - n + 2 \text{ operations.}$$

The multiplication of two $\mathcal{R}_p$-matrices requires

$$N_{R\cdot R}(p) = 3n - 1 \text{ operations.}$$

3.7 Matrix Inversion

In the following, we want to approximate the inverse M^{-1} of a matrix $M \in \mathcal{H}_p$. For this purpose, we define the inversion mapping $inv : D_p \subset \mathcal{H}_p \to \mathcal{H}_p$ recursively (D_p : domain of inv). For $p = 0$ we define $inv(M) := M^{-1}$ as the exact inverse of the 1×1-matrix M, provided that $M \neq 0$. Let inv be defined on $D_{p-1} \subset \mathcal{H}_{p-1}$. The (exact) inverse of M with the block structure (3.1d) is

$$M^{-1} = \begin{bmatrix} M_{11}^{-1} + M_{11}^{-1}M_{12}S^{-1}M_{21}M_{11}^{-1} & -M_{11}^{-1}M_{12}S^{-1} \\ -S^{-1}M_{21}M_{11}^{-1} & S^{-1} \end{bmatrix} \tag{3.7}$$

involving the *Schur complement* $S := M_{22} - M_{21}M_{11}^{-1}M_{12}$. The representation (3.7) and therefore also the following algorithm requires M_{11} to be regular.

Exercise 3.5. (a) If M is positive definite, then M_{11} is regular.
(b) If M and M_{11} are regular, then also the Schur complement S is regular.

In (3.7) we replace M_{11}^{-1} by $inv(M_{11})$. Multiplications by M_{12} and M_{21} can be performed exactly, since these block matrices belong to $\mathcal{R}_{p-1}$. Additions (here also subtractions are called additions) are performed is the sense of $\oplus_1$. Hence, S as well as all matrix blocks from (3.7) can be computed approximately. This defines $inv(M)$ completely. The exact sequence of operations is

matrix operation	cost	expression to be approximated
$M_{11} \mapsto N_{11} := inv(M_{11}) \in \mathcal{H}_{p-1}$	N_{inv}	M_{11}^{-1}
$M_{21}, N_{11} \mapsto X_{21} := M_{21} \cdot N_{11} \in \mathcal{R}_{p-1}$	$N_{R\cdot H}$	$M_{21}M_{11}^{-1}$
$N_{11}, M_{12} \mapsto X_{12} := N_{11} \cdot M_{12} \in \mathcal{R}_{p-1}$	$N_{H\cdot R}$	$M_{11}^{-1}M_{12}$
$X_{21}, M_{12} \mapsto X_{22} := X_{21} \cdot M_{12} \in \mathcal{R}_{p-1}$	$N_{R\cdot R}$	$M_{21}M_{11}^{-1}M_{12}$
$M_{22}, X_{22} \mapsto \hat{S} := M_{22} \ominus_1 X_{22} \in \mathcal{H}_{p-1}$	N_{H+R}	$M_{22} - M_{21}M_{11}^{-1}M_{12}$
$\hat{S} \mapsto T := inv(\hat{S}) \in \mathcal{H}_{p-1}$	N_{inv}	S^{-1}
$T, X_{21} \mapsto Z_{21} := -T \cdot X_{21} \in \mathcal{R}_{p-1}$	$N_{H\cdot R}$	$-S^{-1}M_{21}M_{11}^{-1}$
$X_{12}, T \mapsto Z_{12} := -X_{12} \cdot T \in \mathcal{R}_{p-1}$	$N_{R\cdot H}$	$-M_{11}^{-1}M_{12}S^{-1}$
$X_{12}, Z_{21} \mapsto X_{11} := X_{12} \cdot Z_{21} \in \mathcal{R}_{p-1}$	$N_{R\cdot R}$	$-M_{11}^{-1}M_{12}S^{-1}M_{21}M_{11}^{-1}$
$N_{11}, X_{11} \mapsto Z_{11} := N_{11} \oplus_1 X_{11} \in \mathcal{H}_{p-1}$	N_{H+R}	$M_{11}^{-1}+M_{11}^{-1}M_{12}S^{-1}M_{21}M_{11}^{-1}$

