The algorithmic complexity of the minimization of the number of segments in multileaf collimator field segmentation

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Abstract

Intensity maps are nonnegative matrices describing the intensity modulation of beams in radiotherapy. In order to use a multileaf collimator in the static mode for the realization of the intensity modulation one has to determine a segmentation, i.e. a representation of an intensity map as a positive combination of special matrices corresponding to fixed positions of the multileaf collimator, called segments. We consider the problem to construct segmentations with the minimal total number of monitor units and the minimal number of segments. Neglecting machine—dependent constraints like the interleaf collision constraint and assuming that the entries of the intensity map are bounded by a constant, we prove that a segmentation with minimal number of segments under the condition that the number of monitor units is minimal, can be determined in time polynomial in the matrix dimensions. The results of our algorithm are compared with Engel's [9] heuristic for the reduction of the number of segments.

Key words: leaf sequencing, radiation therapy optimization, intensity modulation, multileaf collimator, IMRT

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1 Introduction

In recent years intensity modulated radiation therapy (IMRT) has become an important method in cancer therapy. The objective in the treatment planning is to irradiate the tumor as efficient as possible without damaging the organs near to it. A modern way to realize intensity modulated radiation fields is the usage of a multileaf collimator (MLC). An MLC consists of two opposite banks of metal leaves which can be shifted towards each other and so open or close certain parts of the irradiated area. In this paper we assume that the desired intensity is already determined. After discretization an intensity function can be considered as an $m \times n$ matrix A with nonnegative integer entries. We consider the problem to realize this intensity modulation with an MLC in the static mode (step and shoot). This means that the radiation is switched off when the leaves of the collimator are moving. In other words we have to determine a (finite) set of leaf positions with corresponding irradiation times such that the superposition of the homogeneous fields yields the given intensity matrix. Two important criteria for the quality of the segmentation are the total number of monitor units (TNMU) and the number of segments (NS) which should both be as small as possible. In general, it is not possible to minimize both parameters simultaneously (see [13] for a counterexample). Instead we first determine the minimal TNMU and among all the realizations with this TNMU we search for one with minimal NS. In the literature there are several leaf sequencing algorithms ([2,4,6-10,14,16-18]), some of them providing the optimal TNMU but a large NS, others reducing the NS heuristically at the price of an increased TNMU. The algorithms also differ in the extend to which they include additional machine—dependent constraints like the interleaf collision constraint. In principle both, TNMU and NS, can be optimized by integer programming [15]. But due to the NP-completeness of integer programming this is applicable only for small problem sizes. See [13] for a survey and a comparison of the different segmentation algorithms. In this paper we neglect machine-dependent constraints and focus on the question for the complexity of the NS-minimization.

Throughout the paper we use the notation $[n] := \{1, 2, ..., n\}$ for positive integers n. Let $A = (a_{i,j})$ denote the given $m \times n$ -intensity matrix. For brevity of notation we put $a_{i,0} = a_{i,n+1} = 0$ for $i \in [m]$. We define a segment to be a 0 - 1-matrix describing a leaf position of the MLC. This is made precise in the following definition.

Definition 1. A segment is an $m \times n$ -matrix $S = (s_{i,j})$, such that there exist

integers l_i , r_i $(i \in [m])$ with the following properties:

$$l_i \le r_i + 1 \qquad (i \in [m]), \tag{1}$$

$$s_{i,j} = \begin{cases} 1 & \text{if } l_i \le j \le r_i \\ 0 & \text{otherwise} \end{cases} \qquad (i \in [m], \ j \in [n]), \tag{2}$$

The interpretation is that $l_i - 1$ and $r_i + 1$ are the positions of the i-th left and right leaf, respectively. So a 1-entry indicates that the corresponding region receives radiation while a 0-entry indicates a region that is covered by a leaf. Now for a nonnegative integer matrix A, a segmentation of A is a representation of A as a positive integer combination of segments, i.e. $A = \sum_{i=1}^{k} u_i S_i$ with segments S_i (i = 1, 2, ..., k) and positive integers u_i (i = 1, 2, ..., k).

Example 1. A segmentation with 10 MU for a benchmark matrix from [15] is

$$\begin{pmatrix}
450145 \\
241314 \\
232124 \\
533253
\end{pmatrix} = 3 \begin{pmatrix}
0000011 \\
0000011 \\
0000011
\end{pmatrix} + 3 \begin{pmatrix}
1100000 \\
0100000 \\
0100000
\end{pmatrix} + 1 \begin{pmatrix}
0000111 \\
0000111 \\
000011
\end{pmatrix}
+ 1 \begin{pmatrix}
0000111 \\
0000100 \\
0111000
\end{pmatrix} + 1 \begin{pmatrix}
0100000 \\
1100000 \\
111110
\end{pmatrix}
+ 1 \begin{pmatrix}
1110000 \\
0111110 \\
0111110
\end{pmatrix}
(3)$$

Now the segmentation problem can be formulated as follows.

Segmentation problem: Given the nonnegative integer matrix A, find a segmentation $A = \sum_{i=1}^{k} u_i S_i$ with in first instance minimal TNMU $\sum_{i=1}^{k} u_i$ and in second instance minimal number of segments k.

There are several efficient algorithms for determining TNMU-optimal segmentations [6, 9, 14]. According to [9] the minimal TNMU equals

$$c(A) := \max_{i \in [m]} \sum_{j=1}^{n} \max\{0, a_{i,j} - a_{i,j-1}\}.$$

$$(4)$$

The problem of minimizing the number of segments is NP-complete in the strong sense even for single row matrices. The NP-hardness was shown in [2] by reduction of 2-Partition ([11]). Woeginger gave an unpublished proof of the NP-hardness in the strong sense by a reduction of 3-Partition ([11]). In [13] the NS-minimization for one row has been reduced to the bipartite case of Minimum Edge-Cost Flow ([11]). For special instances of Minimum Edge-Cost Flow there is a reduction in the reverse direction and this yields a new point of view on Woegingers argument which is presented below. The following special case of Minimum Edge-Cost Flow has been shown to be strongly NP-complete in [3] by a reduction of 3-Partition.

Instance: A complete bipartite graph $G = (U \cup V, E)$ with |U| = 3|V| and a function $w : U \to I\!\!N \setminus \{0\}$.

Question: Is there a flow function $f: E \to IN$ such that

$$\forall x \in U \quad \sum_{y \in V} f(xy) = w(x), \tag{5}$$

$$\forall y \in V \quad \sum_{x \in U} f(xy) = 3\overline{w}, \quad \text{where } \overline{w} = \frac{1}{|U|} \sum_{x \in U} w(x), \quad (6)$$

$$|\{xy \in E : f(xy) > 0\}| \le |U|. \tag{7}$$

This problem can be reduced to the NS-minimization problem as follows. We put q = |V|, n = 4q, denote the elements of U by u_1, \ldots, u_{3q} , the elements of V by v_1, \ldots, v_q , and define the row vector $\mathbf{a} = \begin{pmatrix} a_1 & \cdots & a_n \end{pmatrix}$ as follows.

$$a_i = \sum_{j=1}^{i} w(u_j)$$
 for $1 \le i \le 3q$,
 $a_i = 3(n-i)\overline{w}$ for $3q+1 \le i \le n$.

Theorem 1 (Woeginger). There is a segmentation of a with 3q segments (and this segmentation is necessarily TNMU-optimal) iff there is a function $f: E \to IN$ satisfying (5)–(7)

Proof. " \Rightarrow ": Suppose there is a segmentation

$$\boldsymbol{a} = \sum_{j=1}^{3q} c_j \boldsymbol{s}^{(j)} \tag{8}$$

where the segments are described by

$$s_i^{(j)} = \begin{cases} 1 & \text{if } l_j \le i \le r_j \\ 0 & \text{otherwise.} \end{cases} (j \in [3q], i \in [n]).$$

By Lemma 1 from [13] we may assume that $l_j \leq 3q \leq r_j$ for all $j \in [3q]$. Moreover, $a_i > a_{i-1}$ for all $i \in [3q]$ (with $a_0 = 0$) implies that for each $i \in [3q]$ there is some $j \in [3q]$ with $l_j = i$, hence we may assume $l_i = i$ and $c_i = a_i - a_{i-1}$ for $i \in [3q]$, and this assures the TNMU-optimality of the segmentation. Let

$$f(u_i v_{r_i - 3q + 1}) = c_i \qquad (i \in [3q])$$

and f(xy) = 0 for all the remaining edges xy. Observe that $a_n = 0$, so $r_i < n$ for all i and $1 \le r_i - 3q + 1 \le q$. Clearly, (7) is satisfied. Now fix $i \in [3q]$. From (8) and the fact that j = i is the only index with $l_j = i$ we obtain that

$$w(u_i) = a_i - a_{i-1} = c_i = f(u_i v_{r_i}) = \sum_{y \in V} f(u_i y),$$

so (5) is satisfied. Now fix i, $3q + 1 \le i \le n$. From (8) we obtain

$$3\overline{w} = a_{i-1} - a_i = \sum_{j \in [3q]: r_j = i-1} c_j$$

$$= \sum_{j \in [3q]: r_j = i-1} f(u_j v_{i-3q}) = \sum_{j=1}^{3q} f(u_j v_{i-3q}),$$

thus (6) is satisfied.

