Double Soules pairs and matching Soules bases

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Abstract

We consider two generalizations of the notion of a Soules basis matrix. A pair of nonsingular $n \times n$ matrices $(P, Q)$ is called a double Soules pair if the first columns of $P$ and $Q$ are positive, $PQ^T = I$, and $PAQ^T$ is nonnegative for every $n \times n$ nonnegative diagonal matrix $A$ with nonincreasing diagonal elements. In a paper by Chen, Han, and Neumann an algorithm for generating such pairs was given. Here we characterize all such pairs, and discuss some implications of the characterization. We also consider pairs of matrices $(U, V)$ such that $U$ and $V$ each consists of $k$ orthonormal columns, the first of which is positive, and $UAV$ is nonnegative for every $k \times k$ nonnegative diagonal matrix $A$ with nonincreasing diagonal elements. We call such pairs matching Soules pairs. We characterize all such pairs, and make some observations regarding the nonnegative matrices and generalized inverses generated by them.

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1. Introduction

A Soules basis matrix is an orthogonal matrix $R$ with a positive first column which has the property:

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\[ RAR^T \] is nonnegative for every nonnegative diagonal matrix \( A \) with nonincreasing diagonal elements.

In [9], Soules constructed for any positive unit vector \( x \) such a matrix \( R \) with \( x \) as its first column. In this construction the \( k \)th column of \( R \) consisted of \( n - k + 1 \) positive entries, followed by one negative entry, followed by zeros. This sign pattern was called sign pattern \( \mathcal{N} \). In [3], Elsner, Nabben and Neumann described all \( n \times n \) Soules basis matrices, and considered the nonnegative matrices generated as \( A = RAR^T \), where \( R \) is a Soules basis matrix and \( A = \text{diag}(\lambda_1, \ldots, \lambda_n) \), \( \lambda_1 \geq \cdot \cdot \cdot \lambda_n \geq 0 \). Such matrices \( A \) will be called here (symmetric) Soules matrices.

Symmetric Soules matrices have some attractive properties – see [3] for some of these, and also [2,8]. We mention here one trivial property (see [2,1]): If \( A = RAR^T \) is a Soules matrix, where \( A = \text{diag}(\lambda_1, \ldots, \lambda_n) \), then \( RAR^T \) is the singular value decomposition of \( A \) and the best approximation of rank at most \( k \), which is the matrix given by \( RA_k R^T \), where \( A_k = \text{diag}(\lambda_1, \ldots, \lambda_k, 0, \ldots, 0) \), is, again, a Soules matrix and therefore a nonnegative matrix. So Soules matrices have the property that their best rank \( k \) approximations are nonnegative for every \( k \). Moreover, every such approximation can be factored as \( BB^T \) where \( B \in \mathbb{R}^{n \times k} \) is nonnegative (see [8]).

Nonnegative matrices of the form \( A = RAR^T \), where \( R \) is a Soules basis matrix and \( A \) is a diagonal matrix whose diagonal entries are nonincreasing but not necessarily nonnegative are also of interest. They were used to study the nonnegative inverse eigenvalue problem for symmetric matrices (see [7,6]).

These issues motivate generalizations of Soules bases and matrices. Chen, Han and Neumann considered in [2] the following generalization: A pair of nonsingular \( n \times n \) matrices \( (P, Q) \) is called a double Soules pair\(^1\) if the first columns of \( P \) and \( Q \) are positive, \( PQ^T = I \), and \( PAQ^T \) is nonnegative for every nonnegative diagonal matrix \( A \) with nonincreasing diagonal elements. An algorithm was provided for generating double Soules pairs \( (P, Q) \), where both \( P \) and \( Q \) have sign pattern \( \mathcal{N} \), and some properties of double Soules pairs (mainly of this pattern) were studied.

In Section 2 we will show how to construct all double Soules pairs, and discuss the properties of the nonnegative matrices generated by them. (We call a matrix \( A = PAQ^T \) generated by such a pair a double Soules matrix.)

In Section 3 we consider another generalization of Soules bases: We characterize all pairs \((U, V)\) where \( U \in \mathbb{R}^{m \times k} \) and \( V \in \mathbb{R}^{n \times k} \) each have orthonormal columns, the first of which is positive, and for every \( A = \text{diag}(\lambda_1, \ldots, \lambda_k) \), where \( \lambda_1 \geq \cdot \cdot \cdot \geq \lambda_k \geq 0 \), the matrix \( UAV^T \) is nonnegative. Such pairs will be called pairs of matching Soules bases. If \( A = UAV^T \), where \( (U, V) \) is a matching Soules pair, and \( A \) is as above, then \( A \) is a nonnegative matrix with the diagonal elements of \( A \) as its singular values. If \( m = n \) and \( U = V \), then \( A \) is a symmetric Soules matrix. Other matching Soules pairs generate matrices \( A \) which are non-square, or square and not symmetric. At the end of Section 3 we discuss the sign pattern of the Moore–Penrose generalized inverse of any nonnegative matrix generated by a matching Soules pair.

First we recall the description of Soules basis matrices. The following terminology and notations will be used: \( \langle n \rangle = \{1, \ldots, n\} \). For a vector \( x \in \mathbb{R}^n \), \( \|x\| \) denotes the Euclidean norm of \( x \), and

\[
\text{supp } x = \{1 \leq i \leq n | x_i \neq 0 \}, \\
\text{supp}_+ x = \{1 \leq i \leq n | x_i > 0 \}, \\
\text{supp}_- x = \{1 \leq i \leq n | x_i < 0 \}.
\]

\(^1\) The definition here slightly deviates from the one in [2].
If $\alpha$ is an ordered subset of $\langle n \rangle$, we denote by $x[\alpha]$ the vector obtained from $x$ by erasing all entries $x_i$, $i \notin \alpha$. $A^{(i)}$ denotes the $i$th column of the matrix $A$.

