When Can Matrix Query Languages Discern Matrices?

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Abstract

We investigate when two graphs, represented by their adjacency matrices, can be distinguished by means of sentences formed in MATLANG, a matrix query language which supports a number of elementary linear algebra operators. When undirected graphs are concerned, and hence the adjacency matrices are real and symmetric, precise characterisations are in place when two graphs (i.e., their adjacency matrices) can be distinguished. Turning to directed graphs, one has to deal with asymmetric adjacency matrices. This complicates matters. Indeed, it requires to understand the more general problem of when two arbitrary matrices can be distinguished in MATLANG. We provide characterisations of the distinguishing power of MATLANG on real and complex matrices, and on adjacency matrices of directed graphs in particular. The proof techniques are a combination of insights from the symmetric matrix case and results from linear algebra and linear control theory.

2012 ACM Subject Classification Theory of computation → Database query languages (principles); Mathematics of computing → Graph theory

Keywords and phrases matrix query languages, linear algebra, expressive power

Digital Object Identifier 10.4230/LIPIcs.ICDT.2020.12

Acknowledgements I want to thank Lieven Le Bruyn for inspiring discussions and for pointing me to the connections to linear control theory.

1 Introduction

The integration of linear algebra functionalities inside relational database systems is currently high on the agenda [4, 5, 6, 12, 19, 31, 33, 34, 35, 36, 39, 40]. The need for such an integration is due to the increased importance of linear algebra for scalable machine learning and data analytics. From a query language perspective, it is challenging to combine classical relational data operators with linear algebra operators. The Lara language is one such proposal [29] and its connections to classical database query languages has been recently explored [3]. Logics extended with linear algebra operators have been considered as well in an attempt to find logics capturing PTIME and to study the descriptive complexity of linear algebra [15, 16, 17, 18, 22, 26, 27]. An even more basic question is to design a query language for matrices and linear algebra alone. In recent work, a query language for matrices, MATLANG, was introduced in which some basic linear operators are supported [8, 7]. The design of MATLANG is motivated by operations commonly supported by linear algebra packages. It can be seen as a linear algebraic counterpart of the relational algebra on K-relations [9], where K is a semiring representing the domain of matrix entries. We here continue the study of the expressive power of MATLANG. What is known so far is that when MATLANG is regarded as a query language on graphs, i.e., queries in MATLANG take the adjacency matrix of a (directed/undirected) graph as input and return an adjacency matrix, then its expressive power is bounded by aggregate logic with only three non-numerical variables. Furthermore, when asked whether two undirected graphs G and H are *indistinguishable by means of sentences* in MATLANG, denoted by $G \equiv_{\mathsf{MATLANG}} H$, then this precisely corresponds

23rd International Conference on Database Theory (ICDT 2020).
Editors: Carsten Lutz and Jean Christoph Jung; Article No. 12; pp. 12:1–12:18
Leibniz International Proceedings in Informatics
LIPICS Schloss Dagstuhl – Leibniz-Zentrum für Informatik, Dagstuhl Publishing, Germany

to these graphs being C^3-equivalent [20]. Here, C^3 is the three-variable fragment of first-order logic with counting. With a sentence in MATLANG one means a query which returns scalars on input matrices, in analogy with sentences in logic. A more fine-grained analysis of the impact of each of the operators in MATLANG as a graph query language was provided in [20]. In particular, if $\mathcal{L}$ is a subset of the operators in MATLANG, then $\mathsf{ML}(\mathcal{L})$ refers to the fragment of MATLANG supporting only those operators in $\mathcal{L}$. Precise characterisations were obtained for when two *undirected* graphs G and H are indistinguishable by sentences in $\mathsf{ML}(\mathcal{L})$, denoted by $G \equiv_{\mathsf{ML}(\mathcal{L})} H$ [20]. In particular, a fragment $\mathsf{ML}(\mathcal{L})$ was identified such that $G \equiv_{\mathsf{ML}(\mathcal{L})} H$ if and only if $G \equiv_{\mathsf{C}^2} H$, where C^2 is the two-variable fragment of first-order logic with counting. We remark that $G \equiv_{\mathsf{C}^2} H$ is known to correspond to G and H being *fractional isomorphic* [10, 30, 37, 38], i.e., there exists a doubly stochastic matrix (non-negative and rows and columns sum up to one) S such that $A_G \cdot S = S \cdot A_H$, where A_G and A_H denote adjacency matrices of G and H, respectively. In [20], for each fragment $\mathsf{ML}(\mathcal{L})$ a proper class of matrices was identified such that for undirected graphs G and H, $G \equiv_{\mathsf{ML}(\mathcal{L})} H$ if and only if $A_G \cdot X = X \cdot A_H$ for some matrix X in that class. For example, for the fragment corresponding to C^2-equivalence this class consists of all doubly stochastic matrices. Such characterisations enable to assess the expressive power of the fragment $\mathsf{ML}(\mathcal{L})$. Indeed, graph properties expressible by sentences in $\mathsf{ML}(\mathcal{L})$ should be invariant under such transformations X. All of the above relates to undirected graphs only.

It seems natural to ask what changes when *directed* graphs (or *digraphs*, for short) are considered, and this is the focus of this paper. More precisely, we investigate how the operators in MATLANG interact with adjacency matrices of directed graphs. Compared to the undirected graph case, the adjacency matrices are *not necessarily symmetric* anymore (i.e. the entry A_{ij} in a matrix A may be different from entry A_{ji}). As a consequence, one cannot rely on properties of symmetric matrices, the most important being that symmetric matrices are diagonalisable. Some of the results in [20] relied on this. Furthermore, whereas algebraic graph theory provides a comprehensive insight in the properties of undirected graphs, which underly some of the results in [20], this is less so for directed graphs.

To obtain characterisations for digraphs, we are faced with the more general question of when two *general matrices* (complex or real) can be discerned by sentences in our fragments $\mathsf{ML}(\mathcal{L})$. We identify two techniques that allow us to answer this question:

- A technique from linear algebra for testing when two matrices A and B are related by means of an invertible matrix X, i.e., such that $A \cdot X = X \cdot B$ holds. This technique only works for fragments containing the *trace* operator ($\mathsf{tr}(\cdot)$), which takes the sum of the diagonal entries of a matrix, and *complex conjugate transposition* (*), which switches rows and columns, followed by complex conjugation. We describe this technique in detail and apply it for fragments $\mathsf{ML}(\mathcal{L})$ supporting $\mathsf{tr}(\cdot)$ and * in Section 5.
- A technique originating from the study of linear systems in control theory which allows to *reduce* matrices A and B to their so-called *minimal realisations* $\hat{A}$ and $\hat{B}$, for which the existence of an invertible matrix X such that $\hat{A} \cdot X = X \cdot \hat{B}$ holds is guaranteed. We show that this allows to link the original matrices A and B as well, and connect it to indistinguishability by our fragments. Neither trace nor complex conjugate transposition is needed here. We detail this technique and consider fragments without trace or complex conjugate transposition in Section 6.

The main observation is that many of the results from [20] graciously generalise to general matrices and to adjacency matrices of digraphs in particular. This is especially true for fragments including the trace operator. The differences here are subtle and mostly relate to the absence of complex conjugate transposition. This is not surprising. After all, this is the only operator in MATLANG that has access to the possible asymmetry of matrices. For trace-less fragments, the generalisations are less straightforward, due to the minimal realisation approach. We show, however, that the general results reported in this paper collapse to precisely the same results as for the undirected graph case, when *normal* matrices are used (normal matrices A satisfy $A^* \cdot A = A \cdot A^*$ and they are known to inherit most of the properties of symmetric matrices). As a pleasant side-effect, we thus recover results reported in [20] as special cases of the more general approach used in this paper.

2 Background

We denote by $\mathbb{R}$ ($\mathbb{C}$) the set of real (complex) numbers. The set of $m \times n$-matrices over the real (complex) numbers is denoted by $\mathsf{Mat}_{m\times n}(\mathbb{R})$ ($\mathsf{Mat}_{m\times n}(\mathbb{C})$). Vectors are elements of $\mathsf{Mat}_{m\times 1}(\mathbb{R})$ (or $\mathsf{Mat}_{m\times 1}(\mathbb{C})$), or $\mathsf{Mat}_{1\times m}(\mathbb{R})$ (or $\mathsf{Mat}_{1\times m}(\mathbb{C})$). The entries of an $m \times n$-matrix A are denoted by A_{ij}, for $i \in [1, m]$ and $j \in [1, n]$. The entries of a vector v are denoted by v_i, for $i \in [1, m]$. We often identify $\mathsf{Mat}_{1\times 1}(R)$ with $\mathbb{R}$, and $\mathsf{Mat}_{1\times 1}(\mathbb{C})$ with $\mathbb{C}$ and refer to these as scalars. The following classes of matrices are of interest in this paper: *square* matrices (elements in $\mathsf{Mat}_{n\times n}(\mathbb{R})$ or $\mathsf{Mat}_{n\times n}(\mathbb{C})$), *symmetric* matrices (such that $A_{ij} = A_{ji}$ for all i and j), *doubly stochastic* matrices ($A_{ij} \in \mathbb{R}$, $A_{ij} \geq 0$, $\sum_{j=1}^{n} A_{ij} = 1$ and $\sum_{i=1}^{m} A_{ij} = 1$ for all i and j), *doubly quasi-stochastic* matrices ($\sum_{j=1}^{n} A_{ij} = 1$ and $\sum_{i=1}^{m} A_{ij} = 1$ for all i and j), *orthogonal* matrices ($A \in \mathsf{Mat}_{n\times n}(\mathbb{R})$, $A^{\mathsf{t}} \cdot A = I_{n\times n} = A \cdot A^{\mathsf{t}}$, where A^{t} denotes the *transpose* of A obtained by switching rows and columns of A and $I_{n\times n}$ is the *identity matrix* in $\mathsf{Mat}_{n\times n}(\mathbb{R})$), *unitary* matrices ($A \in \mathsf{Mat}_{n\times n}(\mathbb{C})$, $A^* \cdot A = I_{n\times n} = A \cdot A^*$), and *normal* matrices ($A^* \cdot A = A \cdot A^*$). The matrix $J_{m\times n} \in \mathsf{Mat}_{m\times n}(\mathbb{R})$ denotes the matrix consisting of all ones and $O_{m\times n} \in \mathsf{Mat}_{m\times n}(\mathbb{R})$ denotes the zero matrix. We use I, J and O for $I_{n\times n}$, $J_{m\times n}$ and $O_{m\times n}$, respectively, when the dimensions are clear from the context. We assume familiarity with standard concepts of linear algebra and refer to [2, 28] for more background. A *directed graph* or *digraph* $G = (V, E)$ is defined as usual. The *order* of a digraph is its number of vertices. An *adjacency matrix* of a digraph G of order n, denoted by A_G, is an $n \times n$-matrix whose entries $(A_G)_{ij}$ are set to 1 if and only if $(i, j) \in E$, all other entries are set to 0. We regard *undirected* graphs as digraphs such that $(v, w) \in E$ implies that also $(w, v) \in E$, i.e., their adjacency matrices are symmetric. Strictly speaking, to define an adjacency matrix one requires an ordering on the vertices in G. In this paper, any ordering will do and we thus speak about "the" adjacency matrix of a (di)graph.