" \Leftarrow ": Suppose there is a function f satisfying (5)–(7). By (5) and (7), for each $j \in [3q]$ there is exactly one $k(j) \in [q]$ with $f(u_j v_{k(j)}) > 0$. For $j \in [3q]$, put

$$c_j = f(u_j v_{k(j)}), \quad l_j = j, \quad r_j = 3q + k(j) - 1,$$

and define segments $\boldsymbol{s}^{(j)}$ by

$$s_i^{(j)} = \begin{cases} 1 & \text{if } l_j \le i \le r_j \\ 0 & \text{otherwise.} \end{cases} (j \in [3q], i \in [n]).$$

This yields a segmentation of \boldsymbol{a} : for $i \leq 3q$ we have $s_i^{(j)} = 1$ iff $l_j \leq i$, so

$$\sum_{j=1}^{3q} c_j s_i^{(j)} = \sum_{j=1}^i c_j = \sum_{j=1}^i \sum_{v \in V} f(u_j v) = \sum_{j=1}^i w(u_j) = a_i,$$

and for i > 3q we have $s_i^{(j)} = 1$ iff $r_j \ge i$, and so

$$\sum_{j=1}^{3q} c_j s_i^{(j)} = \sum_{t=i}^{n-1} \sum_{j \in [3q]: r_j = t} c_j = \sum_{t=i}^{n-1} \sum_{j \in [3q]: k(j) = t - 3q + 1} c_j$$

$$= \sum_{t=i}^{n-1} \sum_{j=1}^{3q} f(u_j v_{t-3q+1}) = (n-i)\overline{w} = a_i.$$

This shows that the NS-minimization is NP-hard. But the reduction essentially depends on the fact that the entries can become arbitrary large. In this paper we show that the NS-minimization problem can be solved in time polynomial in the matrix dimensions m and n if the maximal entry L of the intensity matrix is bounded. This seems to be a reasonable assumption in practice: for instance the authors of [18] report, that they obtained matrices with 7 nonzero intensity levels when they applied a preliminary version of the CORVUS inverse treatment planning system (NOMOS corporation) to a very complex head and neck tumor case. The algorithm proposed here is an application of the dynamic programming principle (see [5]). The paper is organized as follows. The cases of single row intensity maps and multiple row intensity maps are treated seperately in Sections 2 and 3, respectively. For both cases we describe polynomial algorithms for the construction of segmentations with minimal TNMU and minimal NS. In Section 4 we test our algorithm with randomly generated matrices and with matrices from clinical practice, and we compare the results with the heuristic method from [9].

2 Single row intensity maps

First we give an exact formulation of the problem L-ONE ROW-MIN MU-MIN NS:

Instance: A vector $\mathbf{a} = (a_1 \ a_2 \dots a_n)$ of integers with $0 \le a_i \le L$ $(i = 1, \dots, n)$.

Problem: Find a segmentation with in first instance minimal TNMU and in second instance minimal NS!

We put $a_0 = a_{n+1} = 0$. Let

$$P = \{i \in [n] : a_i \ge a_{i-1} \text{ and } a_i > a_{i+1}\},\$$

$$Q = \{i \in [n] : a_i < a_{i-1} \text{ and } a_i \le a_{i+1}\}.$$

Clearly, |P| = |Q| + 1 if $a_n \neq 0$ and |P| = |Q| if $a_n = 0$. If $a_n \neq 0$ denote the elements of P and Q by p_1, \ldots, p_t and q_1, \ldots, q_{t-1} such that

$$p_1 < q_1 < p_2 < q_2 < \dots < q_{t-1} < p_t,$$

and put $q_0 = 0$ and $q_t = n + 1$. If $a_n = 0$ denote the elements of P and Q by p_1, \ldots, p_t and q_1, \ldots, q_t such that

$$p_1 < q_1 < p_2 < q_2 < \dots < q_{t-1} < p_t < q_t$$

From the results of [9] it follows that in a TNMU-optimal segmentation

$$oldsymbol{a} = \sum_{j=1}^k c_j oldsymbol{s}^{(j)}$$

every segment is of the form

$$s_i^{(j)} = \begin{cases} 1 & \text{for } l_j \le i \le r_j, \\ 0 & \text{otherwise,} \end{cases}$$

with $q_{\tau-1} < l_j \le p_{\tau}$ and $p_{\tau'} \le r_j < q_{\tau'}$ for some $\tau, \tau' \in [t]$. Since the order of the segments is not relevant, we may order them in such a way that $r_1 \le \cdots \le r_k$. For $\tau \in [t-1]$, let $k_0(\tau)$ be the unique index with $r_j < q_{\tau}$ for $j \le k_0(\tau)$ and $r_j \ge q_{\tau}$ for $j > k_0(\tau)$, and put

$$oldsymbol{a}^{(au)} = oldsymbol{a} - \sum_{j=1}^{k_0(au)} c_j oldsymbol{s}^{(j)}.$$

Also put $k_0(0) = 0$, $k_0(t) = k$, $\boldsymbol{a}^{(0)} = \boldsymbol{a}$ and $\boldsymbol{a}^{(t)} = \boldsymbol{0}$. For $j > k_0(\tau)$, from $r_j \geq q_{\tau}$ it follows that for $i \leq q_{\tau}$,

$$s_i^{(j)} = 1 \iff l_j \le i.$$

In particular, for $i = 1, \ldots, q_{\tau} - 1$ and $j = k_0(\tau) + 1, \ldots, k$,

$$s_i^{(j)} = 1 \implies s_{i+1}^{(j)} = 1.$$
 (9)

For $0 \le \tau \le t - 1$, we have

$$oldsymbol{a}^{(au)} = \sum_{j=k_0(au)+1}^k c_j oldsymbol{s}^{(j)},$$

hence (9) implies that

$$a_1^{(\tau)} \le a_2^{(\tau)} \le \dots \le a_{q_{\tau}}^{(\tau)},$$

and the multisets

$$U_{\tau} = \{ a_i^{(\tau)} - a_{i-1}^{(\tau)} : 1 \le i \le q_{\tau}, \ a_i^{(\tau)} \ne a_{i-1}^{(\tau)} \}, \tag{10}$$

$$V_{\tau} = \{ a_i^{(\tau)} - a_{i-1}^{(\tau)} : q_{\tau} < i \le p_{\tau+1}, \ a_i^{(\tau)} \ne a_{i-1}^{(\tau)} \}, \tag{11}$$

$$W_{\tau} = \{ a_i^{(\tau)} - a_{i+1}^{(\tau)} : p_{\tau+1} \le i < q_{\tau+1}, \ a_i^{(\tau)} \ne a_{i+1}^{(\tau)} \}$$
 (12)

are partitions of $a_{q_{\tau}}$, $a_{p_{\tau+1}} - a_{q_{\tau}}$ and $a_{p_{\tau+1}} - a_{q_{\tau+1}}$, respectively. Observe that $a_i^{(\tau)} = a_i$ for $i \geq q_{\tau}$, hence V_{τ} and W_{τ} depend only on \boldsymbol{a} , while U_{τ} depends also on the pairs

$$(s^{(1)}, c_1), \ldots, (s^{(k_0(\tau))}, c_{k_0(\tau)}).$$

Considering the sequence $(U_{\tau}, V_{\tau}, W_{\tau})$ $(\tau = 0, ..., t)$, where we add $U_t = V_t = W_t = \emptyset$, we will derive a method to construct the desired segmentation.

Definition 2. For integers u, v and w with $0 \le u \le v \le L$ and $0 \le w < v$, a (u, v, w)-peak is a triple (U, V, W) of unordered partitions of u, v - u and v - w, i.e. a triple of multisets of positive integers with

$$\sum_{x \in U} x = u, \qquad \sum_{x \in V} x = v - u, \quad \sum_{x \in W} x = v - w.$$

In addition, the triple $(\emptyset, \emptyset, \emptyset)$ is called (0, 0, 0)-peak.

Thus for $\tau = 0, \ldots, t$, $(U_{\tau}, V_{\tau}, W_{\tau})$ is an $(a_{q_{\tau}}, a_{p_{\tau+1}}, a_{q_{\tau+1}})$ -peak (where $a_{p_{t+1}} = a_{q_{t+1}} = 0$), and for $\tau \leq t - 1$, the choice of the pairs

$$(\boldsymbol{s}^{(k_0(\tau)+1)}, c_{k_0(\tau)+1}), \dots, (\boldsymbol{s}^{(k_0(\tau+1))}, c_{k_0(\tau+1)})$$

can be considered as the choice of a way to go from the peak $(U_{\tau}, V_{\tau}, W_{\tau})$ to the peak $(U_{\tau+1}, V_{\tau+1}, W_{\tau+1})$. We claim that the number of segments needed for this step does not depend on the particular $\boldsymbol{a}^{(\tau)}$, but only on the multisets $U_{\tau} \cup V_{\tau}$, W_{τ} and $U_{\tau+1}$. To prove this we associate with a (u, v, w)-peak (U, V, W) a vector $\boldsymbol{b} = \begin{pmatrix} b_1 \dots b_{\beta} \end{pmatrix}$ as follows. Put $\alpha = |U| + |V|$, $\beta = \alpha + |W|$, denote the elements of $U \cup V$ by d_1, \dots, d_{α} and the elements of W by $d_{\alpha+1}, \dots, d_{\beta}$, such that

$$d_1 \ge d_2 \ge \dots \ge d_{\alpha}$$
 and $d_{\alpha+1} \ge d_{\alpha+2} \ge \dots \ge d_{\beta}$.