A sequence of partitions $\Pi_1, \ldots, \Pi_k$ of $\langle n \rangle$ will be called a sequence of $S$-partitions of $\langle n \rangle$ if for every $1 \leq l \leq k$, $\Pi_l$ is a partition of $\langle n \rangle$ into $l$ (nonempty) subsets, $\{\pi_{l,1}, \ldots, \pi_{l,l}\}$, and partition $\Pi_l$ is obtained from the partition $\Pi_{l-1}$ by splitting one of the partition sets of $\Pi_{l-1}$ into two sets, and keeping the rest of the partition sets unchanged. We will call the two partition sets of $\Pi_l$ obtained by the splitting the distinguished partition sets of $\Pi_l$, and denote them also by $\gamma_l$ and $\delta_l$. Given a positive vector $x \in \mathbb{R}^n$ and an $S$-partition sequence $\Pi_1, \ldots, \Pi_k$, a vector $z \in \mathbb{R}^n$ will be called a $\{\Pi_l, x\}$-vector if $\supp_+ z = \gamma_l$, $\supp_- z = \delta_l$, $z[\gamma_l]$ is a positive scalar multiple of $x[\gamma_l]$, and $z[\delta_l]$ is a negative scalar multiple of $x[\delta_l]$.

We can now describe all Soules basis matrices. Every such matrix $R$ is determined by a positive unit vector $x$, and a sequence $\Pi_1, \ldots, \Pi_n$ of $S$-partitions of $\langle n \rangle$. The first column of $R$ is $x$, and for $1 \leq l \leq n$ the column $R^{(l)}$, $1 \leq l \leq n$ (the signs in the $l$th column depend on which of the two distinguished sets of $\Pi_l$ was named $\gamma_l$, and $\delta_l$).

We will call a matrix $V \in \mathbb{R}^{n \times k}$ a $k$-partial Soules basis matrix if $V$ has orthonormal columns, its first column is positive, and $VAV^T$ is nonnegative for every nonnegative diagonal matrix $A \in \mathbb{R}^{k \times k}$ with nonincreasing diagonal elements. Obviously, the first $k$ columns of any $n \times n$ Soules basis matrix form a partial Soules basis matrix. By the construction of Soules basis matrices in [3] it is quite clear that any $k$-partial Soules basis matrix consists of the first $k$ columns of some Soules basis matrix (and it clearly follows from Lemma 2 below, when applied to the case $P = Q = V$). That is, a $k$-partial Soules basis matrix is determined, in the manner described in the previous paragraph, by the positive unit vector $x$ which is its first column, and by a sequence of $S$-partitions $\Pi_1, \ldots, \Pi_k$ of $\langle n \rangle$.

Given a partial Soules basis matrix $V \in \mathbb{R}^{n \times k}$ we may generate a $k \times k$ Soules basis matrix $\phi_k^p(V)$ as follows: Let $\Pi_k = \{\pi_{k,1}, \ldots, \pi_{k,k}\}$ be the $k$th partition in a sequence of $S$-partitions determining $V$. For every $1 \leq j \leq k$, $V^{(j)}[\pi_{k,i}]$ is either positive, or negative, or the zero vector. Let $u_{ij} = \|V^{(j)}[\pi_{k,i}]\|$ if $V^{(j)}[\pi_{k,i}]$ is positive or zero, and $u_{ij} = -\|V^{(j)}[\pi_{k,i}]\|$ if $V^{(j)}[\pi_{k,i}]$ is negative. Set $\phi_k^p(V) = \{u_{ij}\}_{i,j=1}^k$. The matrix $\phi_k^p(V)$ is then a $k \times k$ Soules basis matrix. We will say that $\phi_k^p(V)$ is obtained from $V$ by shrinking. Observe that $\phi_k^p(V)$ depends on the numbering of the partition sets of $\Pi_k$. Given $V$, $\phi_k^p(V)$ is only unique up to a permutation of its rows. It is also important to note that there exists a nonnegative matrix $S$, with exactly one positive element in each row, such that $S\phi_k^p(V) = V$. (supp$S^{(j)} = \pi_{k,j}$ and $S^{(j)}[\pi_{k,j}] = x_{[j]}/\|x_{[j]}\|$,

where $x_{[j]} = V^{(j)}[\pi_{k,j}]$. For more details see [8]).

We conclude the introduction with a few more terms and notations: For a vector $x$, $|x|$ denotes the vector whose entries are the absolute values of the elements of $x$. A positive diagonal matrix is a diagonal matrix with all diagonal entries positive. The number of elements in a finite set $\alpha$ is denoted by $|\alpha|$. $I_r$ denotes the $r \times r$ identity matrix.
2. Double Soules pairs

In this section we characterize all double Soules pairs \((P, Q)\). We first observe that if \(R\) is a Soules basis matrix, then for any nonsingular diagonal matrix \(D\) and any positive diagonal matrix \(E\), the matrices \(P = ERD\) and \(Q = E^{-1}RD^{-1}\) constitute a double Soules pair, since
\[
PAQ^T = (ERD)A(D^{-1}R^TE^{-1}) = E(RAR^T)E^{-1}.
\]
Given two positive vectors \(p\) and \(q\) in \(\mathbb{R}^n\) such that \(q^Tp = 1\) and a sequence \(\Pi_1, \ldots, \Pi_n\) of \(S\)-partitions of \(\langle n \rangle\), we obtain a double Soules pair \((P, Q)\) as follows: Let \(x\) be the vector whose \(i\)th entry is \(x_i = \sqrt{p_iq_i}\), \(i = 1, \ldots, n\); Let \(R\) be a Soules basis matrix determined by \(x\) and the given sequence of \(S\)-partitions; Let \(e_i = \sqrt{p_i/q_i}\), \(i = 1, \ldots, n\), and \(E = \text{diag}(e_1, \ldots, e_n)\). Then the pair \((P, Q)\) where \(P = ER\) and \(Q = E^{-1}R\) is a double Soules pair with \(p\) as the first column of \(P\) and \(q\) as the first column of \(Q\).