3 Matrix Query Languages

As described in Brijder et al. [8], matrix query languages can be formalised as compositions of linear algebra operators. By closing such operators under composition "matrix query languages" are formed. More specifically, for a set $\mathcal{L}$ of linear algebra operators $\mathsf{op}_1, \ldots, \mathsf{op}_k$ the corresponding matrix query language is denoted by $\mathsf{ML}(\mathcal{L})$ and consists of expressions formed by the grammar:

$$e := X \mid \mathsf{op}_1(e_1, \ldots, e_{p_1}) \mid \cdots \mid \mathsf{op}_k(e_1, \ldots, e_{p_k}),$$

where X denotes a *matrix variable* which serves to indicate the input to expressions and p_i denotes the number of inputs required by operator op_i. We allow a single matrix variable X in this paper, although some of the results can be generalised to multiple matrix variables.

The semantics of an expression $e(X)$ in $\mathsf{ML}(\mathcal{L})$ is defined inductively, relative to an *assignment* ν of X to a matrix $\nu(X) \in \mathsf{Mat}_{n\times n}(\mathbb{C})$, for some dimension n. In general, rectangular

Table 1 Linear algebra operators (supported in MATLANG [8, 20]) and their semantics. In the last column, $+$, $\times$ and $^{-}$ denote addition, multiplication and complex conjugation of complex numbers, respectively.

matrix multiplication ($\mathsf{op}(e_1, e_2) = e_1 \cdot e_2$)		
$e_1(\nu(X)) = A \in \mathsf{Mat}_{m\times n}(\mathbb{C})$ $e_2(\nu(X)) = B \in \mathsf{Mat}_{n\times o}(\mathbb{C})$	$e_1(\nu(X)) \cdot e_2(\nu(X)) = C \in \mathsf{Mat}_{m\times o}(\mathbb{C})$	$C_{ij} = \sum_{k=1}^{n} A_{ik} \times B_{kj}$
matrix addition ($\mathsf{op}(e_1, e_2) = e_1 + e_2$)		
$e_i(\nu(X)) = A^{(i)} \in \mathsf{Mat}_{m\times n}(\mathbb{C})$	$e_1(\nu(X)) + e_2(\nu(X)) = B \in \mathsf{Mat}_{m\times n}(\mathbb{C})$	$B_{ij} = A^{(1)}_{ij} + A^{(2)}_{ij}$
scalar multiplication ($\mathsf{op}(e) = ce$, $c \in \mathbb{C}$)		
$e(\nu(X)) = A \in \mathsf{Mat}_{m\times n}(\mathbb{C})$	$ce(\nu(X)) = B \in \mathsf{Mat}_{m\times n}(\mathbb{C})$	$B_{ij} = c \times A_{ij}$
Schur-Hadamard product ($\mathsf{op}(e_1, e_2) = e_1 \odot e_2$)		
$e_1(\nu(X)) = A \in \mathsf{Mat}_{m\times m}(\mathbb{C})$ $e_2(\nu(X)) = B \in \mathsf{Mat}_{m\times m}(\mathbb{C})$	$e_1(\nu(X)) \odot e_2(\nu(X)) = C \in \mathsf{Mat}_{m\times m}(\mathbb{C})$	$C_{ij} = A_{ij} \times B_{ij}$
complex conjugate transposition ($\mathsf{op}(e) = e^*$)		
$e(\nu(X)) = A \in \mathsf{Mat}_{m\times n}(\mathbb{C})$	$e(\nu(X))^* = A^* \in \mathsf{Mat}_{n\times m}(\mathbb{C})$	$(A^*)_{ij} = \bar{A}_{ji}$
identity ($\mathsf{op}(e) = \mathsf{Id}(e)$)		
$e(\nu(X)) = A \in \mathsf{Mat}_{m\times m}(\mathbb{C})$	$\mathsf{Id}(e(\nu(X)) = I_{m\times m} \in \mathsf{Mat}_{m\times m}(\mathbb{C})$	$I_{ii} = 1$, $I_{ij} = 0$, $i \neq j$
one-vector ($\mathsf{op}(e) = \mathbb{1}(e)$)		
$e(\nu(X)) = A \in \mathsf{Mat}_{m\times n}(\mathbb{C})$	$\mathbb{1}(e(\nu(X)) = \mathbb{1} \in \mathsf{Mat}_{m\times 1}(\mathbb{C})$	$\mathbb{1}_i = 1$
transpose one-vector ($\mathsf{op}(e) = \mathbb{1}^{\mathsf{t}}(e)$)		
$e(\nu(X)) = A \in \mathsf{Mat}_{m\times n}(\mathbb{C})$	$\mathbb{1}(e(\nu(X)) = \mathbb{1}^{\mathsf{t}} \in \mathsf{Mat}_{1\times m}(\mathbb{C})$	$\mathbb{1}_i = 1$
trace ($\mathsf{op}(e) = \mathsf{tr}(e)$)		
$e(\nu(X)) = A \in \mathsf{Mat}_{m\times m}(\mathbb{C})$	$\mathsf{tr}(e(\nu(X)) = c \in \mathbb{C}$	$c = \sum_{i=1}^{m} A_{ii}$

matrices are allowed but we only focus on square matrices in this paper. We denote by $e\big(\nu(X)\big)$ the result of evaluating $e(X)$ on $\nu(X)$. As expected, $\mathsf{op}_i(e_1(X), \ldots, e_{p_i}(X))(\nu(X)) := \mathsf{op}_i\big(e_1(\nu(X)), \ldots, e_{p_i}(\nu(X))\big)$ for linear algebra operator op_i. In Table 1 we list operators supported in the matrix query language MATLANG [8]. In the table we also show the semantics of the operators and indicate restrictions on the dimensions such that the operators are well-defined.

▶ Remark 1. We use a slightly modified list of operators than used in [8, 20]. For example, we leave out general function applications and only focus on the Schur-Hadamard product ($\odot$). The reason is that once two matrices are indistinguishably with regards to fragments including $\odot$, then adding more general function applications does not increase the distinguishing power [20]. We also leave out the diagonalisation operator (diag) which turns a vector into a diagonal matrix with the input vector on the diagonal. Previous results show that the real distinguishing power for fragments including diag comes from its ability to simulate the Schur-Hadamard product on vectors [20]. We therefore omit diag and use the Schur-Hadamard product on *vectors*, denoted by $\odot_v$, instead. We assume that all fragments include matrix multiplication, addition and scalar multiplication and we do not list these explicitly in the set $\mathcal{L}$ of supported operators. ◀

4 Problem statement

As mentioned in the introduction we want to understand when two matrices can be distinguished by a sentence in fragments $\mathsf{ML}(\mathcal{L})$. We define an expression $e(X)$ in $\mathsf{ML}(\mathcal{L})$ to be a *sentence* if $e(\nu(X))$ returns a scalar in $\mathbb{C}$ for any assignment ν of X. We note that the type system of MATLANG [8] allows to check whether an expression in $\mathsf{ML}(\mathcal{L})$ is a sentence.

▶ **Definition 2.** *Two matrices A and B in $\mathsf{Mat}_{n\times n}(\mathbb{C})$ are said to be* $\mathsf{ML}(\mathcal{L})$-equivalent, *denoted by $A \equiv_{\mathsf{ML}(\mathcal{L})} B$, if and only if $e(A) = e(B)$ for all sentences $e(X)$ in $\mathsf{ML}(\mathcal{L})$.* ◀

For (di)graphs G and H, we write $G \equiv_{\mathsf{ML}(\mathcal{L})} H$ if and only if $A_G \equiv_{\mathsf{ML}(\mathcal{L})} A_H$, where A_G and A_H denote the adjacency matrices of G and H, respectively.

We aim to characterise when $A \equiv_{\mathsf{ML}(\mathcal{L})} B$ holds by determining how A and B relate to each other. A typical characterisation will be *similarity-based*, stating that $A \equiv_{\mathsf{ML}(\mathcal{L})} B$ if and only if $A \cdot X = X \cdot B$ for some matrix X with some specific properties, depending on the fragment $\mathsf{ML}(\mathcal{L})$ under consideration. We will see that for some fragments more complicated relationships than $A \cdot X = X \cdot B$ are needed. When digraphs are concerned, we also provide characterisations in terms of graph properties.