So, for $U = U_{\tau}$, $V = V_{\tau}$ and $W = W_{\tau}$ the d_i $(i = 1, ..., \beta)$ are the absolute values of the nonzero differences of consecutive entries of the initial part $(a_1^{(\tau)} \dots a_{q_{\tau+1}}^{(\tau)})$ of $\boldsymbol{a}^{(\tau)}$. Now \boldsymbol{b} is defined by

$$b_i = \begin{cases} \sum_{j=1}^i d_j & \text{for } 1 \le i \le \alpha, \\ v - \sum_{j=\alpha+1}^i d_j & \text{for } \alpha + 1 \le i \le \beta. \end{cases}$$

In addition, let $b_0 = 0$.

Example 2. The associated vector for any peak with $U \cup V = \{4, 2, 1, 1\}$ and $W = \{2, 2, 1\}$ is $\boldsymbol{b} = (4678643)$.

Lemma 1. Fix some τ , $0 \le \tau \le t - 1$, and let $\mathbf{b} = (b_1 \dots b_{\beta})$ be the vector associated with the $(a_{q_{\tau}}, a_{p_{\tau+1}}, a_{q_{\tau+1}})$ -peak $(U_{\tau}, V_{\tau}, W_{\tau})$, defined according to (10)-(12), where $\alpha = |U_{\tau} \cup V_{\tau}|$ and $\beta = \alpha + |W_{\tau}|$. Also let U' be a partition of $a_{q_{\tau+1}}$, and let c_1, \ldots, c_{ρ} be positive integers with

$$\sum_{j=1}^{\rho} c_j = a_{p_{\tau+1}} - a_{q_{\tau+1}}. \tag{13}$$

Then the following statements are equivalent.

1. There exist integers l_j , r_j with $1 \le l_j \le p_{\tau+1} \le r_j < q_{\tau+1}$ $(j = 1, ..., \rho)$, such that for $\mathbf{a'} = \mathbf{a}^{(\tau)} - \sum_{j=1}^{\rho} c_j \mathbf{s}^{(j)}$, where

$$s_i^{(j)} = \begin{cases} 1 & if \ l_j \le i \le r_j \\ 0 & otherwise \end{cases} \quad (j = 1, \dots, \rho; \ i = 1, \dots, n)$$

we have

(a)
$$0 \le a_1' \le a_2' \le \dots \le a_{q_{\tau+1}}'$$

(b)
$$\{a'_i - a'_{i-1} : 1 \le i \le q_{\tau+1}, \ a'_i \ne a'_{i-1}\} = U' \ (where \ a'_0 = 0).$$

2. There exist integers l'_j , r'_j with $1 \le l'_j \le r'_j \le \beta - 1$ for $j = 1, \ldots, \rho$, such that for $\mathbf{b'} = \mathbf{b} - \sum_{j=1}^{\rho} c_j \mathbf{f}^{(j)}$, where

$$f_i^{(j)} = \begin{cases} 1 & if \ l_j' \le i \le r_j' \\ 0 & otherwise \end{cases} \quad (j = 1, \dots, \rho; \ i = 1, \dots, \beta)$$

we have

(a)
$$b'_1 \leq b'_2 \leq \cdots \leq b'_{\beta} = b_{\beta}$$

(b)
$$\{b_i' - b_{i-1}' : 1 \le i \le \beta, b_i' \ne b_{i-1}'\} = U'$$
 (where $b_0' = 0$).

Proof. Let

$$R_1 = \{i : 1 \le i \le p_{\tau+1}, \ a_i^{(\tau)} \ne a_{i-1}^{(\tau)} \},$$

$$R_2 = \{i : p_{\tau+1} \le i < q_{\tau+1}, \ a_i^{(\tau)} \ne a_{i+1}^{(\tau)} \}.$$

Clearly,

$$U_{\tau} \cup V_{\tau} = \{ a_i^{(\tau)} - a_{i-1}^{(\tau)} : i \in R_1 \} \quad \text{and}$$

$$W_{\tau} = \{ a_i^{(\tau)} - a_{i+1}^{(\tau)} : i \in R_2 \}.$$

But by construction of \boldsymbol{b} we also have

$$U_{\tau} \cup V_{\tau} = \{b_i - b_{i-1} : 1 \le i \le \alpha\}$$
 and $W_{\tau} = \{b_i - b_{i+1} : \alpha \le i \le \beta - 1\}.$

Together this implies that there are bijections

$$\varphi_1: R_1 \to \{1, \ldots, \alpha\}, \quad \varphi_2: R_2 \to \{\alpha, \ldots, \beta - 1\},$$

such that

$$a_i^{(\tau)} - a_{i-1}^{(\tau)} = b_{\varphi_1(i)} - b_{\varphi_1(i)-1} \text{ for } i \in R_1 \text{ and } a_i^{(\tau)} - a_{i+1}^{(\tau)} = b_{\varphi_2(i)} - b_{\varphi_2(i)+1} \text{ for } i \in R_2.$$

It is an easy consequence of the results of [9], that from the assumption (13) it follows that for l_j, r_j $(j = 1, ..., \rho)$ as in the first statement, we have $l_j \in R_1$ and $r_j \in R_2$ for all j and for l'_j, r'_j $(j = 1, ..., \rho)$ as in the second statement we have $l'_j \leq \alpha$ and $r'_j \geq \alpha$ for all j. Suppose that l_j, r_j $(j = 1, ..., \rho)$ satisfy the conditions of the first statement. The difference of the entries number i and i-1 changes only when $l_j = i$ or $r_j = i-1$ for some j. Thus, if $i \notin R_1$ and $i-1 \notin R_2$ we have

$$a'_{i} - a'_{i-1} = a^{(\tau)}_{i} - a^{(\tau)}_{i-1} = 0.$$

Hence, for $i = 1, ..., q_{\tau+1}$.

$$a'_{i} - a'_{i-1} \neq 0 \implies i \in R_1 \text{ or } i - 1 \in R_2.$$

Put

$$C_1(i) = \{ j \in [\rho] : l_j = i \}$$
 for $i \in R_1$,
 $C_2(i) = \{ j \in [\rho] : r_i = i \}$ for $i \in R_2$.

Then

$$a'_{i} - a'_{i-1} = a_{i}^{(\tau)} - a_{i-1}^{(\tau)} - \sum_{j \in C_{1}(i)} c_{j} \quad \text{for } i \in R_{1}$$
$$a'_{i} - a'_{i+1} = a_{i}^{(\tau)} - a_{i+1}^{(\tau)} - \sum_{j \in C_{2}(i)} c_{j} \quad \text{for } i \in R_{2}.$$

By condition (a) of the first statement we have $a'_i - a'_{i+1} \leq 0$ for $i = 0, \ldots, q_{\tau+1} - 1$. For $i \in R_2$ this yields

$$\sum_{j \in C_2(i)} c_j \ge a_i^{(\tau)} - a_{i+1}^{(\tau)},$$

and together with

$$\sum_{i \in R_2} \sum_{j \in C_2(i)} c_j = \sum_{j=1}^{\rho} c_j = a_{p_{\tau+1}} - a_{q_{\tau+1}} = \sum_{i \in R_2} \left(a_i^{(\tau)} - a_{i+1}^{(\tau)} \right)$$

we obtain for $i \in R_2$,

$$\sum_{j \in C_2(i)} c_j = a_i^{(\tau)} - a_{i+1}^{(\tau)}.$$

and thus $a_i' - a_{i+1}' = 0$ for $i \in R_2$. So the only nonzero differences $a_i' - a_{i-1}'$ come from indices $i \in R_1$. Now put $l_j' = \varphi_1(l_j)$ and $r_j' = \varphi_2(r_j)$ $(j = 1, \ldots, \rho)$ and let $\boldsymbol{b'}$ be defined as in the second statement. Then $l_j' = \varphi_1(i)$ iff $j \in C_1(i)$ and $r_j' = \varphi_2(i)$ iff $j \in C_2(i)$, hence for $i \in R_1$ we have

$$b'_{\varphi_1(i)} - b'_{\varphi_1(i)-1} = b_{\varphi_1(i)} - b_{\varphi_1(i)-1} - \sum_{j : l'_j = \varphi_1(i)} c_j$$

$$= b_{\varphi_1(i)} - b_{\varphi_1(i)-1} - \sum_{j \in C_1(i)} c_j$$

$$= a_i - a_{i-1} - \sum_{j \in C_1(i)} c_j$$

$$= a'_i - a'_{i-1},$$

and for $i \in R_2$,

$$\begin{aligned} b'_{\varphi_2(i)} - b'_{\varphi_2(i)+1} &= b_{\varphi_2(i)} - b_{\varphi_2(i)+1} - \sum_{j \ : \ r'_j = \varphi_2(i)} c_j \\ &= b_{\varphi_2(i)} - b_{\varphi_2(i)+1} - \sum_{j \in C_2(i)} c_j \\ &= a_i - a_{i+1} - \sum_{j \in C_2(i)} c_j \\ &= a'_i - a'_{i+1} = 0. \end{aligned}$$

So the second statement holds, and since all the arguments are reversible, we have proved that l_j , r_j $(j=1,\ldots,\rho)$ satisfy the conditions of the first statement iff $l'_j = \varphi_1(l_j)$, $r'_j = \varphi_2(r_j)$ $(j=1,\ldots,\rho)$ satisfy the conditions of the second statement, and this proves the lemma.