and determines $inv(M) = \begin{bmatrix} Z_{11} & Z_{12} \\ Z_{21} & T \end{bmatrix}$. Adding the different costs from above, we obtain the recursion

$$N_{\mathrm{inv}}(p) = 2N_{\mathrm{inv}}(p-1) + 2N_{R\cdot H}(p-1) + 2N_{H\cdot R}(p-1) + 2N_{H+R}(p-1) + 2N_{R\cdot R}(p-1)$$

(very similar to the $N_{H\cdot H}$ recursion). Inserting the values from (3.6), we conclude that

$$N_{\mathrm{inv}}(p) = 2N_{\mathrm{inv}}(p-1) + 25n\log_2 n + 15n - 70.$$

Together with $N_{\mathrm{inv}}(0) = 1$ the statement of the next lemma follows.

Lemma 3.6. *The approximate inversion of a matrix from* $\mathcal{H}_p$ *requires the amount of*

$$\frac{25}{2}p^2 n + \frac{55}{2}pn - 69n + 70 \quad \textit{operations}.$$

3.8 LU Decomposition

An LU decomposition (without pivoting) does not exist for all square matrices. Sufficient conditions are (a) nonvanishing minors, (b) positive definiteness, or (c) the H-matrix property (cf. [119, Criterion 8.5.8]).

The LU factors L and U in $M = LU$ belong to the following matrix formats:

$$\mathcal{H}_{p,L} := \{M \in \mathcal{H}_p : M_{ii} = 1,\ M_{ij} = 0 \text{ for } j > i\},$$
$$\mathcal{H}_{p,U} := \{M \in \mathcal{H}_p : M_{ij} = 0 \text{ for } j < i\}.$$

As in the case of full matrices, the storage requirement for both matrices $L \in \mathcal{H}_{p,L}$ and $U \in \mathcal{H}_{p,U}$ together is the same as the storage cost of a general matrix $M \in \mathcal{H}_p$.

3.8.1 Forward Substitution

Let $L \in \mathcal{H}_{p,L}$ be a normed lower triangular matrix and $y \in \mathbb{R}^{I_p}$ a right-hand side. We want to determine the solution $x \in \mathbb{R}^{I_p}$ of $Lx = y$. For $p \geq 1$, the matrix L has the block structure

$$L = \begin{bmatrix} L_{11} & 0 \\ L_{21} & L_{22} \end{bmatrix} \qquad \text{with } L_{11}, L_{22} \in \mathcal{H}_{p-1,L} \quad \text{and } L_{21} \in \mathcal{R}_{p-1}.$$

Analogously, the vectors $x = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$, $y = \begin{bmatrix} y_1 \\ y_2 \end{bmatrix}$ are block partitioned. The solution of $Lx = y$ is performed by forward substitution, which leads us to the recursion

$$\text{solve } L_{11}x_1 = y_1, \qquad \text{set } z := y_2 - L_{21}x_1, \qquad \text{solve } L_{22}x_2 = z.$$

By Remark 2.9a, the matrix-vector multiplication $L_{21}x_1$ requires $3\frac{n}{2}-1$ operations. The addition of y_2 costs $\frac{n}{2}$ operations, so that the recursion for the work becomes

$$N_{\mathrm{fw}}(p) = 2N_{\mathrm{fw}}(p-1) + 2n - 1\,. \tag{3.8}$$

For $p=0$, the solution of $Lx=y$ is without cost since[1] $x=y$, so that $N_{\mathrm{fw}}(0)=0$. Solving the recursion (3.8) is