5 Fragments with the trace operation

We start with the equivalence of matrices for the fragments $\mathsf{ML}(\mathsf{tr}, {}^*)$, $\mathsf{ML}(\mathsf{tr}, {}^*, \mathbb{1})$ and $\mathsf{ML}(\mathsf{tr}, {}^*, \mathbb{1}, \odot_v)$, and sub-fragments without * but with $\mathbb{1}^{\mathsf{t}}(\cdot)$ instead. We leave out the biggest fragment $\mathsf{ML}(\mathsf{tr}, {}^*, \mathbb{1}, \odot, \mathsf{Id})$ since an inspection of the proof for that fragment (sketched in [20]) shows that it works for arbitrary matrices. In particular, we have that for (di)graphs G and H, $G \equiv_{\mathsf{ML}(\mathsf{tr}, {}^*, \mathbb{1}, \odot, \mathsf{Id})} H$ if and only if $G \equiv_{\mathsf{C}^3} H$. For all fragments considered, pairs of undirected graphs are known that separate them [20]. We provide *new separating pairs* when there is a distinction between graphs and digraphs. We will see that this occurs when * is not supported. We next outline a general proof strategy for characterising equivalence for fragments with the trace operation and complex conjugate transposition (Section 5.1). This strategy will then be applied to the various fragments under consideration (Section 5.2).

5.1 Proof strategy

We use Specht's Theorem (see e.g., [32] or Theorem 2.2.6 in [28]) as the basis for our proof strategy. It can be stated as follows. Let $\mathcal{A} = A_1, \ldots, A_k$ and $\mathcal{B} = B_1, \ldots, B_k$ be two sequences of k matrices in $\mathsf{Mat}_{n\times n}(\mathbb{C})$ which are closed under *, i.e., each A_i^* is in $\mathcal{A}$, and similarly, each B_i^* is in $\mathcal{B}$. Then, $\mathcal{A}$ and $\mathcal{B}$ are called *(simultaneously) unitary similar* if there exists a unitary matrix U such that for all $i \in [1, k]$, $A_i \cdot U = U \cdot B_i$. Specht's Theorem provides necessary and sufficient conditions for this to hold. More precisely, $\mathcal{A}$ and $\mathcal{B}$ are simultaneously unitary similar if and only if $\mathsf{tr}(w(A_1, \ldots, A_k)) = \mathsf{tr}(w(B_1, \ldots, B_k))$ for all words $w(x_1, \ldots, x_k)$ over variables $x_1, \ldots, x_k$. As an example of what $w(A_1, \ldots, A_k)$ means, if $\mathcal{A} = A, A^*$ and $w(x, y) = xxyx$, then $w(A, A^*) = A \cdot A \cdot A^* \cdot A$. So, variables in words are substituted by matrices and concatenation is interpreted as matrix multiplication. The real analogue of Specht's Theorem is as follows [32]: Let $\mathcal{A}$ and $\mathcal{B}$ be two sequences of k matrices in $\mathsf{Mat}_{n\times n}(\mathbb{R})$ which are closed under transposition. Then, $\mathcal{A}$ and $\mathcal{B}$ are called *(simultaneously) orthogonal similar* if there exists a (real) orthogonal matrix Q such that $A_i \cdot Q = Q \cdot B_i$ for all $i \in [1, k]$. Again, this is equivalent to requiring $\mathsf{tr}(w(A_1, \ldots, A_k)) = \mathsf{tr}(w(B_1, \ldots, B_k))$ for all words $w(x_1, \ldots, x_k)$ over variables $x_1, \ldots, x_k$[1].

We can use Specht's Theorem to characterise $\mathsf{ML}(\mathcal{L})$-equivalence for fragments with trace and *, as follows. Let A and B be two matrices in $\mathsf{Mat}_{n\times n}(\mathbb{C})$. Let $\Sigma = e_1(X), \ldots, e_k(X)$ be a finite sequence of expressions such that (i) each $e_i(X)$ is in $\mathsf{ML}(\mathcal{L})$; (ii) each $e_i(X) \in \Sigma$

[1] For both the complex and real version of Specht's Theorem there are bounds on the length of words that one needs to consider, a rough bound being $2n^2$ [32]. Some recent progress and tighter bounds are reported in [41]. These quantitative bounds do not play a role in what follows.

evaluates to a matrix, i.e., $e_i(A) \in \mathsf{Mat}_{n\times n}(\mathbb{C})$ (and hence also $e_i(B) \in \mathsf{Mat}_{n\times n}(\mathbb{C})$); and (iii) when $e_i(X) \in \Sigma$ also $(e_i(X))^* \in \Sigma$, i.e., Σ is closed under *.

Given $\Sigma = e_1(X), \dots, e_k(X)$ and A and B, we then construct two sequences of matrices in $\mathsf{Mat}_{n\times n}(\mathbb{C})$: $\Sigma(A) := e_1(A), \dots, e_k(A)$ and $\Sigma(B) := e_1(B), \dots, e_k(B)$. Clearly, these sequences are closed under complex conjugation by the definition of Σ. Let $w(x_1, \dots, x_k)$ be a word over $x_1, \dots, x_k$. For each such word we consider the $\mathsf{ML}(\mathcal{L})$-*sentence*:

$$e_w(X) := \mathsf{tr}\big(w(e_1(X), \dots, e_k(X))\big).$$

Then, $A \equiv_{\mathsf{ML}(\mathcal{L})} B$ implies that $e_w(A) = e_w(B)$ for any word $w(x_1, \dots, x_k)$ and hence, by Specht's Theorem, there exists a unitary matrix U such that $e_i(A) \cdot U = U \cdot e_i(B)$ for all $i \in [1, k]$. We will always assume that in Σ, $e_1(X) := X$, such that $A \equiv_{\mathsf{ML}(\mathcal{L})} B$ implies that $A \cdot U = U \cdot B$ and $e_i(A) \cdot U = U \cdot e_i(B)$ for $i \in [2, k]$.

The sequences Σ of $\mathsf{ML}(\mathcal{L})$-expressions which we will use ensure that the unitary/orthogonal matrix is restricted such that *similarity is preserved* by the operators in $\mathsf{ML}(\mathcal{L})$. This allows, by induction on the structure of expressions in $\mathsf{ML}(\mathcal{L})$, to show that when $\Sigma(A)$ and $\Sigma(B)$ are simultaneously unitary equivalent, then $A \equiv_{\mathsf{ML}(\mathcal{L})} B$. We will not detail these inductive proofs as they are similar to those underlying the results in [20].

5.2 Results

$\mathsf{ML}(\mathsf{tr}, ^*)$-equivalence

For undirected graphs it is known that $G \equiv_{\mathsf{ML}(\mathsf{tr},^*)} H$ if and only if $A_G \cdot Q = Q \cdot A_H$ for an orthogonal matrix Q [20]. The proof relies on the Spectral Theorem of symmetric matrices (see e.g., Theorem 2.5.3 in [28]), which does not apply for general matrices and, in particular, for adjacency matrices of directed graphs. Instead, we here follow our proof strategy. Let A and B be matrices in $\mathsf{Mat}_{n\times n}(\mathbb{C})$. To apply Specht's Theorem, we consider the sequence $\Sigma = e_1(X) := X, e_2(X) := X^*$. Hence, $\Sigma(A) = A, A^*$ and $\Sigma(B) = B, B^*$ and $A \equiv_{\mathsf{ML}(\mathsf{tr},^*)} B$ implies that $A \cdot U = U \cdot B$ and $A^* \cdot U = U \cdot B^*$ for a unitary matrix U. This shows one direction of the following proposition. The other direction is shown by induction on the structure of expressions and uses that $\mathsf{tr}(\cdot)$ is invariant under similarity, i.e., $\mathsf{tr}(A) = \mathsf{tr}(P^{-1} \cdot A \cdot P)$ for any matrix A and invertible matrix P in $\mathsf{Mat}_{n\times n}(\mathbb{C})$.

▶ **Proposition 3.** *Let A and B be matrices in $\mathsf{Mat}_{n\times n}(\mathbb{C})$. Then $A \equiv_{\mathsf{ML}(\mathsf{tr},^*)} B$ if and only if A and B are unitary similar. When A and B are real matrices, then orthogonal similarity can be used.* ◀

Proposition 3 holds in particular for adjacency matrices representing digraphs, hereby generalising the characterisation for undirected graphs. We can say a bit more by rephrasing the trace conditions underlying Specht's Theorem in terms of so-called *semi-walks* in digraphs.

Let π be a string in $\{\leftarrow, \rightarrow\}^*$ of length k. A *semi-walk ρ of type π* in a digraph $G = (V, E)$ is a sequence of $k+1$ vertices $v_1, v_2, \dots, v_{k+1}$ in V such that for each pair of consecutive vertices v_i and v_{i+1}, (v_i, v_{i+1}) is an edge in G if $\pi_i =$"$\rightarrow$" or (v_{i+1}, v_i) is an edge if $\pi_i =$"$\leftarrow$". A *closed* semi-walk of type π is a semi-walk of that type which starts and ends in the same vertex. Let $w(x, y)$ be a word of length k over variables x and y. We define the *type of* $w(x, y)$ as the string $\pi(w) \in \{\leftarrow, \rightarrow\}^k$ such that $\pi(w)_i =$"$\rightarrow$" if the ith symbol in $w(x, y)$ is x, and $\pi(w)_i =$"$\leftarrow$" if the ith symbol of $w(x, y)$ is y. It is now readily verified that $\mathsf{tr}(w(A_G, A_G^{\mathsf{t}}))$ counts the number of closed semi-walks of type $\pi(w)$ in the digraph G represented by adjacency matrix A_G.