In fact the proof shows even more than just the equivalence of the two statements: knowing l'_j and r'_j $(j=1,\ldots,\rho)$ and R_1 and R_2 , we can determine the l_j , r_j $(j=1,\ldots,\rho)$ and $R'=\{i:1\leq i\leq q_{\tau+1},\ a_i^{(\tau+1)}\neq a_{i-1}^{(\tau+1)}\}$ in a number of steps that is bounded by a constant.

Example 3. Suppose $a^{(\tau)} = (2\ 2\ 3\ 7\ 7\ 9\ 8\ 5\ 5\ 12)$ with $U_{\tau} = \{2,1\}, V_{\tau} = \{4,2\}, W_{\tau} = \{3,1\}, R_1 = \{1,3,4,6\}$ and $R_2 = \{6,7\}$. The associated vector is $b = (4\ 6\ 8\ 9\ 6\ 5)$ and bijections as in the proof of Lemma 1 are given by

$$\varphi_1: \qquad 1 \mapsto 2, \qquad 3 \mapsto 4, \qquad 4 \mapsto 1, \qquad 6 \mapsto 3,$$

 $\varphi_2: \qquad 6 \mapsto 5, \qquad 7 \mapsto 4.$

Now from

$$(444555) = (468965) - (022200) - (001110) - (001100),$$

where we have

$$l'_1 = 2, \ r'_1 = 4, \qquad l'_2 = 3, \ r'_2 = 5, \qquad l'_3 = 3, \ r'_3 = 4,$$

we obtain

$$l_1 = 1, r_1 = 7, l_2 = 6, r_2 = 6, l_3 = 6, r_3 = 7,$$

corresponding to

Lemma 1 motivates the following definitions.

Definition 3. Let $\boldsymbol{b} = (b_1 \dots b_\beta)$ be the vector associated with some (u, v, w)–peak (U, V, W) where $\alpha = |U \cup V|$ and $\beta = \alpha + |W|$, and let U' be a partition of w. Let T be the set of positive integers ρ such that there are integers $l_1, \ldots, l_\rho, r_1, \ldots, r_\rho$ and coefficients $c_1, \ldots, c_\rho \in IV \setminus \{0\}$ such that

1.
$$\sum_{j=1}^{\rho} c_j = v - w$$
,

2.
$$1 \le l_j \le r_j \le \beta - 1$$
 for $j = 1, 2, \dots, \rho$.

and for $\boldsymbol{b'} = \boldsymbol{b} - \sum_{j=1}^{\rho} c_j \boldsymbol{f}^{(j)}$, where

$$f_i^{(j)} = \begin{cases} 1 & \text{if } l_j \le i \le r_j, \\ 0 & \text{otherwise,} \end{cases} \quad (j = 1, \dots, \rho; \ i = 1, \dots, \beta)$$

we have

3.
$$b'_1 \le b'_2 \le \dots \le b'_{\beta} = b_{\beta} = w$$
 and

4.
$$\{b'_i - b'_{i-1} : 1 \le i \le \beta, b'_i \ne b'_{i-1}\} = U' \text{ (with } b'_0 = 0\text{)}.$$

Then we define

$$\rho(\boldsymbol{b}, U') = \left\{ \begin{array}{ll} \min T & \text{if } T \neq \emptyset, \\ \infty & \text{if } T = \emptyset. \end{array} \right.$$

Definition 4. Let (U, V, W) and (U', V', W') be a (u, v, w)-peak and a (u', v', w')-peak, respectively, where u' = w. Then we put

$$\delta((U, V, W), (U', V', W')) = \rho(b, U'),$$

where \boldsymbol{b} is the vector associated with (U, V, W).

In order to model the segmentation process we define a digraph $G = (\mathcal{V}, \mathcal{E})$. The vertex set is

$$\mathcal{V} = \{ (\tau, U, V_{\tau}, W_{\tau}) : 0 \le \tau \le t, U \text{ is a partition of } a_{q_{\tau}} \},$$

where

$$V_{\tau} = \{ a_i - a_{i-1} : q_{\tau} < i \le p_{\tau+1}, \ a_i \ne a_{i-1} \},$$

$$W_{\tau} = \{ a_i - a_{i+1} : p_{\tau+1} \le i < q_{\tau+1}, \ a_i \ne a_{i+1} \}$$

for $0 \le \tau \le t$. Observe that there is only one vertex with first component 0, namely $(0,\emptyset,V_0,W_0)$ corresponding to $\boldsymbol{a}^{(0)}=\boldsymbol{a}$ and there is only one vertex with first component t, namely $(t,\emptyset,\emptyset,\emptyset)$ corresponding to the zero vector. In general, the vertices with first component τ represent the possibilities for (U_τ,V_τ,W_τ) , and by the observation before Definition 2 for each τ there is only one choice for V_τ and W_τ , depending only on \boldsymbol{a} . In the arc set $\mathcal E$ we include all arcs of the form

$$((\tau, U, V_{\tau}, W_{\tau}), (\tau + 1, U', V_{\tau+1}, W_{\tau+1}))$$

for $\tau = 0, \dots, t-1$. Figure 1 shows G for $\boldsymbol{a} = (132434)$, where the vertices are labeled as follows.

$$a = (0, \emptyset, \{1, 2\}, \{1\}), \quad b = (1, \{2\}, \{2\}, \{1\}), \quad c = (1, \{1, 1\}, \{2\}, \{1\}),$$

$$d = (2, \{3\}, \{1\}, \{4\}), \quad e = (2, \{2, 1\}, \{1\}, \{4\}), \quad f = (2, \{1, 1, 1\}, \{1\}, \{4\}),$$

$$g = (3, \emptyset, \emptyset, \emptyset).$$

We define the arc weights in G to be the distances of the corresponding peaks, i.e.

$$\delta((\tau, U, V_{\tau}, W_{\tau}), (\tau + 1, U', V_{\tau+1}, W_{\tau+1})) = \delta((U, V_{\tau}, W_{\tau}), (U', V_{\tau+1}, W_{\tau+1}))$$

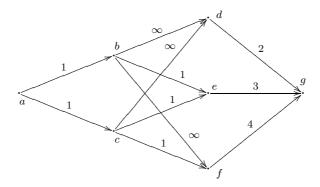


Figure 1: The digraph for the vector **a**.

for $0 \le \tau \le t-1$ and all partitions U and U' of $a_{q_{\tau}}$ and $a_{q_{\tau+1}}$, respectively. Observe that in this definition we used the fact that (U, V_{τ}, W_{τ}) and $(U', V_{\tau+1}, W_{\tau+1})$ are an $(a_{q_{\tau}}, a_{p_{\tau+1}}, a_{q_{\tau+1}})$ -peak and an $(a_{q_{\tau+1}}, a_{p_{\tau+2}}, a_{q_{\tau+2}})$ -peak, respectively. This assures that the condition u' = w in the definition of δ is satisfied. For instance, the segment $(1 \ 1 \ 0 \ 0 \ 0)$ corresponds to the arc (a, b), since

$$a - (110000) = (022434),$$

while $(0\ 1\ 0\ 0\ 0\ 0)$ corresponds to the arc (a,c), since

$$a - (010000) = (122434).$$

In general, an arc of weight ρ corresponds to a linear combination of ρ segments. Now with a segmentation we can associate a path

$$(0, \emptyset, V_0, W_0), (1, U_1, V_1, W_1), \dots, (t, \emptyset, \emptyset, \emptyset)$$
 (14)

in G.

Example 4. The segmentation

$$a = (110000) + (011100) + (011111) + 2(000111) + (000001)$$

corresponds to the path (a, b, e, g) in Figure 1 as follows.

With these definitions the minimal number of segments needed to realize a segmentation corresponding to (14) equals the weight of this path.

Lemma 2. In time O(1) we can determine the values $\rho(\mathbf{b}, U')$ for all vectors \mathbf{b} that are associated with some (u, v, w)-peak and for all partitions U' of w. In addition we obtain values c_j , l'_j , r'_j $(j = 1, ..., \rho(\mathbf{b}, U'))$ satisfying the conditions of Definition 3.

Proof. The total number of vectors \boldsymbol{b} associated with some (u, v, w)-peaks when u, v and w run through all the possible values is

$$\sum_{v=1}^{L} \sum_{w=0}^{v-1} \mathcal{P}_v \mathcal{P}_{v-w}$$

where \mathcal{P}_i is the number of partitions of $i \in \mathbb{N}$. Fix one of these vectors \mathbf{b} . We consider all the sets $S = \{(l'_j, r'_j, c_j) : j = 1, \ldots, \rho\} \ (\rho \in \mathbb{N})$, such that the vectors $\mathbf{f}^{(1)}, \ldots, \mathbf{f}^{(\rho)}$, defined as in Definition 3 and the coefficients c_1, \ldots, c_ρ satisfy the conditions in Definition 3. We claim that there are at most

$$v^{v-w} \le L^L$$

possibilities for S. Writing $\sum_{k=1}^{c_j} \boldsymbol{f}^{(j)}$ for $c_j \boldsymbol{f}^{(j)}$ we can express $\sum_{j=1}^{\rho} c_j \boldsymbol{f}^{(j)}$ as a sum of $\sum_{j=1}^{\rho} c_j = v - w$ (0,1)-vectors. In order to satisfy Conditions 1 and 3 of Definition 3, for $i = \alpha, \ldots, \beta - 1$, in exactly $b_i - b_{i+1}$ of these (0,1)-vectors there must be 0 at position i+1 and a 1 at position i. So we may assume that the v-w right leaf positions are fixed. Since for each right leaf position there are at most v left leaf positions the claim follows. For each S the resulting partition U' of w can be computed in O(1) steps, since ρ is bounded by $v-w \leq L$, and β is bounded by 2L. Thus the number of peaks

is bounded by a constant, the number of sets S to be checked for each peak is bounded by a constant, for each of these sets the number of steps for the checking is bounded by a constant, and this completes the proof.