We will show that every double Soules pair \((P, Q)\) is of the above form. That is, \(P = ERD\) and \(Q = E^{-1}RD^{-1}\) for some Soules basis matrix \(R\) and positive diagonal matrices \(E\) and \(D\). At the end of the section we remark on some implications of this characterization.

In the proof of some of the observations above we shall need the following lemma:

**Lemma 1.** Let \(x, y, u, v \in \mathbb{R}^n\), \(x\) and \(y\) positive. Suppose
\[
\begin{bmatrix} x & u \\ y & v \end{bmatrix} \begin{bmatrix} y & v \\ x & u \end{bmatrix} \geq 0, \tag{1}
\]
\[
\begin{bmatrix} y & v \end{bmatrix} \begin{bmatrix} x & u \end{bmatrix} = I_2. \tag{2}
\]
Then

(a) \(\text{supp}_+u = \text{supp}_+v\), \(\text{supp}_-u = \text{supp}_-v\), and (using \(\alpha\) to denote the first set and \(\beta\) to denote latter) \(\alpha \cup \beta = \langle n \rangle\).

(b) There exist positive numbers \(s\) and \(t\) such that
\[
\begin{align*}
  u[\alpha] &= sx[\alpha], \\
  u[\beta] &= -tx[\beta],
\end{align*}
\]
\[
\begin{align*}
  v[\alpha] &= \frac{1}{t}y[\alpha], \\
  v[\beta] &= -\frac{1}{s}y[\beta],
\end{align*}
\]
and
\[
\frac{t}{s} = \frac{y[\alpha]^Tx[\alpha]}{y[\beta]^Tx[\beta]}. \tag{3}
\]

(c) There exist positive vectors \(a, b \in \mathbb{R}^{|\alpha|}, c, d \in \mathbb{R}^{|\beta|}\) such that \(c^Ta = 1\) and \(d^Tb = 1\) and
\[
\begin{bmatrix} x & u \end{bmatrix} \begin{bmatrix} y & v \end{bmatrix}^T
\]
is a direct sum of \(ac^T\) and \(bd^T\). Moreover, \(a, b, c, d\) are scalar multiples of \(x[\alpha], x[\beta], y[\alpha]\) and \(y[\beta]\), respectively.

**Proof.** Conditions (1) and (2) mean that
\[
\begin{align*}
  y^Tx &= 1, \tag{3} \\
  y^Tu &= 0, \tag{4} \\
  v^Tu &= 1, \tag{5} \\
  v^Tx &= 0. \tag{6}
\end{align*}
\]
and
\[ xy^T \geq -uv^T. \] (7)

Let
\[ \alpha_1 = \{ i \in \langle n \rangle | u_i > 0 \text{ and } v_i > 0 \}, \]
\[ \alpha_2 = \{ i \in \langle n \rangle | u_i < 0 \text{ and } v_i < 0 \}, \]
\[ \alpha_3 = \{ i \in \langle n \rangle | u_i > 0 \text{ and } v_i < 0 \}, \]
\[ \alpha_4 = \{ i \in \langle n \rangle | u_i < 0 \text{ and } v_i > 0 \}, \]
\[ \alpha_5 = \{ i \in \langle n \rangle | u_i > 0 \text{ and } v_i = 0 \}, \]
\[ \alpha_6 = \{ i \in \langle n \rangle | u_i < 0 \text{ and } v_i = 0 \}, \]
\[ \alpha_7 = \{ i \in \langle n \rangle | u_i = 0 \text{ and } v_i > 0 \}, \]
\[ \alpha_8 = \{ i \in \langle n \rangle | u_i = 0 \text{ and } v_i < 0 \}, \]
\[ \alpha_9 = \{ i \in \langle n \rangle | u_i = 0 \text{ and } v_i = 0 \}. \]

Some of these sets may be empty, but (4) and (6) imply that \( \text{supp}_+ u, \text{supp}_- u, \text{supp}_+ v \) and \( \text{supp}_- v \) are not empty. That is,
\[ \alpha_1 \cup \alpha_3 \cup \alpha_5 \neq \emptyset, \] (8)
\[ \alpha_2 \cup \alpha_4 \cup \alpha_6 \neq \emptyset, \] (9)
\[ \alpha_1 \cup \alpha_4 \cup \alpha_7 \neq \emptyset, \] (10)
\[ \alpha_2 \cup \alpha_3 \cup \alpha_8 \neq \emptyset. \] (11)

And by (5),
\[ \alpha_1 \cup \alpha_2 \neq \emptyset. \] (12)

For any vector \( z \in \mathbb{R}^n \), we denote \( z_{[i]} = |z_{\alpha_i}| \). For the sake of clarity, we may assume that for each \( i \) the set \( \alpha_i \) consists of consecutive integers, and \( \alpha_{i+1} \) consists of subsequent consecutive integers. (This is equivalent to row permutation of the matrices \([x \ u]\) and \([y \ v]\), and simultaneous permutation of rows and columns of the product matrices in (1) and (2).) That is,
\[
\begin{align*}
\end{align*}
\]

Eqs. (3)–(7) then translate to
\[
\sum_{i=1}^{9} y_{[i]}^T x_{[i]} = 1, \tag{13}
\]
\[
\sum_{i=1,3,5} y_{[i]}^T u_{[i]} = \sum_{i=2,4,6} y_{[i]}^T u_{[i]}, \tag{14}
\]
If $\alpha_1 \neq \emptyset$, consider the inequalities in (17), for $i = 1$, $j = 2, 3, 8$, and multiply each of them by $v_{[1]}^T$ on the left and $x_{[j]}$ from the right, to obtain

$$v_{[1]}^T x_{[1]} y_{[j]}^T x_{[j]} \geq v_{[1]}^T u_{[1]} v_{[j]}^T x_{[j]}, \quad j = 2, 3, 8.$$  