▶ **Corollary 4.** *Let G and H be digraphs of the same order. Then, $G \equiv_{\mathsf{ML}(\mathsf{tr},^*)} H$ if and only if G and H have the same number of closed semi-walks of any type.* ◀

We remark that when G and H are undirected graphs, semi-walks are simply walks and the type is just the length of the walk. In this case, Corollary 4 implies that $G \equiv_{\mathsf{ML}(\mathsf{tr},^*)} H$ if and only if G and H have the same number of closed walks of any length, as reported in [20]. For undirected graphs, it was furthermore shown that $G \equiv_{\mathsf{ML}(\mathsf{tr},^*)} H$ if and only if $G \equiv_{\mathsf{ML}(\mathsf{tr})} H$ [20]. After all, complex conjugate transposition on symmetric real matrices does not have any effect. By contrast, we will see that the presence of * has an impact on digraphs. First, however, we look into $\mathsf{ML}(\mathsf{tr})$-equivalence.

▶ **Proposition 5.** *Let A and B be in $\mathsf{Mat}_{n\times n}(\mathbb{C})$. Then, $A \equiv_{\mathsf{ML}(\mathsf{tr})} B$ if and only if A and B have the same characteristic polynomial.*

Proof. It is well-known that $\mathsf{tr}(A^k) = \mathsf{tr}(B^k)$, for any k, is equivalent to A and B having the same characteristic polynomial (and thus eigenvalues) (see e.g., Problem 2.4.P10 in [28]), and having $\mathsf{tr}(A^k) = \mathsf{tr}(B^k)$, for any k, is clearly equivalent to $A \equiv_{\mathsf{ML}(\mathsf{tr})} B$. ◀

We can complement this proposition for digraphs G and H by: $G \equiv_{\mathsf{ML}(\mathsf{tr})} H$ if and only if G and H have the same number of closed semi-walks of type "$\rightarrow^k$", for any k.

Proposition 5 immediately implies that a simple similarity-based characterisation of $\mathsf{ML}(\mathsf{tr})$-equivalence does not exist. Indeed, suppose that $A \equiv_{\mathsf{ML}(\mathsf{tr})} B$ would be equivalent to $A \cdot X = X \cdot B$ for some unitary/orthogonal matrix X, then A and B must have the same Jordan normal form (up to reordering of the Jordan blocks). Matrices with the same characteristic polynomial, however, do not necessarily have the same Jordan normal form.

▶ **Example 6.** Consider the digraphs G_1 ($\bullet\!\rightarrow\!\bullet\ \ \bullet$) and H_1 ($\bullet\!\rightarrow\!\bullet\!\rightarrow\!\bullet$) with adjacency matrices $A_{G_1} = \left[\begin{smallmatrix} 0&1&0\\ 0&0&0\\ 0&0&0 \end{smallmatrix}\right]$ and $A_{H_1} = \left[\begin{smallmatrix} 0&1&0\\ 0&0&1\\ 0&0&0 \end{smallmatrix}\right]$, respectively. These matrices are in Jordan normal form, but different. So A_{G_1} and A_{H_1} cannot be similar using an invertible matrix. From the diagonals, however, we can see that both have z^3 (eigenvalue 0 with multiplicity 3) as characteristic polynomial. Hence, $A_{G_1} \equiv_{\mathsf{ML}(\mathsf{tr})} A_{H_1}$ by Proposition 5 (alternatively, one simply observes that both digraphs have no closed semi-walks of type "$\rightarrow^k$" for any k.). ◀

We next show that $\mathsf{ML}(\mathsf{tr})$- and $\mathsf{ML}(^*, \mathsf{tr})$-equivalence of *normal matrices* relate just like for undirected graphs. This is not surprising. Normal matrices are known to inherit many properties of symmetric matrices (see e.g., Section 2.5 in [28]).

▶ **Proposition 7.** *Let A and B be normal matrices in $\mathsf{Mat}_{n\times n}(\mathbb{C})$. Then, $A \equiv_{\mathsf{ML}(\mathsf{tr},^*)} B$ if and only if $A \equiv_{\mathsf{ML}(\mathsf{tr})} B$.*

Proof. (sketch) We note that $A \equiv_{\mathsf{ML}(\mathsf{tr},^*)} B$ trivially implies $A \equiv_{\mathsf{ML}(\mathsf{tr})} B$. The reverse implication holds because if A and B are normal matrices, then $A^* = p(A)$ and $B^* = p(B)$ for some polynomial $p(z)$ (see e.g., Problem 2.5.P26 in [28]). Intuitively, this implies that we can eliminate occurrences of A^* in $\mathsf{tr}(w(A, A^*))$, hereby reducing such expressions to linear combinations of $\mathsf{tr}(A^k)$ for some k's, and $\mathsf{ML}(\mathsf{tr})$-equivalence guarantees that $\mathsf{tr}(A^k) = \mathsf{tr}(B^k)$ for all k. Specht's Theorem and Proposition 3 then imply that $A \equiv_{\mathsf{ML}(\mathsf{tr},^*)} B$. ◀

The digraphs G_1 ($\bullet\!\rightarrow\!\bullet\ \ \bullet$) and H_1 ($\bullet\!\rightarrow\!\bullet\!\rightarrow\!\bullet$), with non-normal adjacency matrices, show that Proposition 7 does not hold in general. Indeed, note that G_1 has one closed semi-walk of type "$\rightarrow\leftarrow$", whereas H_1 has two such walks. Hence, $G_1 \not\equiv_{\mathsf{ML}(\mathsf{tr},^*)} H_1$ by Corollary 4.

$\mathsf{ML}(\mathsf{tr},{}^*,\mathbb{1})$-equivalence

Whereas the trace operator enables counting closed semi-walks in (di)graphs, the inclusion of the $\mathbb{1}(\cdot)$-operator enables to count the number of not necessarily closed (semi-)walks. Indeed, one can use sentences $(\mathbb{1}(X))^* \cdot w(X, X^*) \cdot \mathbb{1}(X)$ in $\mathsf{ML}(\mathsf{tr},{}^*,\mathbb{1})$ to count the number of semi-walks of the type of the word $w(x, y)$ when evaluated on an adjacency matrix of a digraph. It was shown that for undirected graphs, $G \equiv_{\mathsf{ML}(\mathsf{tr},{}^*,\mathbb{1})} H$ if and only if $A_G \cdot Q = Q \cdot A_H$ for an orthogonal doubly quasi-stochastic matrix Q if and only if G and H have the same number of closed and not necessarily closed walks of any length [20]. The proof relied on the Spectral Theorem for symmetric matrices. Our proof strategy, however, allows to generalise this result to digraphs and general matrices.

Let A and B be matrices in $\mathsf{Mat}_{n\times n}(\mathbb{C})$. To apply Specht's Theorem we use the sequence $\Sigma = e_1(X) := X, e_2(X) := X^*, e_3(X) := \mathbb{1}(X) \cdot (\mathbb{1}(X))^*$. Hence, $\Sigma(A) = A, A^*, J$ and $\Sigma(B) = B, B^*, J$ and $A \equiv_{\mathsf{ML}(\mathsf{tr},{}^*,\mathbb{1})} B$ implies $A \cdot U = U \cdot B$ (and thus also $A^* \cdot U = U \cdot B^*$) and $J \cdot U = U \cdot J$ for a unitary matrix U. We note that $J \cdot U = U \cdot J$ implies that U can be chosen such that $A \cdot U = U \cdot B$ and $U \cdot \mathbb{1} = \mathbb{1}$ hold (see Lemma 4 in [42]). In other words, U can be chosen to be unitary and doubly quasi-stochastic. It is easily verified, along the same lines as in [20], by induction on the structure of expressions, that the existence of such a unitary matrix also implies $A \equiv_{\mathsf{ML}(\mathsf{tr},{}^*,\mathbb{1})} B$. We thus have shown:

▶ **Proposition 8.** *Let A and B be matrices in $\mathsf{Mat}_{n\times n}(\mathbb{C})$. Then $A \equiv_{\mathsf{ML}(\mathsf{tr},{}^*,\mathbb{1})} B$ if and only if $A \cdot U = U \cdot B$ for a unitary doubly quasi-stochastic matrix U. When A and B are real matrices, we can use an orthogonal doubly quasi-stochastic matrix instead.* ◀

Specialised to adjacency matrices of digraphs G and H, we can further complement this by:

▶ **Corollary 9.** *Let G and H be digraphs of the same order. Then, $G \equiv_{\mathsf{ML}(\mathsf{tr},{}^*,\mathbb{1})} H$ if and only if G and H have the same number of semi-walks of any type and the same number of closed semi-walks of any type.*

Proof. (sketch) The only if direction requires some explanation. Suppose that A_G and A_H have the same number of semi-walks of any type and the same number of closed semi-walks of any type. We argue that $\mathsf{tr}(w(A_G, A_G^*, J)) = \mathsf{tr}(w(A_H, A_H^*, J))$ for any word $w(x, y, z)$. Specht's Theorem together with Proposition 8 then imply that $G \equiv_{\mathsf{ML}(\mathsf{tr},{}^*,\mathbb{1})} H$. It is easily verified that $\mathsf{tr}(w(A_G, A_G^*, J))$ is either of the form $\mathsf{tr}(w'(A_G, A_G^*))$ (when J does not occur) or can be reduced to an expression of the form $c \prod_{i\in[1,k]} \mathsf{tr}(w_i(A_G, A_G^*) \cdot J)$ for some $c \in \mathbb{N}$. We note that $\mathsf{tr}(w_i(A_G, A_G^*) \cdot J) = \mathbb{1}^{\mathsf{t}} \cdot w_i(A_G, A_G^*) \cdot \mathbb{1}$. Hence, in both cases $\mathsf{tr}(w(A_G, A_G^*, J))$ is fully determined by the number of semi-walks and closed semi-walks in G. Similarly, for $\mathsf{tr}(w(A_H, A_H^*, J))$. ◀

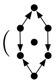
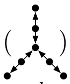
For undirected graphs, $G \equiv_{\mathsf{ML}(\mathsf{tr},{}^*,\mathbb{1})} H$ was also shown to be equivalent to $G \equiv_{\mathsf{ML}(\mathsf{tr},\mathbb{1},\mathbb{1}^{\mathsf{t}})} H$ [20] and to A_G and A_H, and their complements $\bar{A}_G$ and $\bar{A}_H$, having the same characteristic polynomial [43]. Here, the *complement* $\bar{A}$ of a matrix A is defined as $J - A - I$, similarly for $\bar{B}$ of B. The latter equivalence extends more generally:

▶ **Proposition 10.** *Let A and B be matrices in $\mathsf{Mat}_{n\times n}(\mathbb{C})$. Then, $A \equiv_{\mathsf{ML}(\mathsf{tr},\mathbb{1},\mathbb{1}^{\mathsf{t}})} B$ if and only if A and B, and $\bar{A}$ and $\bar{B}$ have the same characteristic polynomial.*

Proof. This is an immediate consequence of the following identity (see e.g., [21]) linking characteristic polynomials of A and $\bar{A}$ to the walk generating function: $\frac{p_A(z)}{p_{\bar{A}}(z)} = 1 - \sum_{k\geq 0}(-z-1)^k \mathsf{tr}(A^k \cdot J)$, where $p_A(z)$ and $p_{\bar{A}}(z)$ denote the characteristic polynomials of A and $\bar{A}$, respectively. Indeed, when $A \equiv_{\mathsf{ML}(\mathsf{tr},\mathbb{1})} B$ holds, $p_A(z) = p_B(z)$ (by Proposition 5) and also

$\mathsf{tr}(A^k \cdot J) = \mathsf{tr}(B^k \cdot J)$. Hence, the identity above tells that $p_{\bar{A}}(z) = p_{\bar{B}}(z)$. Conversely, if $p_A(z) = p_B(z)$ and $p_{\bar{A}}(z) = p_{\bar{B}}(z)$ we must have that $\mathsf{tr}(A^k \cdot J) = \mathsf{tr}(B^k \cdot J)$. It is readily verified, as in the proof of Corollary 9, that this implies that $A \equiv_{\mathsf{ML}(\mathsf{tr},\mathbb{1},\mathbb{1}^{\mathsf{t}})} B$ holds. ◀

Clearly, for digraphs, $\mathsf{ML}(\mathsf{tr}, \mathbb{1}, \mathbb{1}^{\mathsf{t}})$-equivalence coincides with the digraphs having the same number of semi-walks and closed semi-walks of type "$\rightarrow^k$", for any k. However, no simple similarity-based characterisation of $\mathsf{ML}(\mathsf{tr}, \mathbb{1}, \mathbb{1}^{\mathsf{t}})$-equivalence for digraphs exists.

▶ **Example 11.** We use again the Jordan normal form argument as in Example 6. Indeed, the digraphs G_2 () and H_2 () are easily seen to be $\mathsf{ML}(\mathsf{tr}, \mathbb{1}, \mathbb{1}^{\mathsf{t}})$-equivalent (they have no closed semi-walks of type "$\rightarrow^k$", have both 7 semi-walks of length 0, 6 semi-walks of type "$\rightarrow$" and no semi-walks of type "$\rightarrow^k$", for $k > 1$). Nevertheless, one can verify that their Jordan normal forms are different. So no invertible matrix X can exist such that $A_{G_2} \cdot X = X \cdot A_{H_2}$. ◀

We can say a bit more by allowing more complicated ways of linking A and B. We develop this further in Section 6 when focusing on $\mathsf{ML}(\mathbb{1}, \mathbb{1}^{\mathsf{t}})$-equivalence. So, stay tuned.

A similar proof as for Proposition 7 shows that normal matrices simplify matters:

▶ **Corollary 12.** *Let A and B be normal matrices in $\mathsf{Mat}_{n\times n}(\mathbb{C})$. Then, $A \equiv_{\mathsf{ML}(\mathsf{tr},^*,\mathbb{1})} B$ if and only if $A \equiv_{\mathsf{ML}(\mathsf{tr},\mathbb{1},\mathbb{1}^{\mathsf{t}})} B$.* ◀

We thus recover and generalise the characterisation for $\mathsf{ML}(\mathsf{tr}, \mathbb{1}, \mathbb{1}^{\mathsf{t}})$-equivalence of undirected graphs [20] to normal matrices. We note that graphs G_2 and H_2 show that Corollary 12 does not extend to non-normal matrices. Indeed, $G_2 \equiv_{\mathsf{ML}(\mathsf{tr},\mathbb{1},\mathbb{1}^{\mathsf{t}})} H_2$ but $G_2 \not\equiv_{\mathsf{ML}(\mathsf{tr},^*,\mathbb{1})} H_2$. For example, G_2 has 8 semi-walks of type "$\leftarrow\rightarrow\leftarrow\rightarrow$" while H_2 has 48 semi-walks of that type. So, Corollary 9 implies that $G_2 \not\equiv_{\mathsf{ML}(\mathsf{tr},^*,\mathbb{1})} H_2$.

$\mathsf{ML}(\mathsf{tr}, ^*, \mathbb{1}, \odot_v)$-equivalence

We next include pointwise vector multiplication ($\odot_v$), i.e., the Schur-Hadamard product on vectors. The proof of the characterisation of $\mathsf{ML}(\mathsf{tr}, ^*, \mathbb{1}, \odot_v)$-equivalence obtained for undirected graphs in [20] generalises easily to digraphs and general matrices. The key insight for undirected graphs was that pointwise multiplication of vectors allows to compute so-called *equitable partitions* of undirected graphs. On graphs, equitable partitions correspond to the partition obtained by vertex colour refinement [23]. For digraphs and general matrices, equitable partitions and colour refinement have been considered as well (see e.g., [1, 25, 42, 24]). We only need to use this general notion of equitable partition, and the proofs in [20] carry over almost verbatim.

Let $A \in \mathsf{Mat}_{n\times n}(\mathbb{C})$. A partition $[n] = \biguplus_{i\in[1,q]} V_i$ is *row-equitable* for A if there are complex numbers r_{ij} such that for all $k \in V_i$, $\sum_{\ell\in V_j} A_{k\ell} = r_{ij}$. That is, the sum of row entries of A for columns in V_j is constant (r_{ij}) and independent of the chosen row in V_i. Similarly, a partition $[n] = \biguplus_{i\in[1,q]} V_i$ is *column-equitable* for A if there are complex numbers c_{ij} such that for all $k \in V_i$, $\sum_{\ell\in V_j} A_{\ell k} = c_{ij}$. A partition $[n] = \biguplus_{i\in[1,q]} V_i$ is *equitable* for A if it is both row- and column-equitable[2] for A. We remark that any matrix has an equitable partition given by the trivial one consisting of singleton elements.

[2] For symmetric matrices, such as adjacency matrices of undirected graphs, the notions of row- and column-equitability coincide.

In the following we represent partitions by *indicator vectors*. More specifically, if $[n] = \biguplus_{i\in[1,q]} V_i$ is a partition, then we represent it by binary vectors $\mathbb{1}_{V_1}, \ldots, \mathbb{1}_{V_q}$ such that $\mathbb{1}_{V_i}$ holds a 1 at row j if $j \in V_i$ and holds a 0 otherwise.

A matrix may have multiple equitable partitions, but only a unique *coarsest* one. That is, there is unique equitable partition of which any other equitable partition is a refinement. We can relate two matrices based on equitable partitions. More precisely, matrices A and B in $\mathsf{Mat}_{n\times n}(\mathbb{C})$ are said to have a *common equitable partition* if there exists partitions $[n] = \biguplus_{i\in[1,q]} V_i$ and $[n] = \biguplus_{i\in[1,q]} W_j$ which are equitable for A and B, respectively, and if r_{ij} and r'_{ij} denote the complex numbers for row-equitability of the two partitions, and c_{ij} and c'_{ij} the complex numbers for column-equitability, then $r_{ij} = r'_{ij}$ and $c_{ij} = c'_{ij}$ for $i, j \in [1, q]$. We can compute equitable partitions in $\mathsf{ML}(^*, \mathbb{1}, \odot_v)$ (the trace operator is not needed) and we can test for the existence of a common equitable partition:

▶ **Proposition 13** ([20]). *Let A and B be matrices in $\mathsf{Mat}_{n\times n}(\mathbb{C})$. Let $[n] = \biguplus_{i\in[1,q]} V_i$ be the coarsest equitable partition for A. There exists expressions $\mathsf{equit}_j(X) \in \mathsf{ML}(\mathbb{1}, ^*, \odot_v)$, depending on A, such that $\mathbb{1}_{V_j} = \mathsf{equit}_j(A)$ for $j \in [1, q]$. Furthermore, $A \equiv_{\mathsf{ML}(^*,\mathbb{1},\odot_v)} B$ implies that A and B have a common equitable partition witnessed by the partitions represented by $\mathsf{equit}_i(A)$ and $\mathsf{equit}_i(B)$, for $i \in [1, q]$.*

Proof. Compared to the proof for undirected graphs [20] we now need to use * to ensure both row- and column-equitability. The presence of $\odot_v$ allows one to simulate the colour refinement process on matrices (see e.g., [24, 42]) by: extracting the indicator vectors from matrices, and by intersecting indicator vectors in order to create a refined partition. ◀