$$N_{\mathrm{fw}}(p) = 2n\log_2 n - n + 1 \qquad (n = 2^p).$$

3.8.2 Backward Substitution

The cost for solving the equation $Ux = y$ with $U \in \mathcal{H}_{p,U}$ is denoted by $N_{\mathrm{bw}}(p)$. The recursion formula $N_{\mathrm{bw}}(p) = 2N_{\mathrm{bw}}(p-1) + 2n - 1$ is identical with that for N_{fw}, only the starting value changes into $N_{\mathrm{bw}}(0) = 1$. This yields

$$N_{\mathrm{bw}}(p) = 2n\log_2 n + 1 \qquad (n = 2^p).$$

Below we need a variant of the backward substitution: the solution of $x^{\mathsf{T}}U = y^{\mathsf{T}}$ with respect to x. It is equivalent to $U^{\mathsf{T}}x = y$, where U^{T} is a lower triangular matrix. Since U^{T} is not normed, we again obtain the work $N_{\mathrm{bw}}(p)$ from above.

3.8.3 Cost of the LU Decomposition

The ansatz $L = \begin{bmatrix} L_{11} & 0 \\ L_{21} & L_{22} \end{bmatrix} \in \mathcal{H}_{p,L}$ and $U = \begin{bmatrix} U_{11} & U_{12} \\ 0 & U_{22} \end{bmatrix} \in \mathcal{H}_{p,U}$ for $LU = M = \begin{bmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{bmatrix} \in \mathcal{H}_p$ leads to the four equations

$$M_{11} = L_{11}U_{11}, \quad M_{12} = L_{11}U_{12}, \quad M_{21} = L_{21}U_{11}, \quad M_{22} = L_{21}U_{12} + L_{22}U_{22}\,.$$

Hence, the following subproblems are to be solved:

(1) determine the LU decomposition of M_{11} (result: L_{11}, U_{11}),
(2) compute $U_{12} := L_{11}^{-1}M_{12}$ and $L_{21} := M_{21}U_{11}^{-1}$,
(3) compute the LU decomposition of $M_{22} - L_{21}U_{12}$ (result: L_{22}, U_{22}).

Since $M_{12} \in \mathcal{R}_{p-1}$, we have $M_{12} = ab^{\mathsf{T}}$ for suitable $a, b \in \mathbb{R}^{I_{p-1}}$. The representation of $U_{12} \in \mathcal{R}_{p-1}$ is given by $a'b^{\mathsf{T}}$ with $a' = L_{11}^{-1}a$. Obviously, we obtain a' via forward substitution from $L_{11}a' = a$ with the cost $N_{\mathrm{fw}}(p-1)$. Analogously, the (exact) computation of $L_{21} = M_{21}U_{11}^{-1} \in \mathcal{R}_{p-1}$ costs $N_{\mathrm{bw}}(p-1)$. This yields

[1] Here we exploit the fact that L is normed lower triangular, i.e., $L_{ii} = 1$ for all $i \in I$.

a recursive definition of the computational work:

$$\begin{aligned} N_{LU}(p) &= 2N_{LU}(p-1) + N_{\text{fw}}(p-1) + N_{\text{bw}}(p-1) \\ &\quad + N_{R\cdot R}(p-1) + N_{H+R}(p-1) \\ &= 2N_{LU}(p-1) + \left[n(p-1) - \frac{n}{2} + 1\right] + [n(p-1)+1] \\ &\quad + \left[3\frac{n}{2} - 1\right] + \left[17\frac{n}{2}(p-1) + 39\frac{n}{2} - 38\right] \\ &= 2N_{LU}(p-1) + \frac{21}{2}np + 10n - 37 \end{aligned}$$

with the starting value $N_{LU}(0) = 0$. The solution is

$$N_{LU}(p) = \frac{21}{4} n \log_2^2 n + \frac{61}{4} n \log_2 n - 37\,(n-1)\,.$$

Note that the work is clearly lower than for the computation of the inverse with $N_{\text{inv}}(p) = \frac{25}{2} n \log_2^2 n + \ldots$.