Summing the three inequalities yields (using (15))

$$v_{[1]}^T x_{[1]} \sum_{j=2,3,8} y_{[j]}^T x_{[j]} \geq v_{[1]}^T u_{[1]} \sum_{j=2,3,8} v_{[j]}^T x_{[j]} = v_{[1]}^T u_{[1]} \sum_{j=1,4,7} v_{[j]}^T x_{[j]} \geq v_{[1]}^T u_{[1]} v_{[1]}^T x_{[1]}.$$  

Hence if $\alpha_1 \neq \emptyset$ we have

$$\sum_{j=2,3,8} y_{[j]}^T x_{[j]} \geq v_{[1]}^T u_{[1]}.$$  

If in addition $\alpha_2 = \emptyset$, (20) implies that

$$1 = \sum_{j=1}^{9} y_{[j]}^T x_{[j]} \geq \sum_{j=2,3,8} y_{[j]}^T x_{[j]} \geq v_{[1]}^T u_{[1]} \geq v_{[1]}^T u_{[1]} - \sum_{i=3,4} v_{[i]}^T u_{[i]} = 1,$$  

where the right equality is (16), for $\alpha_2 = \emptyset$. But then all the inequalities in (21) are equalities. In particular, the equality in the left inequality means that $\alpha_j = \emptyset$ for $j \neq 2, 3, 8$, which contradicts (10).

We have shown that if $\alpha_1 \neq \emptyset$ then also $\alpha_2 \neq \emptyset$. Similarly, if $\alpha_2 \neq \emptyset$, consider the inequalities (18), for $i = 2, j = 1, 4, 7$, multiply by $v_{[2]}^T$ on the left and $x_{[j]}$ on the right and sum the three inequalities to obtain

$$\sum_{j=1,4,7} y_{[j]}^T x_{[j]} \geq v_{[2]}^T u_{[2]}.$$  

Then use (16) to deduce that if $\alpha_2 \neq \emptyset$ then also $\alpha_1 \neq \emptyset$.

By (12) we conclude that both $\alpha_1$ and $\alpha_2$ are nonempty. Eqs. (20) and (22) then imply that

$$1 = \sum_{j=1}^{9} y_{[j]}^T x_{[j]} \geq \sum_{j=2,3,8} y_{[j]}^T x_{[j]} \geq v_{[1]}^T u_{[1]} \geq v_{[1]}^T u_{[1]} - \sum_{i=3,4} v_{[i]}^T u_{[i]} = 1,$$  

where the right equality is (23), for $i \neq 2, 3, 4, 7, 8$, by the equality in the left equality, and $\alpha_3 = \alpha_4 = \emptyset$, by the equality in the last inequality. The equality in

$$\sum_{i=1,4,7} v_{[i]}^T x_{[i]} = \sum_{i=1,4,7} v_{[i]}^T x_{[i]},$$  

$$\sum_{i=1,2} v_{[i]}^T u_{[i]} - \sum_{i=3,4} v_{[i]}^T u_{[i]} = 1.$$  

Thus all the inequalities in (23) are equalities. In particular $\alpha_i = \emptyset$, for $i \neq 1, 2, 3, 4, 7, 8$, by the equality in the left equality, and $\alpha_3 = \alpha_4 = \emptyset$, by the equality in the last inequality.
the middle inequality implies equality in (20) and (22). Equality in (20) in turn implies equality in 
the last inequality of (19), and therefore \( \alpha_7 = \emptyset \). Similarly, equality in (22) implies that \( \alpha_8 = \emptyset \). Hence
\[
\supp u = \alpha_1 = \supp v, \quad \supp u = \alpha_2 = \supp v,
\]
and \( \alpha_1 \cup \alpha_2 = \langle n \rangle \). This proves (a).

By the positivity of the vectors \( x_1 \) and \( v_2 \), the equality in (20) also implies equality in (17), 
for \( i = 1 \) and \( j = 2 \). It follows that \( u_{11} = s x_1 \), for some \( s > 0 \), and \( v_{22} = \frac{1}{t} y_2 \). Similarly,
equality in (22) implies equality in (18), for \( i = 2 \) and \( j = 1 \), and therefore \( u_{22} = t x_2 \), for some
\( t > 0 \), and \( v_{11} = \frac{1}{t} y_1 \). Eq. (14) now reads \( y_{11}^T u_{11} = y_{22}^T u_{22} \), that is
\[
sv_{11}^T x_1 = tv_{22}^T x_2.
\]
Hence we get that
\[
\frac{t}{s} = \frac{y_{11}^T x_1}{y_{22}^T x_2},
\]
and (b) is proved.

Finally,
\[
\begin{bmatrix} x & u \end{bmatrix} \begin{bmatrix} y & v \end{bmatrix}^T = \begin{bmatrix} x_1 & u_1 \\ x_2 & -u_2 \end{bmatrix} \begin{bmatrix} y_{11}^T & y_{12}^T \\ v_{11}^T & -v_{12}^T \end{bmatrix} = \begin{bmatrix} x_1 y_{11}^T + u_1 v_{11}^T & x_1 y_{12}^T - u_1 v_{12}^T \\ x_2 y_{11}^T - u_2 v_{11}^T & x_2 y_{12}^T + u_2 v_{12}^T \end{bmatrix}
\]
But
\[
x_{11} y_{11}^T + u_{11} v_{11}^T = \left( 1 + \frac{s}{t} \right) x_1 y_{11}^T = \left( 1 + \frac{y_{12}^T x_2}{y_{11}^T x_1} \right) x_1 y_{11}^T = \frac{x_{11} y_{11}^T}{y_{11}^T x_{11}}
\]
Similarly
\[
x_{22} y_{22}^T + u_{22} v_{22}^T = \frac{x_{22} y_{22}^T}{y_{22}^T x_{22}}
\]
and
\[
x_{11} y_{11}^T - u_{11} v_{12}^T = 0, \quad x_{22} y_{22}^T - u_{22} v_{11}^T = 0.
\]
To finish the proof of part (c) take
\[
a = \frac{x_{11}}{\sqrt{y_{11}^T x_{11}}}, \quad b = \frac{x_{22}}{\sqrt{y_{22}^T x_{22}}}, \quad c = \frac{y_{11}}{\sqrt{y_{11}^T x_{11}}}, \quad d = \frac{y_{22}}{\sqrt{y_{22}^T x_{22}}}.
\]