Lemma 3. In time O(n) we can determine the arc weights $\delta(e)$ for all $e \in \mathcal{E}$ and for each arc e a sequence

$$(\boldsymbol{s}^{(1)}, c_1), \ldots, (\boldsymbol{s}^{(\delta(e))}, c_{\delta(e)})$$

realizing its weight.

Proof. By Lemma 2 we may assume that we know all the $\rho(\boldsymbol{b}, U')$. First we determine in time O(n) the sets

$$P = \{p_1, \dots, p_t\},$$

$$Q = \{q_0, \dots, q_t\},$$

$$R_{1,\tau} = \{i : q_\tau < i \le p_{\tau+1}, \ a_i \ne a_{i-1}\} \qquad (\tau = 0, \dots, t-1),$$

$$R_{2,\tau} = \{i : p_{\tau+1} \le i < q_{\tau+1}, \ a_i \ne a_{i+1}\} \qquad (\tau = 0, \dots, t-1),$$

and the partitions V_{τ} and W_{τ} ($\tau=0,\ldots,t$). By induction, we assume that we have already determined the weights of the arcs up to layer τ for some τ , $0 \le \tau \le t-1$. The number of vertices in layers τ and $\tau+1$ are bounded by $\mathcal{P}_{a_{q_{\tau}}}$ and $\mathcal{P}_{a_{q_{\tau+1}}}$, respectively. So the number of arcs is bounded by \mathcal{P}_L^2 . Fix some $(\tau, U_{\tau}, V_{\tau}, W_{\tau})$ and $(\tau+1, U_{\tau+1}, V_{\tau+1}, W_{\tau+1})$. Also by induction, we assume that we know the set

$$R_1 = \{i : 1 \le i \le p_{\tau+1}, \ a_i^{(\tau)} \ne a_{i-1}^{(\tau)}\}$$

for some possible $\boldsymbol{a}^{(\tau)}$ corresponding to $(\tau, U_{\tau}, V_{\tau}, W_{\tau})$. Now by Lemma 1 (and its proof) we obtain

$$\delta((\tau, U_{\tau}, V_{\tau}, W_{\tau}), (\tau + 1, U_{\tau+1}, V_{\tau+1}, W_{\tau+1}))$$

and a sequence realizing this value in constant time from the corresponding data for \boldsymbol{b} and U' where \boldsymbol{b} is the vector associated with $(U_{\tau}, V_{\tau}, W_{\tau})$ and $U' = U_{\tau+1}$. If $\tau \leq t-2$ this also yields

$$R'_1 = \{i : 1 \le i \le p_{\tau+2}, \ a_i^{(\tau+1)} \ne a_{i-1}^{(\tau+1)}\}$$

for some possible $\boldsymbol{a}^{(\tau+1)}$ corresponding to $(\tau+1,U_{\tau+1},V_{\tau+1},W_{\tau+1})$. So the weights for all arcs between adjacent layers can be determined in time O(1). And since the number of layers t+1 is bounded by n, the lemma is proved. \square

Now the search for a segmentation with minimal NS amounts to the search for a path of minimal weight in a layered digraph with at most n layers where the number of vertices per layer is bounded by the constant \mathcal{P}_L . This can be done in time O(n) ([12]). Thus we have proved

Theorem 2. L-One Row-Min MU-Min NS can be solved in time O(n).

3 Multiple row intensity maps

In this subsection we generalize the basic idea of the preceding subsection to prove that for bounded L the NS-minimization is polynomially solvable also for multiple row matrices. The problem L-MIN MU-MIN NS is:

Instance: An integer matrix $A = (a_{i,j})_{\substack{1 \le i \le m \\ 1 \le j \le n}}$ with $0 \le a_{i,j} \le L$ $(i \in [m], j \in [n])$.

Problem: Find a segmentation of A with in first instance minimal TNMU and in second instance minimal NS!

Assume we have already determined the minimal TNMU c. From a segmentation of A we obtain a partition $c = c_1 + c_2 + \cdots + c_k$ where c_i is the coefficient of the i-th segment $(i = 1, \ldots, k)$. First we consider the problem to check for a given partition if there is a segmentation of A with coefficients c_1, \ldots, c_k . This problem can be solved by checking the rows of A independently. For the moment we omit the row index and denote by $\mathbf{a} = \begin{pmatrix} a_1 & \cdots & a_n \end{pmatrix}$ a fixed row of A and we put $a_0 = a_{n+1} = 0$. Compared to the single row case an additional difficulty in the multiple row case arises from the fact that the minimal TNMU that would be sufficient for a segmentation of \mathbf{a} might be smaller than c. As a consequence we can not use Lemma 1, where condition (13) is essential. Here the order of the elements of the considered partition must be taken into consideration. For instance, for $\mathbf{b} = \begin{pmatrix} 2 & 5 & 0 \end{pmatrix}$ there is a segmentation with coefficients 4, 1 and 1, namely

$$b = 4(010) + (110) + (100),$$

while there is no segmentation with these coefficients for b' = (350). So instead of peaks we have to consider ordered peaks to be defined below. Also, in order to describe the segmentation, we attach to a peak a multiset X of coefficients, and call the result an *extended ordered peak*. This is made precise in the following definition.

Definition 5. For integers v and w with $0 \le w < v \le L$ an extended ordered (v, w)-peak is a pair (\boldsymbol{b}, X) of an integer vector $\boldsymbol{b} = (b_1 \ b_2 \dots b_{\beta})$, such that there is an integer α with $1 \le \alpha < \beta$ and

$$0 < b_1 < b_2 < \dots < b_{\alpha} = v,$$

 $v = b_{\alpha} > b_{\alpha+1} > \dots > b_{\beta} = w,$

and a multiset X of positive integers. In addition, a pair (\boldsymbol{b},X) , where $\boldsymbol{b}=()$ is the empty tuple and X is a multiset of positive integers is called extended ordered (0,0)-peak.

Example 5. ((2 5 7 4 3), $\{1, 2, 2, 3, 3\}$) is an extended ordered (7, 3)-peak (with $\alpha = 3, \beta = 5$).

Let p_1, \ldots, p_t and q_0, \ldots, q_t be defined as in the preceding section. Then for a segmentation

$$oldsymbol{a} = \sum_{j=1}^k c_j oldsymbol{s}^{(j)}$$

we can define $k_0(\tau)$ and $\boldsymbol{a}^{(\tau)}$ $(\tau=0,\ldots,t)$ as before. Now for $\tau=0,\ldots,t$, we associate with $\boldsymbol{a}^{(\tau)}$ an extended ordered $(a_{p_{\tau+1}},a_{q_{\tau+1}})$ -peak $(\boldsymbol{b}^{(\tau)},X_{\tau})$ as follows. For $\tau< t$, let

$$I_{\tau} = \{i : 1 \le i \le p_{\tau+1}, \ a_i^{(\tau)} \ne a_{i-1}^{(\tau)}\},$$

$$J_{\tau} = \{i : p_{\tau+1} < i \le q_{\tau+1}, \ a_i^{(\tau)} \ne a_{i-1}^{(\tau)}\},$$

denote the elements of I_{τ} by i_1, \ldots, i_{α} and the elements of J_{τ} by $i_{\alpha+1}, \ldots, i_{\beta}$ such that $i_1 < i_2 < \cdots < i_{\beta}$, and put

$$b_0 = 0, \quad b_l = a_{i_l} \quad (l = 1, \dots, \beta).$$

Let $X_0 = \{c_1, ..., c_k\}$ and

$$X_{\tau+1} = X_{\tau} \setminus \{c_{k_0(\tau)+1}, c_{k_0(\tau)+2}, \dots, c_{k_0(\tau+1)}\}$$
 $(\tau = 0, \dots, t-1).$

Now for $\tau < t$, $(\boldsymbol{b}^{(\tau)}, X_{\tau})$ describes the initial part of $\boldsymbol{a}^{(\tau)}$ (up to column $q_{\tau+1}$) together with the coefficients available for the remaining segments. In the final state $(\tau = t)$ we have the zero row $\boldsymbol{a}^{(t)} = 0$ and a multiset X_t of coefficients, that are not needed for the considered row. With the zero row we associate the empty tuple $\boldsymbol{b}^{(t)} = ()$, and thus we obtain from any segmentation a sequence $(\boldsymbol{b}^{(0)}, X_0), (\boldsymbol{b}^{(1)}, X_1), \ldots, (\boldsymbol{b}^{(t)}, X_t)$ of extended ordered peaks.

Example 6. Suppose a = (243163061) is a row in an intensity matrix with minimal TNMU c = 18, and we are checking the partition c = 5 + 3 + 2 + 2 + 2 + 1 + 1 + 1 + 1. Then from the segmentation

we obtain

au	$oldsymbol{a}^{(au)}$	$\boldsymbol{b}^{(\tau)}$	$X_{ au}$
0	(243163061)	(2431)	${5,3,2,2,2,1,1,1,1}$
1	$(0\ 1\ 1\ 1\ 6\ 3\ 0\ 6\ 1)$	(1630)	$\{5,3,2,2,1,1,1\}$
2	$(0\ 0\ 0\ 0\ 0\ 0\ 0\ 6\ 1)$	(610)	$\{5,2,1,1\}$
3	(0 0 0 0 0 0 0 0	()	$\{2,1\}$

That the vectors $\boldsymbol{b}^{(\tau)}$ provide enough information to construct the segmentation, follows from the simple observation, that w.l.o.g. a *plateau*, i.e. a sequence of consecutive entries of equal value

$$a_{i_1} = a_{i_1+1} = \dots = a_{i_2}$$

can be considered as one single entry. This is intuitively clear and proved formally in the next lemma.