Exercise 3.7. Formulate the Cholesky decomposition (cf. (1.1b)) for a positive definite matrix $M \in \mathcal{H}_p$.

3.9 Further Properties of the Model Matrices and Semiseparability

As remarked, the inversion mapping inv from §3.7 is usually an approximation. However, there is an important case in which inv is exact.

Proposition 3.8 (tridiagonal matrices). *Let $M \in \mathbb{R}^{I_p \times I_p}$ be tridiagonal.*
(a) Then $M \in \mathcal{H}_p$ holds exactly.
(b) If in addition, M is regular, then also the exact inverse M^{-1} belongs to $\mathcal{H}_p$.
(c) Assume that all principal submatrices $M|_{I_q \times I_q}$ $(0 \le q \le p)$ are regular. Then the result $inv(M)$ from §3.7 is well-defined and yields the exact inverse M^{-1}.

The proof will follow after Corollary 3.16.

Proposition 3.8 can easily be generalised to band matrices with band width $r > 1$ (i.e., r upper and r lower off-diagonals) by replacing the rank-1-matrices $\mathcal{R}_p = \mathcal{R}(1, I_p, I_p)$ in the definition of $\mathcal{H}_p$ by rank-r matrices $\mathcal{R}(r, I_p, I_p)$.

The statement from above exploits the fact that the inverse of tridiagonal matrices has special properties. A question in the reverse direction is: Under which conditions does a matrix have a tridiagonal inverse? This leads us to the term *semiseparability*. Since tridiagonal matrices (or band matrices with a certain band width) arise from one-dimensional boundary value problems, semiseparability is closely related to one-dimensional boundary value problems and does not help for two or more spatial variables.

Since in the literature the term semiseparability is not uniquely defined (cf. Vandebril et al. [240]), we do not give a definition. Instead, Definition 3.9 describes a set $\mathcal{S}_r$ which comes close to the semiseparable matrices. For our purposes a weaker condition defining the set $\mathcal{M}_{r,\tau}$ will be sufficient (cf. Definition 3.12). In particular, the $\mathcal{S}_r$ matrices and $\mathcal{M}_{r,\tau}$ matrices defined here have interesting invariance properties with respect to various operations.

Definition 3.9. Let I be ordered and $1 \leq r < \#I$. $M \in \mathbb{R}^{I\times I}$ belongs to $\mathcal{S}_r$ if $\operatorname{rank}(M|_b) \leq r$ holds for any block $b \subset I \times I$ which is contained in the strictly upper triangular part $\{(i,j) : i < j\}$ or in the strictly lower triangular part.

Obviously, any matrix $M \in \mathbb{R}^{I\times I}$ belongs to $\mathcal{S}_r$ with $r = \#I - 1$.

Remark 3.10. (a) Tridiagonal matrices belong to $\mathcal{S}_1$.

(b) Band matrices with at most r upper and r lower off-diagonals belong to $\mathcal{S}_r$.

(c) Let $D \in \mathbb{R}^{I\times I}$ be diagonal. Then M and $M + D$ belong to $\mathcal{S}_r$ with identical r.

(d) Any matrix $M \in \mathcal{S}_r \cap \mathbb{R}^{n\times n}$ ($n = 2^p$) can be exactly represented in the format $\mathcal{H}_p$ if instead of (3.1c) the local rank r is chosen.

Proof. (a) is the special case $r = 1$ of (b).

Part (b) follows since $M|_b$ contains at most r nonzero rows.

For part (c) note that the diagonal is irrelevant for the definition of $\mathcal{S}_r$.

For part (d) consider a block of the partition of $\mathcal{H}_p$. Off-diagonal blocks b belong strictly to one of the triangular parts so that $M|_b$ has rank $\leq r$ and can be represented exactly by $\mathcal{R}(r, b)$. Diagonal blocks b of size 1×1 are trivial. □

The following exercise is connected with another definition of semiseparable matrices.