From Lemma 1 we deduce:
Lemma 2. If \( P, Q \in \mathbb{R}^{n \times k} \) have positive first columns, \( P^{(1)} = p \) and \( Q^{(1)} = q \) and, for every \( 1 \leq r \leq k \),

\[
\begin{bmatrix}
P^{(1)} & \cdots & P^{(r)} \\
Q^{(1)} & \cdots & Q^{(r)}
\end{bmatrix}^T \begin{bmatrix}
Q^{(1)} & \cdots & Q^{(r)} \\
P^{(1)} & \cdots & P^{(r)}
\end{bmatrix} \geq 0, \tag{24}
\]

Then there exist a sequence \( d_1 = 1, d_2, \ldots, d_k \) of positive numbers and an \( S \)-partition sequence \( \Pi_1, \ldots, \Pi_k \) of \( \begin{pmatrix} n \end{pmatrix} \) such that, for each \( i = 1, \ldots, k \), the \( i \)th column of \( P \) is a \( \{\Pi_i, p\} \)-vector, the \( i \)th column of \( Q \) is a \( \{\Pi_i, q\} \)-vector, such that for \( i = 1, \ldots, k \),

\[
\begin{align*}
P^{(i)}[\gamma_i] &= d_i \sqrt{q[\delta_i]^T p[\delta_i] / q[\gamma_i]^T p[\gamma_i]}, \\
P^{(i)}[\delta_i] &= -d_i \sqrt{q[\gamma_i]^T p[\gamma_i] / q[\delta_i]^T p[\delta_i]}, \\
Q^{(i)}[\gamma_i] &= \frac{1}{d_i} \sqrt{q[\delta_i]^T p[\delta_i] / q[\gamma_i]^T p[\gamma_i]}, \\
Q^{(i)}[\delta_i] &= -\frac{1}{d_i} \sqrt{q[\gamma_i]^T p[\gamma_i] / q[\delta_i]^T p[\delta_i]}, \tag{26}
\end{align*}
\]

where \( \gamma_i \) and \( \delta_i \) are the distinguished sets of partition \( \Pi_i \).

Moreover, \( [P^{(1)} \cdots P^{(k)}] [Q^{(1)} \cdots Q^{(k)}]^T \) is a direct sum of \( k \) matrices \( a[i]b[i]^T \), \( i = 1, \ldots, k \), where \( a[i], b[i] \in \mathbb{R}^{n \times k} \) are positive scalar multiples of the vectors \( p[n \times \Pi_i] \) and \( q[n \times \Pi_i] \), respectively, and \( \Pi_i = \{n \times \Pi_{i-1}, \ldots, \Pi_{i-1}, \Pi_{i+1}, \ldots, \Pi_k\} \).

Proof. By induction on \( k \). For \( k = 2 \), this is Lemma 1, where we write \( \gamma_2 \) for \( \alpha \) and \( \delta_2 \) for \( \beta \), and take \( \Pi_2 = \{\gamma_2, \delta_2\} \). Note that in part (b) of the lemma we may write

\[
s = d_2 \sqrt{q[\delta_2]^T p[\delta_2] / q[\gamma_1]^T p[\gamma_1]},
\]

for some positive \( d_2 \), and obtain that

\[
t = d_2 \sqrt{q[\gamma_1]^T p[\gamma_1] / q[\delta_2]^T p[\delta_2]}.
\]

Now assume the result holds for \( k - 1 \). By the induction hypothesis, \( [P^{(1)} \cdots P^{(k-1)}] \)

\[
\begin{bmatrix}
P^{(1)} & \cdots & P^{(k-1)} \\
Q^{(1)} & \cdots & Q^{(k-1)}
\end{bmatrix}^T
\]

is a direct sum of \( k - 1 \) matrices \( a[i]b[i]^T \), \( i = 1, \ldots, k - 1 \), where \( a[i], b[i] \) are positive vectors such that \( b[i]^T a[i] = 1 \) and \( a[i], b[i] \in \mathbb{R}^{n \times \Pi_{k-1,i}} \), where \( \Pi_{k-1} = \{n \times \Pi_{k-1,1}, \ldots, \Pi_{k-1,k-1}\} \). Since \( P^{(k)} \) is orthogonal to the positive vector \( q \) and \( Q^{(k)} \) is orthogonal to the positive \( p \), each of \( P^{(k)} \) and \( Q^{(k)} \) has both positive and negative entries. The matrix

\[
\begin{bmatrix}
P^{(1)} & \cdots & P^{(k)} \\
Q^{(1)} & \cdots & Q^{(k)}
\end{bmatrix}^T
\]