Lemma 4. Let $\boldsymbol{a} = \sum_{j=1}^k c_j \boldsymbol{s}^{(j)}$ be a segmentation with

$$s_i^{(j)} = \begin{cases} 1 & \text{if } l_j \le i \le r_j \\ 0 & \text{otherwise} \end{cases} \qquad (j = 1, \dots, k).$$

There are integers l'_j and r'_j (j = 1, ..., k) with the following properties.

1. We have
$$\mathbf{a} = \sum_{j=1}^{k} c_j \mathbf{s}^{\prime(j)}$$
 where

$$s_i^{\prime(j)} = \begin{cases} 1 & \text{if } l_j' \le i \le r_j' \\ 0 & \text{otherwise} \end{cases} \qquad (j = 1, \dots, k).$$

2.

$$a_i = a_{i-1} \implies s_i^{\prime(j)} = s_{i-1}^{\prime(j)} \qquad (i = 2, \dots, n; \ j = 1, \dots, k).$$
 (15)

Proof. In order to satisfy the last condition, we have to replace the segments with $s_i^{(j)} \neq s_{i-1}^{(j)}$ but $a_i = a_{i-1}$ for some i. Our strategy is to modify the given segments as follows. For each plateau we choose one representative, for instance the rightmost entry, and adapt the entries for each segment to the chosen column. This corresponds to the following shifting of the leaves: if the left leaf covers a part of the plateau it is shifted to the right until the whole plateau is open, and if the right leaf covers a part of the plateau it is shifted to the left until the whole plateau is covered.

First observe that $s_i^{(j)}$ can differ from $s_{i-1}^{(j)}$ only if $i = l_j$ or $i - 1 = r_j$. So for (15) it is sufficient that, for all j, we have

$$a_{l'_{i}} \neq a_{l'_{i}-1}$$
 and $a_{r'_{i}} \neq a_{r'_{i}+1}$. (16)

Suppose $a_{l_j} = a_{l_j-1}$ for some j. Then $i_1 < l_j \le i_2$ for some i_1, i_2 with

$$a_{i_1} = a_{i_1+1} = \dots = a_{i_2} = a$$
 and $a_{i_1-1}, a_{i_2+1} \neq a$. (17)

Since we want to adapt the entries of the segment to the rightmost column i_2 we have to shift the left leaf to the left and put $l'_j = i_1$. Similarly, if $a_{r_j} = a_{r_j+1}$, then $i_1 \leq r_j < i_2$ for some i_1 , i_2 with (17), and in order to adapt the entries of the segment to column i_2 , we have to shift the right leaf to the left and put $r'_j = i_1 - 1$. In summary, for $j \in [k]$ we put

$$l'_{j} = \begin{cases} l_{j} & \text{if } a_{l_{j}} \neq a'_{l_{j}-1} \\ \max\{i < l_{j} : a_{i} \neq a_{l_{j}}\} + 1 & \text{if } a_{l_{j}} = a'_{l_{j}-1} \end{cases}$$

$$r'_{j} = \begin{cases} r_{j} & \text{if } a_{r_{j}} \neq a'_{r_{j}+1} \\ \max\{i < r_{j} : a_{i} \neq a_{r_{j}}\} & \text{if } a_{r_{j}} = a'_{r_{j}+1} \end{cases}$$

Then (16) is valid for all j, hence (15) is satisfied. In order to check the first condition of the lemma, fix some $i \in [n]$. If $s_i^{\prime(j)} = s_i^{(j)}$ for all j, then

$$\sum_{j=1}^{k} c_j s_i^{\prime(j)} = \sum_{j=1}^{k} c_j s_i^{(j)} = a_i.$$

So assume $s_i'^{(j)} \neq s_i^{(j)}$ for some j. By construction this can be the case only if $a_i = a_{i-1}$ or $a_i = a_{i+1}$. Now let i_1 and i_2 be the indices with $i_1 \leq i \leq i_2$,

$$a_{i_1} = a_{i_1+1} = \dots = a_i = \dots = a_{i_2}$$
 and $a_{i_1-1}, a_{i_2+1} \neq a_i$.

We claim that $s_i'^{(j)} = s_{i_2}^{(j)}$ (j = 1, ..., k). If $s_{i_2}^{(j)} = 0$, $l_j > i_2$ or $r_j < i_2$. By construction, in the first case $l_j' > i_2$ and in the second case $r_j' < i_1$, so in both cases $s_i'^{(j)} = 0$. If $s_{i_2}^{(j)} = 1$, $l_j \le i_2$ and $r_j \ge i_2$. By construction, $l_j' \le i_1$ and $r_j' \ge i_2$, hence $s_i'^{(j)} = 1$ and the claim is proved. From this follows

$$\sum_{j=1}^{k} c_j s_i^{\prime(j)} = \sum_{j=1}^{k} c_j s_{i_2}^{(j)} = a_{i_2} = a_i,$$

and since this argument works for any $i \in [n]$ the first condition of the lemma is satisfied.

By Lemma 4 applied to $\mathbf{a}^{(\tau)}$, w.l.o.g. we may assume that $a_{l_j}^{(\tau)} \neq a_{l_j-1}^{(\tau)}$ and $a_{r_j}^{(\tau)} \neq a_{r_j+1}^{(\tau)}$ for all $j > k_0(\tau)$. With this assumption the next lemma, whose proof is obvious, justifies that we use the $\mathbf{b}^{(\tau)}$ instead of the $\mathbf{a}^{(\tau)}$.

Lemma 5. For fixed τ , $0 \le \tau \le t-1$, let $\boldsymbol{b}^{(\tau)}$ and X_{τ} be defined as described above and let $\{c_1, \ldots, c_{\rho}\} \subseteq X_{\tau}$ be fixed. If $a_{q_{\tau+1}} \ne 0$ let $\boldsymbol{g} = (g_1 \ldots g_{\gamma})$ be some vector with

$$0 < g_1 < \dots < g_{\gamma} = a_{q_{\tau+1}}$$
.

Then the following statements are equivalent.

1. There exist integers l_j , r_j with $1 \leq l_j \leq r_j < q_{\tau+1}$, $a_{l_j}^{(\tau)} \neq a_{l_j-1}^{(\tau)}$ and $a_{r_j}^{(\tau)} \neq a_{r_j+1}^{(\tau)}$ $(j = 1, ..., \rho)$ such that for $\mathbf{a'} = \mathbf{a}^{(\tau)} - \sum_{j=1}^{\rho} c_j \mathbf{s}^{(j)}$, where

$$s_i^{(j)} = \begin{cases} 1 & \text{if } l_j \le i \le r_j \\ 0 & \text{otherwise} \end{cases} \quad (j = 1, \dots, \rho; \ i = 1, \dots, n)$$

we have

- (a) $0 \le a_1' \le a_2' \le \dots \le a_{q_{\tau+1}}' = a_{q_{\tau+1}}$
- (b) If $a_{q_{\tau+1}} \neq 0$ there are exactly γ indices $1 \leq i_1 < \cdots < i_{\gamma} \leq q_{\tau+1}$ with $a'_{i_*} \neq a'_{i_*-1}$ (where $a'_0 = 0$) and we have

$$(a_{i_1} \quad a_{i_2} \quad \dots \quad a_{i_{\gamma}}) = \boldsymbol{g}.$$

2. There exist integers l'_j , r'_j with $1 \le l'_j \le r'_j \le \beta - 1$ for $j = 1, ..., \rho$, such that for $\mathbf{b'} = \mathbf{b} - \sum_{j=1}^{\rho} c_j \mathbf{f}^{(j)}$, where

$$f_i^{(j)} = \begin{cases} 1 & \text{if } l_j' \le i \le r_j' \\ 0 & \text{otherwise} \end{cases} \quad (j = 1, \dots, \rho; \ i = 1, \dots, \beta)$$

we have

- (a) $b'_1 \le b'_2 \le \dots \le b'_{\beta} = b_{\beta} = a_{q_{\tau+1}}$
- (b) If $a_{q_{\tau+1}} \neq 0$ there are exactly γ indices $1 \leq i_1 < \dots < i_{\gamma} \leq \beta$ with $b'_{i_*} \neq b'_{i_*-1}$ (where $b'_0 = 0$) and we have

$$(b_{i_1} \quad b_{i_2} \quad \dots \quad b_{i_{\gamma}}) = \boldsymbol{g}.$$

Now for $\tau = 0, 1, \dots, t-1$ the choice of the pairs

$$(s^{k_0(\tau)+1}, c_{k_0(\tau)+1}), \ldots, (s^{k_0(\tau+1)}, c_{k_0(\tau+1)})$$

can be viewed as a way to go from the extended ordered $(a_{p_{\tau+1}}, a_{q_{\tau+1}})$ -peak $(\boldsymbol{b}^{(\tau)}, X_{\tau})$ to the extended ordered $(a_{p_{\tau+2}}, a_{q_{\tau+2}})$ -peak $(\boldsymbol{b}^{(\tau+1)}, X_{\tau+1})$ (with $a_{p_{t+1}} = a_{q_{t+1}} = 0$).