Exercise 3.11. Let $I = \{1, \ldots, n\}$. Show: (a) If there are (general, not triangular) matrices $M^{\mathrm{up}}, M^{\mathrm{low}} \in \mathcal{R}(r, I, I)$ such that $M_{ij} = \left\{ \begin{matrix} M^{\mathrm{up}}_{ij} & \text{for } j > i \\ M^{\mathrm{low}}_{ij} & \text{for } j < i \end{matrix} \right\}$, then $M \in \mathcal{S}_r$.

(b) Assume that for all indices $1 \leq \nu \leq n - r$ and the corresponding blocks $b = \{1, \ldots, \nu\} \times \{\nu + 1, \ldots, n\}$, the first column of $M|_b$ is linearly dependent on the other ones. Then there is an $M^{\mathrm{up}} \in \mathcal{R}(r, I, I)$ such that $M_{ij} = M^{\mathrm{up}}_{ij}$ for $j > i$. Formulate a corresponding condition so that also $M_{ij} = M^{\mathrm{low}}_{ij}$ for $j < i$ with an $M^{\mathrm{low}} \in \mathcal{R}(r, I, I)$.

In the sequel, we study a matrix family $\mathcal{M}_{r,\tau}$ with weaker properties. In particular, I need not be ordered.

Definition 3.12. Let $\emptyset \neq \tau \subsetneqq I$ be an index subset, $\tau' := I\backslash\tau$ its complement, and $r \in \mathbb{N}$. A matrix A belongs to $\mathcal{M}_{r,\tau}(I)$ if $\operatorname{rank}(A|_{\tau\times\tau'}) \leq r$ and $\operatorname{rank}(A|_{\tau'\times\tau}) \leq r$. If the reference to I is not necessary, we also write $\mathcal{M}_{r,\tau}$ instead of $\mathcal{M}_{r,\tau}(I)$.

If the indices are ordered so that the indices from τ precede those from τ', we obtain the block partition

$$A = \begin{array}{c|c|c|c} & \tau & \tau' = I\backslash\tau & \\ \hline & A_{11} & A_{12} & \tau \\ \hline & A_{21} & A_{22} & \tau' \\ \hline \end{array} . \tag{3.9}$$

Definition 3.12 states that $\operatorname{rank}(A_{12}) \leq r$ and $\operatorname{rank}(A_{21}) \leq r$.

The connection to $\mathcal{S}_r$ is given by the next remark.

Remark 3.13. Let $I = \{1, \ldots, n\}$ be ordered. $M \in \mathbb{R}^{I\times I}$ belongs to $\mathcal{S}_r$ if and only if for all $i < n$ the property $M \in \mathcal{M}_{r,\tau}(I)$ holds, where $\tau = \{1, \ldots, i\}$.

In the following, the matrix operations $*, ^{-1}, \pm$ are understood in their exact form, i.e., without any truncation error.

Lemma 3.14. *(a) Let $A \in \mathcal{M}_{r_A,\tau}(I)$ and $B \in \mathcal{M}_{r_B,\tau}(I)$. Then $A \cdot B \in \mathcal{M}_{r,\tau}(I)$ holds with $r = r_A + r_B$.*

(b) Let $A \in \mathcal{M}_{r,\tau}(I)$ be regular. Then $A^{-1} \in \mathcal{M}_{r,\tau}(I)$ holds with the same r.

(c) Let $A \in \mathcal{M}_{r,\tau}(I)$. Then also $A + D \in \mathcal{M}_{r,\tau}(I)$ holds for all diagonal matrices $D \in \mathbb{R}^{I\times I}$.

(d) Let $A \in \mathcal{M}_{r,\tau}(I)$ with $\emptyset \neq \tau \subset I' \subsetneqq I$. Then the principal submatrix $A|_{I'\times I'}$ belongs to $\mathcal{M}_{r,\tau}(I')$. The same statement holds for the Schur complement $S_{I'} = A|_{I'\times I'} - A|_{I'\times I''} * (A|_{I''\times I''})^{-1} * A|_{I''\times I'}$ ($I'' := I\backslash I'$), provided that it is regular.