\[
= [P^{(1)} \cdots P^{(k-1)}] [Q^{(1)} \cdots Q^{(k-1)}]^T + P^{(k)} Q^{(k)^T}
\]
is nonnegative. Hence if \( i \) and \( j \) belong to different partition sets in \( \Pi_{k-1} \), then necessarily the product of the \( i \)th entry of \( P^{(k)} \) and the \( j \)th entry of \( Q^{(k)} \) must be nonnegative. Thus if the \( i \)th entry of \( P^{(k)} \) is positive, then \( \text{supp}_+ Q^{(k)} \) is contained in the same partition set of \( \Pi_{k-1} \) as \( i \). This in turn implies that all of \( \text{supp}_+ P^{(k)} \) is contained in that same partition set. Similarly, \( \text{supp}_- P^{(k)} \) and \( \text{supp}_- Q^{(k)} \) are contained in the same partition set. But either \( \text{supp}_+ Q^{(k)} \cap \text{supp}_+ P^{(k)} = \emptyset \) or \( \text{supp}_- Q^{(k)} \cap \text{supp}_- P^{(k)} = \emptyset \) since \( Q^{(k)T} P^{(k)} = 1 \). This implies that \( \text{supp} P^{(k)} \) and \( \text{supp} Q^{(k)} \) are both contained in the same partition set of \( \Pi_{k-1} \), say \( \pi_{k-1, i} \). Applying Lemma 1 to \( x = a_{[i]} \), \( y = b_{[i]} \), \( u = P^{(k)}[\pi_{k-1, i}] \), and \( v = Q^{(k)}[\pi_{k-1, i}] \) yields the required result. □

We can now state:

**Theorem 1.** A pair \((P, Q)\) of \( n \times n \) matrices is a double Soules pair if and only if there exist an \( n \times n \) Soules matrix \( R \) and positive diagonal \( n \times n \) matrices \( E \) and \( D \) such that \( P = ERD \) and \( Q = E^{-1}RD^{-1} \).

**Proof.** The if part was observed at the beginning of the section. The only if part: As mentioned in [1, Observation 3.2], \( PAP^T \geq 0 \) for every \( n \times n \) nonnegative diagonal matrix \( A \) with nonincreasing diagonal elements if and only if (24) holds for every \( 1 \leq r \leq n \). Given a double Soules pair \((P, Q)\) with first columns \( p \) and \( q \), respectively, apply Lemma 2 (with \( k = n \)). Now let \( D = \text{diag}(d_1, \ldots, d_n) \) and \( E = \text{diag}(e_1, \ldots, e_n) \), where \( e_i = \sqrt{\frac{p_i}{q_i}} \). It is easy to see that \( P = ERD \) and \( Q = E^{-1}RD^{-1} \), where \( R \) is a Soules basis matrix determined by the first column \( x \) whose entries are \( x_i = \sqrt{p_iq_i} \), \( i = 1, \ldots, n \), and the sequence of \( S \)-partitions \( \Pi_1, \ldots, \Pi_n \) obtained in the lemma. □

Let \( A = PAP^T \) be generated by a double Soules pair \((P, Q)\) and a diagonal matrix \( A \) with nonincreasing diagonal elements. Theorem 1 implies that \( A \) is diagonally similar to a symmetric matrix \( B = BAR^T \) for some Soules basis matrix \( R \). In fact, \( A = EBE^{-1} \), where \( E \) is a positive diagonal matrix. This observation immediately implies that many of the properties of Soules matrices hold also for double Soules matrices. Here are some examples. We assume now that \( A \) and \( B \) are as above, with \( A \) nonnegative (that is, \( A \) is a double Soules matrix and the diagonally similar \( B \) is a Soules matrix).

- In [3] it was proved that if \( X \) is a nonsingular Soules matrix then for every nonincreasing function \( f : (0, \infty) \rightarrow (0, \infty) \) the matrix \( f(X) \) is a nonsingular \( M \)-matrix, and hence if \( X \) is nonsingular Soules matrix then all the powers of its inverse are \( M \)-matrices. In [2] the same result was proved for double Soules matrices. In view of our observation we can now deduce the result for double Soules matrices from the one on Soules matrices, since \( f(A) = Ef(B)E^{-1} \), where \( E \) is a positive diagonal matrix.

Matrices all of whose powers are irreducible nonnegative \( M \)-matrices were studied in [5] and named **MMA**-matrices. It was shown there that every **MMA**-matrix is diagonally similar to a symmetric **MMA**-matrix by a positive diagonal matrix. As mentioned in [3], the results of [3] and [4] combined yield that the nonsingular symmetric **MMA**-matrices are exactly the inverses of irreducible nonsingular symmetric Soules matrices. The observation that the double Soules matrices are the matrices which are diagonally similar (by a positive diagonal matrix) to symmetric Soules matrices shows that the nonsingular **MMA**-matrices are the inverses of irreducible nonsingular double Soules matrices.
In [3] it was proved that for any nonsingular Soules matrix $X$, there exists a positive diagonal matrix $D$ such that $DXD$ is a strictly ultrametric matrix. When applying this to $B$, we obtain that if the double Soules matrix $A$ is nonsingular, then there exist positive diagonal matrices $D_1$ and $D_2$ such that $D_1AD_2$ is a strictly ultrametric matrix. ($D_1 = DE$ and $D_2 = E^{-1}D$, where $DBD$ is strictly ultrametric.) (see [3] for the symmetric Soules case, definition and references, and some more references in [2]).

In [8] it was shown that if $X$ is a Soules matrix of rank $k$, then $X = CC^T$, where $C \in \mathbb{R}^{n \times k}$ nonnegative matrix. This implies, in view of Theorem 1, that if $A$ is an $n \times n$ double Soules matrix of rank $k$, then there exist nonnegative matrices $V \in \mathbb{R}^{n \times k}$ and $H \in \mathbb{R}^{k \times n}$ such that $A = VH$ (that is, the nonnegative rank of $A$ is equal to its rank). Indeed, $A = EBE^{-1}$, where $B$ is a symmetric Soules matrix, and $B = CC^T$, where $C \in \mathbb{R}^{n \times k}$ nonnegative matrix. So $A = VH$, where $V = EC$ and $H = CE^{-1}$. We add that by [8] an explicit factorization may be given for $B$: Take $C = RA_k\phi^m_k(R_k)^T$, where $A_k$ consists of the first $k$ columns of $A$, and $R_k$ consists of the first $k$ columns of $R$. This yields an explicit factorization of $A$.