Definition 6. Let $0 \le w < v$ and let (\boldsymbol{b}, X) be an extended ordered (v, w)–peak, and let v', w' be integers with $w \le v' \le L$ and $0 \le w' < v'$ or v' = w' = 0. In addition let X' be a submultiset of X and denote the elements of X' by $x_1, \ldots, x_{|X'|}$. We call an extended ordered (v', w')–peak $(\boldsymbol{b'}, X \setminus X')$ accessible from (\boldsymbol{b}, X) if there are integers $l'_1, \ldots, l'_{|X'|}, r'_1, \ldots, r'_{|X'|}$ such that

1.
$$1 \le l'_j \le r'_j \le \beta - 1$$
 for $j = 1, ..., |X'|$ (where $\boldsymbol{b} = (b_1 ... b_\beta)$).

and for $\boldsymbol{b''} = \boldsymbol{b} - \sum_{j=1}^{|X'|} x_j \boldsymbol{f}^{(j)}$, where

$$f_i^{(j)} = \begin{cases} 1 & \text{if } l_j' \le i \le r_j', \\ 0 & \text{otherwise,} \end{cases} \quad (j = 1, \dots, |X'|; \ i = 1, \dots, \beta)$$

we have b'' = 0 if v' = w' = 0 and otherwise

- 2. $b_1'' \le b_2'' \le \dots \le b_{\beta}'' = b_{\beta} = w$ and
- 3. If $i_1 < i_2 < \cdots < i_{\gamma'}$ are the indices with $b''_{i_*} \neq b''_{i_*-1}$ (where $b''_0 = 0$), then

$$b_1' < b_2' < \dots < b_{\gamma'}' = w,$$

and we have

$$\begin{pmatrix} b_{i_1}^{\prime\prime} & b_{i_2}^{\prime\prime} & \dots & b_{i_{\gamma'}}^{\prime\prime} \end{pmatrix} = \begin{pmatrix} b_1^{\prime} & b_2^{\prime} & \dots & b_{\gamma'}^{\prime} \end{pmatrix}.$$

The definition can be interpreted as follows. Assume $a_{p_1} = v$, $a_{q_1} = w$, $a_{p_2} = v'$, $a_{q_2} = w'$, let $\boldsymbol{b}^{(0)}$ be associated with $\boldsymbol{a}^{(0)}$ as above, and let $\boldsymbol{b}' = (b'_1 \dots b'_{\beta'})$ be a vector with

$$0 < b'_1 < \dots < b'_{\alpha'} = v', \ v' = b'_{\alpha'} > \dots > b'_{\beta'} = w'.$$

Then $(\boldsymbol{b'}, X \setminus X')$ is accessible from $(\boldsymbol{b}^{(0)}, X)$ iff we can assign segments $\boldsymbol{s}^{(j)}$ to the elements of X', described by l_j , r_j (j = 1, ..., |X'|) with $r_j < q_1$ for all j, such that for

$$\boldsymbol{a}^{(1)} = \boldsymbol{a}^{(0)} - \sum_{j=1}^{|X'|} x_j \boldsymbol{s}^{(j)}$$

we have $a_1^{(1)} \leq a_2^{(1)} \leq \cdots \leq a_{p_2}^{(1)}$ and the extended ordered (v', w')-peak associated with $\boldsymbol{a}^{(1)}$ is $(\boldsymbol{b'}, X \setminus X')$.

Example 7. Let $\boldsymbol{a} = (0\ 2\ 5\ 7\ 4\ 3\ 3\ 5\ 6\ 8\ 2),\ X = \{5,3,2,2,2,1,1,1\}$ and $X' = \{3,1\}$. The associated extended ordered (7,3)-peak is (\boldsymbol{b},X) where $\boldsymbol{b} = (2\ 5\ 7\ 4\ 3)$. Now we want to determine the extended ordered (8,0)-peaks $(\boldsymbol{b'},X\setminus X')$ that are accessible from (\boldsymbol{b},X) , where

$$b' = (b'_1 \dots b'_{\gamma-1} \ b'_{\gamma} = 3 \ 5 \ 6 \ 8 \ 2).$$

We obtain that $(\mathbf{b'}, X \setminus X')$ and $(\mathbf{b''}, X \setminus X')$ are accessible from (\mathbf{b}, X) , where $\mathbf{b'} = (2\ 3\ 5\ 6\ 8\ 2)$ and $\mathbf{b''} = (1\ 3\ 5\ 6\ 8\ 2)$:

$$(22333) = \mathbf{b} - (03300) - (00110),$$

 $(11333) = \mathbf{b} - (03300) - (11110).$

This corresponds to the following possible beginnings of a segmentation.

and

On the other hand one can check that $((35682), X \setminus X')$ is not accessible from (\boldsymbol{b}, X) and this corresponds to the fact that it is not possible to find (l_1, r_1) and (l_2, r_2) with $r_1, r_2 < 7$ such that after subtracting the corresponding segments with coefficients 3 and 1 from \boldsymbol{a} we obtain a row vector $\boldsymbol{a'}$ with $a'_1 = \cdots = a'_i = 0, \ a'_{i+1} = \cdots = a'_7 = 3$ for some $i, 1 \le i \le 6$. Similar statements can be made for $\boldsymbol{b'} = (1235682)$.

Lemma 6. Let (\mathbf{b}, X) be an extended ordered (v, w)-peak. Then the set of all $(\mathbf{b'}, X \setminus X')$ that are accessible from (\mathbf{b}, X) can be determined in time O(1).

Proof. Observe that the accessibility does not depend on the whole vector b' but only on the initial part $(b'_1 \dots b'_{\gamma'} = w)$. So in order to determine

the accessible extended ordered peaks it is sufficient to determine the pairs $((b'_1 \cdots b'_{\gamma'}), X \setminus X')$ of initial parts and multisets of coefficients. Let $\mathbf{b} = (b_1 \cdots b_{\beta})$ and let α be the unique index with $b_{\alpha} = v$. We have $b_1 < \cdots < b_{\alpha}$ and $b_{\alpha} > \cdots > b_{\beta}$. So for $1 \leq k \leq v - 1$ there are at most two indices i and i' with $1 \leq i, i' \leq \beta - 1$ and $b_i = k, b_{i'} = k$ (namely the first one with $1 \leq i \leq \alpha - 1$ and the second one with $\alpha + 1 \leq i' \leq \beta - 1$). The only index i with $b_i = v$ is $i = \alpha$, and so we have

$$\sum_{i=1}^{\beta-1} b_i \le v + 2 \sum_{k=1}^{\nu-1} k \le L^2.$$

Hence it is sufficient to consider at most \mathcal{P}_{L^2} candidates for X', where each of these has at most L^2 elements. Fix one of these X'. Labeling the elements of X' as in Definition 6, for each $x_j \in X'$ there are at most $\binom{2L-1}{2}$ choices for $\mathbf{f}^{(j)}$. So the total number of choices for the pairs $(\mathbf{f}^{(j)}, x_j)$ that have to be considered is bounded by

$$\left[\binom{2L-1}{2} \right]^{|X'|} \le \left[\binom{2L-1}{2} \right]^{L^2}.$$

For each of these choices the time needed to determine the resulting b'' is bounded by a constant. Precisely, in order to subtract one of the $x_j \mathbf{f}^{(j)}$ we have to do at most 2L subtractions. So after at most $L^2 \cdot 2L$ subtractions we have determined b''. Finally, in order to determine the corresponding $\begin{pmatrix} b'_1 \cdots b'_{\gamma'} \end{pmatrix}$ according to condition 3 of Definition 6, we have to run through the at most 2L entries of b'. This proves the lemma, since the number of steps to determine the required data is bounded by

$$\mathcal{P}_{L^2}\left[\binom{2L-1}{2}\right]^{L^2}(L^2+1)2L.$$

In order to model the segmentation we construct sets $\mathcal{V}_0, \ldots, \mathcal{V}_t$ of extended ordered peaks. Put $\mathcal{V}_0 = \{(\boldsymbol{b}^{(0)}, X_0)\}$ and suppose we have already constructed $\mathcal{V}_0, \ldots, \mathcal{V}_{\tau}$ for some τ with $0 \le \tau < t$. Now we put

$$\mathcal{V}_{\tau+1} = \{ (\boldsymbol{b'}, X') : (\boldsymbol{b'}, X') \text{ is an } (a_{p_{\tau+2}}, a_{q_{\tau+2}}) - \text{peak that}$$
 is accessible from some $(\boldsymbol{b}, X) \in \mathcal{V}_{\tau} \}.$

Here for brevity of notation we put $a_{p_{t+1}} = 1$ and $a_{q_{t+1}} = 0$. The elements of \mathcal{V}_{τ} represent the possibilities for $(\boldsymbol{b}^{(\tau)}, X_{\tau})$. There is a segmentation of the

row with coefficients c_1, \ldots, c_k iff $\mathcal{V}_t \neq \emptyset$. Note that a natural interpretation of this construction is a breadth first search (BFS) in the tree with vertex set $\mathcal{V}_0 \cup \ldots \cup \mathcal{V}_t$ starting at $(\boldsymbol{b}^{(0)}, X_0)$, where two vertices (\boldsymbol{b}, X) and $(\boldsymbol{b'}, X')$ are connected by an edge iff $(\boldsymbol{b}, X) \in \mathcal{V}_{\tau}$, $(\boldsymbol{b'}, X') \in \mathcal{V}_{\tau+1}$ for some τ and $(\boldsymbol{b'}, X')$ is accessible from (\boldsymbol{b}, X) .