Proof. (i) Decompose the matrices A, B, and $C := AB$ as in (3.9). Since $C_{12} = A_{11}B_{12} + A_{12}B_{22}$, we conclude from $\operatorname{rank}(A_{11}B_{12}) \leq \operatorname{rank}(B_{12}) \leq r_B$ and $\operatorname{rank}(A_{12}B_{22}) \leq \operatorname{rank}(A_{12}) \leq r_A$ that $\operatorname{rank}(C_{12}) \leq r_A + r_B$ holds. The inequality $\operatorname{rank}(C_{21}) \leq r_A + r_B$ is proved analogously.

(ii) Let A_{11} be regular. Then the Schur complement $S = A_{22} - A_{21}A_{11}^{-1}A_{12}$ is also regular and the inverse of A from (3.9) is

$$A^{-1} = \begin{bmatrix} A_{11}^{-1} + A_{11}^{-1}A_{12}S^{-1}A_{21}A_{11}^{-1} & -A_{11}^{-1}A_{12}S^{-1} \\ -S^{-1}A_{21}A_{11}^{-1} & S^{-1} \end{bmatrix}$$

(cf. (3.7)). Since $\operatorname{rank}(A^{-1}|_{\tau\times\tau'}) = \operatorname{rank}(-A_{11}^{-1}A_{12}S^{-1}) \leq \operatorname{rank}(A_{12}) \leq r$ and $\operatorname{rank}(A|_{\tau'\times\tau}) \leq \operatorname{rank}(A_{12}) \leq r$, it follows that $A^{-1} \in \mathcal{M}_{r,\tau}(I)$.

(iii) If A_{11} is singular, the matrix $A_\varepsilon := A + \varepsilon I$ is regular for sufficiently small $\varepsilon \neq 0$. Since $\operatorname{rank}\left(A_\varepsilon^{-1}|_{\tau\times\tau'}\right) \leq \operatorname{rank}(A_{12})$ holds independently of ε, it follows that $A_\varepsilon^{-1} \in \mathcal{M}_{r,\tau}(I)$. The limit $\lim_{\varepsilon\to 0} A_\varepsilon^{-1}$ is A^{-1}, since by assumption A is regular. Exercise 2.2 ensures that the rank satisfies $\operatorname{rank}\left(A^{-1}|_{\tau\times\tau'}\right) = \operatorname{rank}\left(\lim_{\varepsilon\to 0} A_\varepsilon^{-1}|_{\tau\times\tau'}\right) \leq \lim_{\varepsilon\to 0} \operatorname{rank}\left(A_\varepsilon^{-1}|_{\tau\times\tau'}\right) \leq \operatorname{rank}\left(A_{12}\right) \leq r$. Together with the analogous inequality $\operatorname{rank}\left(A^{-1}|_{\tau'\times\tau}\right) \leq r$, the statement $A^{-1} \in \mathcal{M}_{r,\tau}(I)$ follows.

(iv) A change of the diagonal does not effect $A|_{\tau\times\tau'}$ and $A|_{\tau'\times\tau}$.

(v) A restriction of the matrix to $I' \times I' \subset I \times I$ can only diminish the rank, so that $A|_{I' \times I'} \in \mathcal{M}_{r,\tau}(I')$.

(vi) Assume A to be regular. The inverse Schur complement $(S_{I'})^{-1}$ is the principal $I' \times I'$-submatrix of A^{-1}. From part (b) we conclude $A^{-1} \in \mathcal{M}_{r,\tau}(I)$, while (v) shows $(S_{I'})^{-1} \in \mathcal{M}_{r,\tau}(I')$. Repeated application of (ii–iii) with $(S_{I'})^{-1}$ instead of A yields the assertion $S_{I'} \in \mathcal{M}_{r,\tau}(I')$. For singular A argue as in (iii). □

A consequence of Lemma 3.14 is the following statement.