Another implication of the characterization in Theorem 1: If $(P, Q)$ is a double Soules pair and $A$ is a diagonal matrix with nonincreasing diagonal elements (not necessarily nonnegative), then the off-diagonal elements in $A = PAQ^T$ are nonnegative. (Since this is known to be true for $RAR^T$, where $R$ is a Soules basis matrix.) The case when the diagonal elements are also nonnegative is of interest – one may hope that such double Soules matrices can be used in studying the nonnegative inverse eigenvalue problem. Unfortunately, the fact that such $A$ is diagonally similar to a symmetric nonnegative matrix generated by Soules basis means that no new spectrums are generated this way.

3. Matching Soules bases

In this section we consider the following question, which is a sort of generalization of Soules matrices to the non-square case (and yields also some new matrices in the square case):

**Question 1.** Let $m$, $n$, and $k$ be integers, $k \leq \min(m, n)$. Characterize all pairs of matrices $(U, V)$ such that: (i) $U \in \mathbb{R}^{m \times k}$ and $V \in \mathbb{R}^{n \times k}$; (ii) each of the two matrices has orthonormal columns and each has a positive first column; and (iii) for every nonnegative diagonal matrix $A \in \mathbb{R}^{k \times k}$ with nonincreasing diagonal elements, the matrix $A = UAV^T$ is nonnegative. We will call such a pair $(U, V)$ a pair of matching Soules ($k$-)bases.

If $(U, V)$ is such a pair, then it can be used to construct an $m \times n$ nonnegative matrix with any given set of singular values, up to $k$ of which are nonzero. Any matrix $A$ thus generated has the property that for every $1 \leq r \leq k$, the best rank $r$ approximation to $A$ is a nonnegative matrix.

**Theorem 2.** Let $U \in \mathbb{R}^{m \times k}$ and $V \in \mathbb{R}^{n \times k}$ be two matrices with orthonormal columns and each with a positive first column. Then $(U, V)$ is a pair of matching Soules bases if and only if $U$ and $V$ are partial Soules basis matrices and $\phi^n_k(U) = P\phi^n_k(V)$ for some permutation matrix $P \in \mathbb{R}^{k \times k}$. 
Proof. If $U$ and $V$ are partial Soules basis matrices, then they can be shrunk to $\phi_k^m(U)$ and $\phi_k^n(V)$, respectively. There exist nonnegative matrices $S$ and $T$, with one positive element in each row, such that $U = S\phi_k^m(U)$ and $V = T\phi_k^n(V)$. Hence if $\phi_k^m(U) = P\phi_k^n(V)$, for some permutation matrix $P$, then we have that

$$UAV^T = (SP)(\phi_k^m(V)A\phi_k^m(V)^T)T^T,$$

is a nonnegative matrix, for every nonnegative diagonal matrix $A$ (with nonincreasing elements), since $\phi_k^m(U)$ is a Soules basis matrix and $S$ and $T$ are nonnegative.

If $(U, V)$ is a pair of matching Soules $k$-bases, then for every diagonal nonnegative $A \in \mathbb{R}^{k \times k}$ with nonincreasing diagonal elements, $UAV^T = (U\sqrt{A}V^T)(U\sqrt{A}V^T)^T$ is nonnegative. Hence $U$ is necessarily a partial Soules basis matrix and, similarly, for $V$. Now consider $\phi_k^m(U)$ and $\phi_k^n(V)$ and let $S$ and $T$ be nonnegative matrices such that $U = S\phi_k^m(U)$ and $V = T\phi_k^n(V)$. Since $UAV^T = S(\phi_k^m(U)A\phi_k^m(V)^T)T^T$ (and each row of $S$ and of $T$ has a unique positive element), the matrix $\phi_k^m(U)A\phi_k^m(V)^T$ is nonnegative for every nonnegative diagonal matrix $A$ with nonincreasing elements. Since $\phi_k^m(U)$ and $\phi_k^n(V)$ are orthogonal $k \times k$ matrices, this implies that $\phi_k^m(U) = P\phi_k^n(V)$ for some permutation matrix $P$ (see discussion of Question 1.3 in [2]).

Remark 1. If $U \in \mathbb{R}^{m \times k}$ is a partial Soules basis matrix, one can construct a matching partial Soules matrix $V \in \mathbb{R}^{n \times k}$ as follows: Shrink $U$ to $\phi_k^m(U)$, and let $u = [u_1, \ldots, u_k]^T$ be the first column of $\phi_k^m(U)$. Now expand $\phi_k^m(U)$ to a matrix $V$: Choose $k$ positive vectors $x_{[1]}$, $\ldots$, $x_{[k]}$, of various lengths which sum up to $n$, and such that $\|x_i\| = u_i$, $i = 1, \ldots, k$. Then let

$$V = \begin{bmatrix}
\frac{x_{[1]}}{\|x_{[1]}\|} & 0 & \cdots & 0 \\
0 & \frac{x_{[2]}}{\|x_{[2]}\|} & \cdots & 0 \\
0 & 0 & \cdots & \frac{x_{[k]}}{\|x_{[k]}\|}
\end{bmatrix} \phi_k^m(U).$$