Lemma 7. For given V_{τ} , the set $V_{\tau+1}$ can be determined in time $O(n^{L+1})$.

Proof. According to [9], the sum of the elements of X_0 , which is the minimal TNMU equals

$$c = \max_{1 \le i \le m} \sum_{j=1}^{n} \max\{0, a_{i,j} - a_{i,j-1}\} \le nL.$$

Now in any partition $c = c_1 + \cdots + c_k$ where the c_i $(i \in [k])$ are the coefficients of a segmentation of A, we have $c_i \leq L$ for $i \in [k]$. Hence such a partition can be described by an L-tuple $(\lambda_1, \ldots, \lambda_L)$ of integers, where λ_r is the number of summands equal to r for $r \in [L]$. Then

$$\lambda_r \le \frac{nL}{r} \quad (r \in [L]),$$

and so there are $O(n^L)$ choices for X_0 . Now the multiset X in

$$(\boldsymbol{b}, X) \in \mathcal{V}_{\tau}$$

is a partition of some c' with $0 \le c' \le c \le nL$ with all summands less than or equal to L. So there are nL possibilities for c', and for each of these there are $O(n^L)$ possible partitions. Thus the number of choices for X is bounded by $O(n^{L+1})$. The vectors \mathbf{b} in the elements of \mathcal{V}_{τ} differ only in the initial part $(b_1 \dots b_{\gamma})$, where $b_{\gamma} = a_{q_{\tau}}$. But these initial parts are in bijection to the ordered partitions of $a_{q_{\tau}}$, and of these there are (see for instance [1])

$$\sum_{i=1}^{a_{q_{\tau}}} \binom{a_{q_{\tau}}-1}{i-1} \le L \binom{L}{\lfloor \frac{L}{2} \rfloor}.$$

Since L is bounded by a constant we obtain that $|\mathcal{V}_{\tau}|$ is bounded by $O(n^{L+1})$. By Lemma 6, for each $(\boldsymbol{b}, X) \in \mathcal{V}_{\tau}$ the set of accessible $(\boldsymbol{b'}, X \setminus X')$ can be determined in time bounded by a constant, and this yields the claim. \square

Lemma 8. For a fixed partition $c = c_1 + \cdots + c_k$, it can be checked in time $O(n^{L+2})$ if there is a segmentation of \boldsymbol{a} with coefficients c_1, \ldots, c_k .

Proof. We only have to check if $\mathcal{V}_t \neq \emptyset$. Since $t \leq n$ the claim is an immediate consequence of Lemma 7.

Now we can prove

Theorem 3. The problem L-Min MU-Min NS can be solved in time $O(mn^{2L+2})$.

Proof. Obviously,

$$c = \max_{1 \le i \le m} \sum_{j=1}^{n} \max\{0, a_{i,j} - a_{i,j-1}\}\$$

can be determined in time O(mn). As in the proof of Lemma 7 the number of partitions of $c = c_1 + \cdots + c_k$ that have to be considered is bounded by $O(n^L)$. By Lemma 8, for a fixed partition $c = c_1 + \cdots + c_k$ it can be checked in time $O(mn^{L+2})$ if there is a segmentation of A with coefficients c_1, \ldots, c_k , and this concludes the proof.

We finish this section with a remark concerning practical aspects of this result. Though the time complexity of the NS-minimization is polynomial in m and n the exponent grows linearly with L and also the L-dependent constants that were used to estimate the time-complexities of the different steps of the algorithm, grow rapidly with L. So we expect an efficient algorithm only for very small L. In the proof of the polynomiality we constructed the whole sets \mathcal{V}_{τ} ($\tau = 1, \ldots, t$), i.e. we performed a BFS as described before Lemma 7. But in order to decide if there is a segmentation with the considered coefficients we need to know only if \mathcal{V}_t is nonempty, and in order to reconstruct a segmentation basically one path from the unique element of \mathcal{V}_0 to some element of \mathcal{V}_t is sufficient. So for practical purposes it is natural to use depth first search (DFS) instead of BFS.

4 Test results

We implemented the algorithm described above and Tables 1 and 2 show test results for random $10 \times 10^-$ and $15 \times 15^-$ matrices, respectively. The computations where done on a 2 GHz workstation and we determined the minimal NS for 1000 randomly generated matrices with maximal entry L. The entry in column 'max. time' is the maximal time needed for one single matrix, and the entry in column 'total time' is the time needed for all the 1000 matrices. For comparison the tables also contain heuristic results that

	exact			heuristic	
L	NS	max. time	total time	NS	total time
3	6.9	1 s	9 s	6.9	$0.9 \mathrm{\ s}$
4	7.6	1 s	13 s	7.8	$1.0 \mathrm{\ s}$
5	8.1	1 s	29 s	8.4	$1.1 \mathrm{\ s}$
6	8.5	21 s	1.7 min	8.9	$1.2 \mathrm{\ s}$
7	8.8	$50 \mathrm{\ s}$	5.6 min	9.3	$1.2 \mathrm{\ s}$
8	9.1	$66 \mathrm{\ s}$	6.2 min	9.7	$1.3 \mathrm{\ s}$
9	9.3	3.4 min	16.1 min	10.0	$1.3 \mathrm{\ s}$
10	9.5	$5.6 \min$	41.3 min	10.3	$1.4 \mathrm{\ s}$
11	9.8	$11.0 \min$	1.3 h	10.6	$1.4 \mathrm{\ s}$
12	9.9	$24.0 \min$	2.0 h	10.9	$1.5 \mathrm{\ s}$
13	10.0	1.4 h	7.0 h	11.1	$1.5 \mathrm{\ s}$

Table 1: Average number of segments for random 10×10 -matrices with maximal entry L. Each entry is averaged over 1000 matrices.

	exact			heuristic	
L	NS	max. time	total time	NS	total time
3	9.7	1 s	16 s	9.8	4.8 s
4	10.7	1 s	31 s	10.9	$5.4 \mathrm{\ s}$
5	11.3	12 s	$175 \mathrm{\ s}$	11.7	$5.8 \mathrm{\ s}$
6	11.8	$54 \mathrm{s}$	18.6 min	12.4	$6.5 \mathrm{\ s}$
7	12.3	$6.5 \min$	1.6 h	13.0	$6.8 \mathrm{\ s}$
8	12.6	4.5 h	7.9 h	13.5	$7.1 \mathrm{\ s}$
9	12.9	24.1 h	37.9 h	14.0	$7.4 \mathrm{\ s}$
10	13.2	10.0 h	44.7 h	14.5	$7.6 \mathrm{\ s}$

Table 2: Average number of segments for random 15×15 -matrices with maximal entry L. Each entry is averaged over 1000 matrices.

were obtained with a slightly improved version of the algorithm described in [9].

In order to evaluate the performance of the heuristic we determined the differences between the heuristic values and the exact minimums. Tables 3 and 4 show the frequencies of the values of the differences when 1000 matrices where treated for each value of L. We conclude that for the considered range

L	0	1	2	3
3	969	31	0	0
4	876	123	1	0
5	780	218	2	0
6	663	331	2	0
7	525	456	19	0
8	437	516	47	0
9	335	603	62	0
10	306	584	104	6
11	262	615	121	2
12	168	654	173	5
13	141	641	213	5

L	0	1	2	3	4
3	940	60	0	0	0
4	809	189	2	0	0
5	609	379	12	0	0
6	453	509	37	1	0
7	327	585	86	2	0
8	250	594	151	5	0
9	150	609	230	11	0
10	85	551	335	28	1

Table 3: Frequencies of the differences between the heuristic number of segments and the exact minimum for 10×10 -matrices.

Table 4: Frequencies of the differences between the heuristic number of segments and the exact minimum for 15×15 -matrices.

of parameters the exact algorithm yields only small improvements in terms of the number of segments, while the computational effort is extremely high already for small values of L. So for practical purposes the heuristic seems to be a good compromise between computation time and accuracy of the optimization. Finally, we also tested our algorithm with 13 clinical matrices, and the results are shown in Table 5.

		exact		heuristic	
case no.	MU	NS	CPU-time	NS	CPU-time
1	16	7	$0.04 \mathrm{\ s}$	8	$0.01 \mathrm{\ s}$
2	16	7	$0.19 \; s$	7	$0.00 \mathrm{\ s}$
3	20	8	$0.39 \mathrm{\ s}$	8	$0.01 \mathrm{\ s}$
4	19	7	$0.04 \mathrm{\ s}$	8	$0.00 \mathrm{\ s}$
5	15	7	$0.01 \mathrm{\ s}$	7	$0.00 \mathrm{\ s}$
6	17	8	$0.70 \mathrm{\ s}$	9	$0.00 \mathrm{\ s}$
7	18	7	$0.03 \mathrm{\ s}$	7	$0.00 \mathrm{\ s}$
8	22	9	$1.30 \; s$	9	$0.01 \mathrm{\ s}$
9	26	9	25.77 s	10	$0.00 \mathrm{\ s}$
10	22	8	$0.62 \mathrm{\ s}$	9	$0.00 \mathrm{\ s}$
11	22	10	$7.88 \mathrm{\ s}$	10	$0.00~\mathrm{s}$
12	23	9	$1.96 \mathrm{\ s}$	10	$0.01 \mathrm{\ s}$
13	23	9	$2.36 \mathrm{\ s}$	9	$0.01 \mathrm{\ s}$

Table 5: Test results for clinical matrices

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