A similarity-based characterisation of $\mathsf{ML}(\mathsf{tr}, ^*, \mathbb{1}, \odot_v)$-equivalence is obtained using Specht's Theorem. We consider the sequence $\Sigma = e_1(X) := X, e_2(X) := X^*, \mathsf{equit}_i(X) \cdot \mathsf{equit}_i^*(X), i \in [1, q]$, such that $\mathsf{equit}_i(A)$ computes indicator vectors of an equitable partition $[n] = \biguplus_{i\in[1,q]} V_i$ of A. Hence, $\Sigma(A) = A, A^*, E_1 = \mathbb{1}_{V_1} \cdot \mathbb{1}^{\mathsf{t}}_{V_1}, \ldots, E_q = \mathbb{1}_{V_q} \cdot \mathbb{1}^{\mathsf{t}}_{V_q}$ and $\Sigma(B) = B, B^*, F_1 = \mathbb{1}_{W_1} \cdot \mathbb{1}^{\mathsf{t}}_{W_1}, \ldots, F_q = \mathbb{1}_{W_q} \cdot \mathbb{1}^{\mathsf{t}}_{W_q}$, where $[n] = \biguplus_{i\in[1,q]} W_i$ is an equitable partition of B. We have that $A \equiv_{\mathsf{ML}(\mathsf{tr},^*,\mathbb{1},\odot_v)} B$ implies the existence of a unitary matrix U such that $A \cdot U = U \cdot B$ and $E_i \cdot U = U \cdot F_i$ for $i \in [1, q]$. The latter conditions imply that U can be chosen such that $\mathbb{1}_{V_i} = U \cdot \mathbb{1}_{W_i}$ for $i \in [1, q]$. That the existence of such a similarity between A and B implies that $A \equiv_{\mathsf{ML}(\mathsf{tr},^*,\mathbb{1},\odot_v)} B$ holds, is not straightforward but the argument given in [20] can be generalised to general matrices. We only need a generalisation of Lemma 2.1 in [11] which states, translated to our setting, that all vectors $e(A)$ which can be computed by means of expressions $e(X)$ in $\mathsf{ML}(\mathsf{tr}, ^*, \mathbb{1}, \odot_v)$ can be written as a linear combination of indicator vectors $\mathbb{1}_{V_i}$, for $i \in [1, q]$. Similarly for $e(B)$. Since $\mathbb{1}_{V_i} = U \cdot \mathbb{1}_{W_i}$, $e(A) = U \cdot e(B)$ and this can be used to show, by induction on the structure of expressions, that $A \equiv_{\mathsf{ML}(\mathsf{tr},^*,\mathbb{1},\odot_v)} B$.

▶ **Proposition 14.** *Let A and B be matrices in $\mathsf{Mat}_{n\times n}(\mathbb{C})$. Then, $A \equiv_{\mathsf{ML}(\mathsf{tr},^*,\mathbb{1},\odot_v)} B$ if and only if $A \cdot U = U \cdot B$ and $\mathbb{1}_{V_i} = U \cdot \mathbb{1}_{W_i}$ for $i \in [1, q]$. For real matrices A and B one can use orthogonal matrices Q such that $\mathbb{1}_{V_i} = Q \cdot \mathbb{1}_{W_i}$, for $i \in [1, q]$* ◀

In the proposition, $\mathbb{1}_{V_i}$ and $\mathbb{1}_{W_i}$, for $i \in [1, q]$, witness that A and B have a common equitable partition. This exactly matches the characterisation given for undirected graphs in [20] but beware that row- and column-equitable partitions are used in this general setting. We observe that $\mathbb{1}_{V_i} = U \cdot \mathbb{1}_{W_i}$ implies that U is doubly quasi-stochastic (simply note that $\mathbb{1} = \sum_{i\in[1,q]} \mathbb{1}_{V_i} = \sum_{i\in[1,q]} \mathbb{1}_{W_i}$). For undirected graphs G and H, we also have that $G \equiv_{\mathsf{ML}(\mathsf{tr},^*,\mathbb{1},\odot_v)} H$ if and only if $G \equiv_{\mathsf{ML}(\mathsf{tr},\mathbb{1},\mathbb{1}^{\mathsf{t}},\odot_v)} H$. This equivalence does not hold in general, however. We remark that $\mathsf{ML}(\mathsf{tr}, \mathbb{1}, \mathbb{1}^{\mathsf{t}}, \odot_v)$- and $\mathsf{ML}(\mathsf{tr}, ^*, \mathbb{1}, \odot_v)$-equivalence do coincide when normal matrices are considered, just as for undirected graphs. It suffices again to observe that * can be eliminated for normal matrices (see e.g., the proof of Proposition 7).

6 Fragments without the trace operator and/or complex conjugate transposition

It should be clear by now that the absence of complex conjugate transposition has an impact when digraphs and general matrices are concerned. Moreover, for fragments that do not support $\mathsf{tr}(\cdot)$, we cannot use the proof strategy based on Specht's Theorem. We follow a different route in this section, inspired by the theory of *linear systems* in control theory (see e.g., [13]) and the notion of *minimal realisation* in particular. The fragments we consider are: $\mathsf{ML}(\mathbb{1},\mathbb{1}^{\mathsf{t}})$, $\mathsf{ML}(^*,\mathbb{1})$, and $\mathsf{ML}(^*,\mathbb{1},\odot_v)$.

6.1 Minimal realisations

In control theory, one analyses linear systems described by a triple $\langle A,C,D\rangle$ with $A\in\mathsf{Mat}_{n\times n}(\mathbb{C})$, $C\in\mathsf{Mat}_{m\times n}(\mathbb{C})$, and $D\in\mathsf{Mat}_{n\times o}(\mathbb{C})$, and one wants to understand the "dynamics" $C\cdot A^k\cdot D$, for $k\geq 0$, of the system. To this aim, one typically finds a *minimal realisation* of $\langle A,C,D\rangle$. That is, a system $\langle\hat{A},\hat{C},\hat{D}\rangle$ with $\hat{A}\in\mathsf{Mat}_{q\times q}(\mathbb{C})$, $\hat{C}\in\mathsf{Mat}_{m\times q}(\mathbb{C})$, and $\hat{D}\in\mathsf{Mat}_{q\times o}(\mathbb{C})$ such that (i) $C\cdot A^k\cdot D=\hat{C}\cdot\hat{A}^k\cdot\hat{D}$, for all $k\geq 0$, i.e., it has the same dynamics; and (ii) the dimension q, also called the *order of the system*, is minimal. The importance of minimal realisations is that they are *unique*, up to unitary similarity. That is, for any two minimal realisations $\langle\hat{A},\hat{C},\hat{D}\rangle$ and $\langle\hat{A}',\hat{C}',\hat{D}'\rangle$ of $\langle A,C,D\rangle$, there exists a unitary matrix $Z\in\mathsf{Mat}_{q\times q}(\mathbb{C})$ such that $\hat{A}=Z^*\cdot\hat{A}'\cdot Z$, $\hat{C}\cdot Z=\hat{C}'$ and $\hat{D}=Z^*\cdot\hat{D}'$. When real matrices are concerned, they are unique up to orthogonal similarity. If one has given two systems $\langle A,C,D\rangle$ and $\langle B,C',D'\rangle$ that have the same dynamics, i.e., $C\cdot A^k\cdot D=C'\cdot B^k\cdot D'$, for $k\geq 0$, then this implies that $\langle A,C,D\rangle$ and $\langle B,C',D'\rangle$ have the same minimal realisation (up to similarity). We use this observation to link the matrices A and B. To see how this relates to $\mathsf{ML}(\mathcal{L})$-equivalence, consider the following examples.

▶ **Example 15.** Let A and B in $\mathsf{Mat}_{n\times n}(\mathbb{C})$. Then, $A\equiv_{\mathsf{ML}(\mathbb{1},\mathbb{1}^{\mathsf{t}})}B$ implies $\mathbb{1}^{\mathsf{t}}\cdot A^k\cdot\mathbb{1}=\mathbb{1}^{\mathsf{t}}\cdot B^k\cdot\mathbb{1}$ for all $k\geq 0$. After all, we can consider sentences $e_k(X):=\mathbb{1}^{\mathsf{t}}(X)\cdot X^k\cdot\mathbb{1}(X)$ in $\mathsf{ML}(\mathbb{1},\mathbb{1}^{\mathsf{t}})$ and $A\equiv_{\mathsf{ML}(\mathbb{1},\mathbb{1}^{\mathsf{t}})}B$ implies that $e_k(A)=e_k(B)$. So, when we consider the systems $\langle A,\mathbb{1}^{\mathsf{t}},\mathbb{1}\rangle$ and $\langle B,\mathbb{1}^{\mathsf{t}},\mathbb{1}\rangle$, $A\equiv_{\mathsf{ML}(\mathbb{1},\mathbb{1}^{\mathsf{t}})}B$ implies that these have the same dynamics and hence, similar minimal realisations. ◀

We note that for $\mathsf{ML}(\mathbb{1},\mathbb{1}^{\mathsf{t}})$-equivalence we only need to consider systems of the form $\langle A,C,D\rangle$ with $C=D^*$. From now on, we denote such a system by $\langle A,D\rangle$ instead of $\langle A,D^*,D\rangle$.