All possible matching $V$’s may be obtained by choosing different $x_{[i]}$’s, and by permuting the rows of the matrix $V$. For example, if

$$U = \begin{bmatrix}
\frac{1}{2} & \frac{1}{2} & \frac{1}{2} \\
\frac{1}{2} & \frac{1}{2} & \frac{1}{2} \\
\frac{1}{2} & \frac{1}{2} & \frac{1}{2}
\end{bmatrix},$$

then we may take

$$V = \begin{bmatrix}
\frac{\sqrt{3}}{2\sqrt{5}} & \frac{1}{2\sqrt{5}} & \frac{\sqrt{3}}{2\sqrt{5}} \\
\frac{\sqrt{3}}{2\sqrt{5}} & \frac{1}{2\sqrt{5}} & \frac{\sqrt{3}}{2\sqrt{5}} \\
\frac{1}{\sqrt{10}} & \frac{\sqrt{3}}{2\sqrt{10}} & \frac{3}{2\sqrt{10}}
\end{bmatrix}.$$
We conclude the paper with two observations on nonnegative matrices generated by matching Soules pairs, which follow from the proof of Theorem 2:

- If \( U = V \) is a partial Soules basis matrix, then \((U, V)\) is a matching Soules pair, and a matrix
  \[ A = UAV^T \]
  is a usual symmetric Soules matrix, with both eigenvalues and singular values equal to the diagonal elements of \(A\).

- If \( m = n = k \), then \( \phi_i^m(U) = U \) and \( \phi_i^n(V) = V \), hence \( U = PV \) for some permutation matrix
  \( P \), and any nonnegative matrix generated by the matching Soules pair \((U, V)\) is a row-permutation
  of a (symmetric) Soules matrix.

- Let \( A = UAV^T \), where \((U, V)\) is a matching Soules pair, \( U \in \mathbb{R}^{m \times k} \) and \( V \in \mathbb{R}^{n \times k} \), and \( A \) is
  a nonnegative diagonal matrix with nonincreasing diagonal elements. If rank \( A = r \), we may
  assume that \( r = k \) (by deleting the last \( k - r \) columns from \( U \) and \( V \) and the corresponding rows
  and columns of \( A \)). Since \( U \) and \( V \) have orthonormal columns, we get that the Moore–Penrose
  generalized inverse of \( A \) is given by
  \[ A^\dagger = (UAV^T)^\dagger = VA^{-1}U^T. \]

But then for some permutation matrix \( P \),
\[ VA^{-1}U^T = T \phi_i^r(V)A^{-1}(SP\phi_i^n(V))^T = T(\phi_i^n(V)A\phi_i^n(V)^T)^{-1}(SP)^T. \]

Since \( \phi_i^n(V)A\phi_i^n(V)^T \) is a nonsingular symmetric Soules matrix, its inverse is an \( M \)-matrix.
And since \( T \) and \( SP \) are nonnegative matrices, each with exactly one positive entry in each row, we get that \( A^\dagger \) also has a special sign pattern: Suppose the \( r \)th partitions of \( U \) and \( V \) are \( \Pi_r = \{ \pi_{r,1}, \ldots, \pi_{r,r} \} \) and \( \Pi_{\bar{r}} = \{ \bar{\pi}_{r,1}, \ldots, \bar{\pi}_{r,r} \} \), respectively. Let \( m_i = |\pi_{r,i}| \) and \( n_i = |\bar{\pi}_{r,i}| \).
Then, since the columns of \( S \) and \( T \) are supported by the partition sets of \( \Pi_r \) and \( \Pi_{\bar{r}} \), we get that the rows and columns of \( A^\dagger \) can be permuted to obtain an \( r \times r \) block matrix, with the \( i, j \) block of size \( n_i \times m_j \). If \( u \) and \( v \) are the first columns of \( U \) and \( V \), respectively, and \( C = (\phi_i^n(V)A\phi_i^n(V)^T)^{-1} \), then the \( i, j \) block of the permuted \( A^\dagger \) is
\[ c_{ij} v_{[i]} u_{[j]}^T, \]
where \( u_{[j]} = u[\pi_{r,j}] / ||u[\pi_{r,j}]|| \) and \( v_{[i]} = v[\pi_{r,i}] / ||v[\pi_{r,i}]|| \). Thus every nonzero block of \( A^\dagger \)
is of rank 1, and all the entries in the block have the same sign. The sign pattern of the blocks
is that of \( C = (\phi_i^n(V)A\phi_i^n(V)^T)^{-1} \). In particular, the diagonal blocks are positive and the off-
diagonal blocks are nonpositive. This observation applies, in particular, to singular symmetric
Soules matrices \( A \). In that case, \( U = V \) and \( P = I_r \), and \( A^\dagger \) is a symmetric matrix with the
described sign pattern.

As an example for the Moore–Penrose inverse of a matching Soules matrix consider the
matching Soules bases \( U \) and \( V \) given in (27) and (28), respectively, in which \( m_1 = 3, m_2 = 1, \)
\( n_1 = 2, \) and \( n_2 = 2. \) Let \( A = \text{diag}(2, 1) \). Then for
\[ A = UAV^T = \begin{bmatrix}
0.4520 & 0.9036 & 0.07905 & 0.2372 \\
0.4520 & 0.9036 & 0.07905 & 0.2372 \\
0.4520 & 0.9036 & 0.07905 & 0.2372 \\
0.1937 & 0.3873 & 0.3953 & 1.186 \\
\end{bmatrix}, \]

we find that

$$
A^\dagger = \begin{bmatrix}
0.1614 & 0.1614 & 0.1614 & -0.09683 \\
0.3227 & 0.3227 & 0.3227 & -0.1937 \\
-0.03953 & -0.03953 & -0.03953 & 0.2767 \\
-0.1186 & -0.1186 & -0.1186 & 0.8300
\end{bmatrix}.
$$

It is readily seen for $i, j = 1, 2$, that the $i, j$th block of $A^\dagger$ has dimensions $n_i \times m_j$ and is of rank 1. Furthermore, the diagonal blocks are positive matrices, while the off-diagonal blocks are negative matrices.

References