Lemma 3.15. *Let R be a rational function $R(x) = P^I(x)/P^{II}(x)$ with polynomials P^I, P^{II} of the respective degrees $d_I, d_{II} \in \mathbb{N}_0$. The eigenvalues of $A \in \mathcal{M}_{r,\tau}(I)$ are supposed to be different from the poles of R. Then the matrix[2] $R(A)$ belongs to $\mathcal{M}_{r_R,\tau}(I)$ with $r_R = r * d_R$, where $d_R := \max(d_I, d_{II})$ is the degree of R.*

Proof. Factorise[3] the polynomials P^I, P^{II} into $P^I(x) = a_I \prod_{i=1}^{d_I} (x - x_i^I)$ and $P^{II}(x) = a_{II} \prod_{i=1}^{d_{II}} (x - x_i^{II})$. For $i \le \min\{d_I, d_{II}\}$, the rational factors $\frac{x - x_i^I}{x - x_i^{II}} = 1 + (x_i^{II} - x_i^I) / (x - x_i^{II})$ appear. According to Lemma 3.14c, replacing x by $A \in \mathcal{M}_{r,\tau}(I)$ yields $R_i(A) := I + (x_i^{II} - x_i^I)(A - x_i^{II} I)^{-1} \in \mathcal{M}_{r,\tau}(I)$. Hence, $R(A)$ is a product of $\min\{d_I, d_{II}\}$ rational factors $R_i(A)$ and additional $\max\{d_I, d_{II}\} - \min\{d_I, d_{II}\}$ factors of the form $A - x_i^I I$ for $d_I > d_{II}$ and $(A - x_i^{II} I)^{-1}$ for $d_I < d_{II}$, which all belong to $\mathcal{M}_{r,\tau}(I)$. By Lemma 3.14a, the product belongs to $\mathcal{M}_{r_R,\tau}(I)$ with $r_R = r d_R$. □

Corollary 3.16. According to Remark 3.13, the previous statements transfer to $\mathcal{S}_r$ matrices. For instance, the inverse of a regular $\mathcal{S}_r$ matrix is again in $\mathcal{S}_r$.

Now we present the postponed *proof of Proposition 3.8.*

Part (a) follows from Remark 3.10a,d, while part (b) follows from Corollary 3.16.

For part (c) it remains to show that the algorithm inv is well-defined and does not introduce any approximation error. We use induction on p. Obviously inv is exact on $\mathcal{H}_0$. Let the statement hold for $p-1$. Decompose $M \in \mathbb{R}^{I_{p-1} \times I_{p-1}}$ according to (3.1a). The submatrices M_{11} and M_{22} are again tridiagonal, where, by assumption, M_{11} is regular and, by the induction hypothesis, $M_{11}^{-1} = inv(M_{11})$ holds. Computing $M_{21} \odot inv(M_{11}) \odot M_{12}$ involves only the intermediate results of rank ≤ 1, which therefore are represented exactly. Lemma 3.14d shows that $S = M_{22} - M_{21} M_{11}^{-1} M_{12}$ as well as S^{-1} belong to $\mathcal{H}_{p-1}$. The regularity of S follows from Exercise 3.5. The exact inverse of M is given by (3.7). Concerning the off-diagonal blocks $-M_{11}^{-1} M_{12} S^{-1}$ and $-S^{-1} M_{21} M_{11}^{-1}$ we remark that not only the final product, but also the intermediate results are exactly represented in $\mathcal{R}_{p-1}$. Hence, inv is also exact on level p.

Connections between $\mathcal{M}_{r,\tau}$ and the weak admissibility will be studied in §9.3.3.

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[2] Concerning matrix functions, we refer to later definitions in §14.1.

[3] x_i^I and x_i^{II} may be complex numbers.

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