▶ **Example 16.** Let A and B in $\mathsf{Mat}_{n\times n}(\mathbb{C})$. Then, $A\equiv_{\mathsf{ML}(^*,\mathbb{1})}B$ implies $\mathbb{1}^{\mathsf{t}}\cdot w(A,A^*)\cdot\mathbb{1}=\mathbb{1}^{\mathsf{t}}\cdot w(B,B^*)\cdot\mathbb{1}$ for all words $w(x,y)$. We are here thus interested in the same systems as before, i.e., $\langle A,\mathbb{1}\rangle$ and $\langle B,\mathbb{1}\rangle$, but have in mind a more general notion of "dynamics" in which arbitrary words $w(x,y)$ are considered. ◀

One can show, following closely the proof for standard minimal realisations (see e.g., Chapter 25 in [14]), that results from control theory extend to this more general setting, provided that we define a *generalised minimal realisation* of $\langle A,D\rangle$ as a system $\langle\hat{A},\hat{D}\rangle$ of minimal order (i.e., the dimension of $\hat{A}$ is minimal) and such that $D^*\cdot w(A,A^*)\cdot D=(\hat{D})^*\cdot w(\hat{A},(\hat{A})^*)\cdot\hat{D}$ for every word $w(x,y)$. One can show that:

▶ **Proposition 17.** *Let $A\in\mathsf{Mat}_{n\times n}(\mathbb{C})$ and $D\in\mathsf{Mat}_{n\times o}(\mathbb{C})$. Then, $\langle A,D\rangle$ has a unique generalised minimal realisation, up to unitary similarity. Furthermore, orthogonal similarity can be used when A and D are real matrices.* ◀

Standard minimal realisations can be computed in several ways. We here use the *Kalman decomposition* method [13]. Let $\langle A, D\rangle$ and $\langle B, D'\rangle$ be two systems such that $D^* \cdot A^k \cdot D = (D')^* \cdot B^k \cdot D'$, for any k. The Kalman decomposition procedure can be used to obtain two special unitary bases U and V in $\mathsf{Mat}_{n\times n}(\mathbb{C})$, leveraging that minimal realisations are similar, such that:

$$U^*{\cdot}A{\cdot}U = \begin{bmatrix} \bigstar_{p\times p} & \bigstar_{p\times q} & \bigstar_{p\times r} \\ O_{q\times p} & \hat{A} & \bigstar_{q\times r} \\ O_{r\times p} & O_{r\times q} & \bigstar_{r\times r} \end{bmatrix}, V^*{\cdot}B{\cdot}V = \begin{bmatrix} \bigstar_{p'\times p'} & \bigstar_{p'\times q} & \bigstar_{p'\times r'} \\ O_{q\times p'} & \hat{A} & \bigstar_{q\times r'} \\ O_{r'\times p'} & O_{r'\times q} & \bigstar_{r'\times r'} \end{bmatrix},$$
$$U^*{\cdot}D = \begin{bmatrix} \bigstar_{p\times o} \\ \hat{D} \\ O_{r\times o} \end{bmatrix}, \text{ and } V^*{\cdot}D' = \begin{bmatrix} \bigstar_{p'\times o} \\ \hat{D} \\ O_{r'\times o} \end{bmatrix},$$

where each occurrence of $\bigstar$ represents a different matrix of dimensions specified in the subscripts. We can see that a minimal realisation $\langle \hat{A}, \hat{D}\rangle$ (of order q) is embedded in these matrices, albeit in different positions. The latter can be phrased by means of matrix transformations. More specifically, one can show that

$$P_A \cdot A \cdot S = S \cdot B \cdot P_B, \tag{1}$$

where P_A and P_B are matrices representing *orthogonal projection operators* on the *controllable and observable spaces* of $\langle A, D\rangle$ and $\langle B, D'\rangle$, respectively, and S is a matrix such that

$$D = S \cdot D' \text{ and } D^* \cdot S = (D')^*. \tag{2}$$

Intuitively, the controllable and observable space of a system $\langle A, D\rangle$, denoted by $\mathsf{CO}_{\langle A,D\rangle}$, consists of all vectors obtained by a linear combination of $A^i \cdot D$, for varying i, and which are *not* in the null space of vectors obtained by a linear combination of $D^* \cdot A^j$, for varying j. When interested in the dynamics $D^* \cdot A^k \cdot D$ only those vectors matter and, in fact, $\hat{A}$ is the matrix representation of A restricted to this space[3]. So, equation (1) is just stating that A and B are related (by matrix S) after appropriate projections are in place. Using properties of projection operators P_A and P_B, and (2), the following can be verified:

▶ **Theorem 18.** *Let A and B be in $\mathsf{Mat}_{n\times n}(\mathbb{C})$ and D and D' in $\mathsf{Mat}_{n\times o}(\mathbb{C})$. Then, $D^* \cdot A^k \cdot D = (D')^* \cdot B^k \cdot D'$, for any k, if and only if there exists a matrix S such that $D = S \cdot D'$ and $D^* \cdot S = (D')^*$ and such that $P_A \cdot A \cdot S = S \cdot B \cdot P_B$ for projection operators P_A and P_B on $\mathsf{CO}_{\langle A,D\rangle}$ ad $\mathsf{CO}_{\langle B,D'\rangle}$, respectively.* ◀

We can further show that this result also holds for our general notion of dynamics, using a *generalised notion of controllable and unobservable space* based on words rather than powers of matrices.

▶ **Proposition 19.** *Let A and B be in $\mathsf{Mat}_{n\times n}(\mathbb{C})$ and D and D' in $\mathsf{Mat}_{n\times o}(\mathbb{C})$. Then, $D^* \cdot w(A, A^*) \cdot D = (D')^* \cdot w(B, B^*) \cdot D'$ for all words $w(x, y)$ if and only if there exists a matrix S such that $D = S \cdot D'$ and $D^* \cdot S = (D')^*$ and such that $P_A \cdot A \cdot S = S \cdot B \cdot P_B$ and $P_A \cdot A^* \cdot S = S \cdot B^* \cdot P_B$ for projection operators P_A and P_B on $\widetilde{\mathsf{CO}}_{\langle A,D\rangle}$ and $\widetilde{\mathsf{CO}}_{\langle B,D'\rangle}$, respectively.* ◀

Here, $\widetilde{\mathsf{CO}}$ indicates that we work with the generalised CO space. In all this, real matrices can be used when A, B, D and D' are real. These results *directly translate* into characterisations of $\mathsf{ML}(\mathcal{L})$-equivalence for the fragments considered in this section.

[3] We refer to any textbook on linear systems, such as [13], for more background.

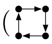
6.2 Results

$\mathsf{ML}(\mathbb{1}, \mathbb{1}^{\mathsf{t}})$-equivalence

For undirected graphs, $G \equiv_{\mathsf{ML}(\mathbb{1},\mathbb{1}^{\mathsf{t}})} H$ if and only if $A_G \cdot S = S \cdot A_H$ for a doubly quasi-stochastic matrix S if and only if G and H have the same number of walks of any length [20]. For general matrices, we can say the following. Let A and B be matrices in $\mathsf{Mat}_{n\times n}(\mathbb{C})$. From Example 15, we know that $A \equiv_{\mathsf{ML}(\mathbb{1},\mathbb{1}^{\mathsf{t}})} B$ implies that the systems $\langle A, \mathbb{1}\rangle$ and $\langle B, \mathbb{1}\rangle$ have the same dynamics. A direct application of Theorem 18 results in:

▶ **Corollary 20.** *Let A and B be matrices in $\mathsf{Mat}_{n\times n}(\mathbb{C})$. Then, $A \equiv_{\mathsf{ML}(\mathbb{1},\mathbb{1}^{\mathsf{t}})} B$ if and only if there is a doubly quasi-stochastic matrix S such that $P_A \cdot A \cdot S = S \cdot B \cdot P_B$ for projection operators P_A and P_B.* ◀

So, the only difference with the undirected graph case is the use of the projection operators. This cannot be avoided, as shown in the example below. We also observe that for digraphs, $G \equiv_{\mathsf{ML}(\mathbb{1},\mathbb{1}^{\mathsf{t}})} H$ is clearly equivalent to G and H having the same number of semi-walks of type "$\rightarrow^k$" for any k, similar as in the undirected graph case.

▶ **Example 21.** Consider directed graphs G_4 () and H_4 (). Both have 4 semi-walks of type "$\rightarrow^k$" for any k, i.e., $\mathbb{1}^{\mathsf{t}} \cdot A_{G_4}^k \cdot \mathbb{1} = 4 = \mathbb{1}^{\mathsf{t}} \cdot A_{H_4}^k \cdot \mathbb{1}$, for all $k \geq 0$. It is an easy exercise to show that there is no doubly quasi-stochastic matrix S such that $A_{G_4} \cdot S = S \cdot A_{H_4}$. We thus have to rely on Corollary 20. It can be verified that the minimal realisations of $\langle A_{G_4}, \mathbb{1}\rangle$ and $\langle A_{H_4}, \mathbb{1}\rangle$ consist of $\langle \hat{A} = [1], \hat{\mathbb{1}} = [2]\rangle$. So, indeed, $4 = [2]^{\mathsf{t}} \cdot [1]^k \cdot [2]$ for any k, as desired. Furthermore,

$$\underbrace{\begin{bmatrix} \frac{1}{4} & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} \\ \frac{1}{4} & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} \\ \frac{1}{4} & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} \\ \frac{1}{4} & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} \end{bmatrix}}_{P_{A_{G_4}}} \cdot A_{G_4} \cdot \underbrace{\begin{bmatrix} \frac{1}{4} & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} \\ \frac{1}{4} & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} \\ \frac{1}{4} & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} \\ \frac{1}{4} & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} \end{bmatrix}}_{S} = \underbrace{\begin{bmatrix} \frac{1}{4} & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} \\ \frac{1}{4} & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} \\ \frac{1}{4} & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} \\ \frac{1}{4} & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} \end{bmatrix}}_{S} \cdot A_{H_4} \cdot \underbrace{\begin{bmatrix} \frac{1}{4} & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} \\ \frac{1}{4} & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} \\ \frac{1}{4} & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} \\ \frac{1}{4} & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} \end{bmatrix}}_{P_{H_4}}.$$

That the same matrices are being used on both sides is just specific for this example. ◀

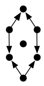
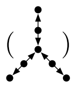
Corollary 20 begs the question why no projection operators are required when undirected graphs are concerned. The reason is that for normal matrices, the transformation matrices involved in the proof of Theorem 18 can be chosen to consist of eigenvectors of A and B (recall that normal matrices have n independent eigenvectors). This allows to simplify the expression $P_A \cdot A \cdot S = S \cdot B \cdot P_B$ into $A \cdot S = S \cdot B$.

▶ **Proposition 22.** *Let A and B be normal matrices in $\mathsf{Mat}_{n\times n}(\mathbb{C})$. Then, $A \equiv_{\mathsf{ML}(*,\mathbb{1})} B$ if and only if $A \equiv_{\mathsf{ML}(\mathbb{1},\mathbb{1}^{\mathsf{t}})} B$ if and only if there exists a doubly quasi-stochastic matrix S such that $A \cdot S = S \cdot B$. For real matrices, S can be assumed to be real.* ◀

This is again analogous to the undirected graph case. We anticipated in Section 5 that will say something more about $\mathsf{ML}(\mathsf{tr}, \mathbb{1}, \mathbb{1}^{\mathsf{t}})$-equivalence. One can verify, by an analysis of expressions, that $A \equiv_{\mathsf{ML}(\mathsf{tr},\mathbb{1},\mathbb{1}^{\mathsf{t}})} B$ if and only if $A \equiv_{\mathsf{ML}(\mathsf{tr})} B$ and $A \equiv_{\mathsf{ML}(\mathbb{1},\mathbb{1}^{\mathsf{t}})} B$. Hence, Proposition 10 and Corollary 20 result in:

▶ **Corollary 23.** *Let A and B be matrices in $\mathsf{Mat}_{n\times n}(\mathbb{C})$. Then, $A \equiv_{\mathsf{ML}(\mathsf{tr},\mathbb{1},\mathbb{1}^{\mathsf{t}})} B$ if and only if A and B have the same characteristic polynomial and $P_A \cdot A \cdot S = S \cdot B \cdot P_B$ for a doubly quasi-stochastic matrix S.* ◀

In other words, compared to Proposition 10, we can replace the condition related to the complements $\bar{A}$ and $\bar{B}$ by the revised similarity condition.

▶ **Example 24.** The digraphs G_2 () and H_2 () from Example 11 are $\mathsf{ML}(\mathsf{tr}, \mathbb{1}, \mathbb{1}^{\mathsf{t}})$-equivalent. They have the same characteristic polynomial ($p_{A_{G_2}}(z) = -z^7 = p_{A_{H_2}}(z)$) and one can verify that the minimal realisation of $\langle A_{G_2}, \mathbb{1}\rangle$ and $\langle A_{H_2}, \mathbb{1}\rangle$ is given by $\hat{A} = \begin{bmatrix} \frac{6}{7} & -\frac{1}{7}(3\sqrt{3}) \\ \frac{4\sqrt{3}}{7} & -\frac{6}{7} \end{bmatrix}$ and $\hat{\mathbb{1}} = \begin{bmatrix} \sqrt{7} \\ 0 \end{bmatrix}$. We see that $\hat{\mathbb{1}}^{\mathsf{t}} \cdot \hat{\mathbb{1}} = 7$, $\hat{\mathbb{1}}^{\mathsf{t}} \cdot \hat{A} \cdot \hat{\mathbb{1}} = 6$ and for $k \geq 2$, $\hat{\mathbb{1}}^{\mathsf{t}} \cdot \hat{A}^k \cdot \hat{\mathbb{1}} = 0$ because $\hat{A}^2 = O$. This is in accordance with Example 11. We have seen that there is no orthogonal similarity between A_{G_2} and A_{H_2}. One can also verify that no doubly quasi-stochastic matrix links these matrices. We thus have to rely on Corollary 20 and one can show that $P_{A_{G_2}} \cdot A_{G_2} \cdot S = S \cdot A_{H_2} \cdot P_{A_{H_2}}$ with

$$P_{A_{G_2}} = P_{A_{H_2}} = \begin{bmatrix} \frac{1}{4} & 0 & \frac{1}{4} & 0 & \frac{1}{4} & 0 & \frac{1}{4} \\ 0 & \frac{1}{3} & 0 & \frac{1}{3} & 0 & \frac{1}{3} & 0 \\ \frac{1}{4} & 0 & \frac{1}{4} & 0 & \frac{1}{4} & 0 & \frac{1}{4} \\ 0 & \frac{1}{3} & 0 & \frac{1}{3} & 0 & \frac{1}{3} & 0 \\ \frac{1}{4} & 0 & \frac{1}{4} & 0 & \frac{1}{4} & 0 & \frac{1}{4} \\ 0 & \frac{1}{3} & 0 & \frac{1}{3} & 0 & \frac{1}{3} & 0 \\ \frac{1}{4} & 0 & \frac{1}{4} & 0 & \frac{1}{4} & 0 & \frac{1}{4} \end{bmatrix},$$

and S the identity matrix. Again, that $P_{A_{G_2}} = P_{A_{H_2}}$ is just a coincidence. ◀

$\mathsf{ML}(^*, \mathbb{1})$-equivalence

Consider two matrices A and B in $\mathsf{Mat}_{n\times n}(\mathbb{C})$ and consider the systems $\langle A, \mathbb{1}\rangle$ and $\langle B, \mathbb{1}\rangle$. As we have seen in Example 16, $A \equiv_{\mathsf{ML}(^*,\mathbb{1})} B$ implies that $\mathbb{1}^{\mathsf{t}} \cdot w(A, A^*) \cdot \mathbb{1} = \mathbb{1}^{\mathsf{t}} \cdot w(B, B^*) \cdot \mathbb{1}$ for every word $w(x, y)$ and hence Proposition 19 applies, resulting in:

▶ **Proposition 25.** *Let A and B be in $\mathsf{Mat}_{n\times n}(\mathbb{C})$. Then, $A \equiv_{\mathsf{ML}(^*,\mathbb{1})} B$ if and only if $P_A \cdot A \cdot S = S \cdot B \cdot P_B$ and $P_A \cdot A^* \cdot S = S \cdot B^* \cdot P_B$ for a doubly quasi-stochastic matrix S and for projection operators P_A and P_B.* ◀

We remark that P_A and P_B are now projection operators on the generalised controllable spaces of $\langle A, \mathbb{1}\rangle$ and $\langle B, \mathbb{1}\rangle$, respectively.

▶ **Example 26.** We do not have a digraph example at hand such that $G \equiv_{\mathsf{ML}(^*,\mathbb{1})} H$ holds and which shows the necessity of the projection operators in Proposition 25. All efforts resulted in $A_G \cdot S = S \cdot A_H$ and $A_G^{\mathsf{t}} \cdot S = S \cdot A_H^{\mathsf{t}}$ for a doubly quasi-stochastic matrix S, i.e., without needing the projection operators. Finding such a digraph example or showing that the projection operators can be eliminated is left as an open problem. ◀

$\mathsf{ML}(^*, \mathbb{1}, \odot_v)$-equivalence

For undirected graphs, $\mathsf{ML}(^*, \mathbb{1}, \odot_v)$-equivalence coincides with the graphs being fractionally isomorphic, with having a common equitable partition, and with being C^2-equivalent [37, 38, 10, 30, 20]. We recall that a fractional isomorphism between graphs G and H is a doubly stochastic matrix S such $A_G \cdot S = S \cdot A_H$.

When considering $\mathsf{ML}(^*, \mathbb{1}, \odot_v)$-equivalence of arbitrary matrices, we simply need to use the corresponding notions of equitable partitions as in Section 5 for $\mathsf{ML}(\mathsf{tr}, ^*, \mathbb{1}, \odot_v)$-equivalence. We can again use Proposition 19 to obtain a characterisation.

▶ **Example 27.** Let A, B in $\mathsf{Mat}_{n\times n}(\mathbb{C})$ and let $\mathbb{1}_{V_i}$ and $\mathbb{1}_{W_i}$, for $i \in [1, q]$, represent common equitable partitions of A and B, respectively. We can obtain these indicator vectors by expressions $\mathsf{equit}_i(X) \in \mathsf{ML}(^*, \mathbb{1}, \odot_v)$, for $i \in [1, q]$ (Proposition 13). Hence, $A \equiv_{\mathsf{ML}(^*,\mathbb{1},\odot_v)} B$ implies that $\mathbb{1}^{\mathsf{t}}_{V_i} \cdot w(A, A^*) \cdot \mathbb{1}_{V_j} = \mathbb{1}^{\mathsf{t}}_{W_i} \cdot w(B, B^*) \cdot \mathbb{1}_{W_j}$ for every word $w(x, y)$ and any $i, j \in [1, q]$. By letting $D = [\mathbb{1}_{V_1} \ldots \mathbb{1}_{V_p}]$ and $D' = [\mathbb{1}_{W_1} \ldots \mathbb{1}_{W_p}]$, $A \equiv_{\mathsf{ML}(^*,\mathbb{1},\odot_v)} B$ implies that $D^* \cdot w(A, A^*) \cdot D = (D')^* \cdot w(B, B^*) \cdot D'$ for every word $w(x, y)$. Hence, $\langle A, D\rangle$ and $\langle B, D'\rangle$ have the same generalised dynamics. ◀

Hence, Proposition 19 implies that $A \equiv_{\mathsf{ML}(^*,\mathbb{1},\odot_v)} B$ if and only if $P_A \cdot A \cdot S = S \cdot B \cdot P_B$ and $P_A \cdot A^* \cdot S = S \cdot B^* \cdot P_B$ for a matrix S satisfying $\mathbb{1}_{V_i} = S \cdot \mathbb{1}_{W_i}$ and $\mathbb{1}^{\mathsf{t}}_{V_i} \cdot S = \mathbb{1}^{\mathsf{t}}_{W_i}$, for all $i \in [1, q]$. We remark again that this implies that S is doubly quasi-stochastic. We can do better, however, and eliminate the projection operators and ensure that S is doubly-stochastic and hence, A and B are fractionally isomorphic.

▶ **Corollary 28.** *Let A and B be matrices in $\mathsf{Mat}_{n\times n}(\mathbb{C})$. Then $A \equiv_{\mathsf{ML}(^*,\mathbb{1},\odot_v)} B$ if and only if there is a doubly stochastic matrix S such that $A \cdot S = S \cdot B$ and $A^* \cdot S = S \cdot B^*$, $\mathbb{1}_{V_i} = S \cdot \mathbb{1}_{W_i}$ and $\mathbb{1}^{\mathsf{t}}_{V_i} \cdot S = \mathbb{1}^{\mathsf{t}}_{W_i}$, for all $i \in [1, q]$, for indicator vectors describing a common equitable partition of A and B.*

Proof. (Sketch). It can be verified that the transformation matrices underlying the proof of Proposition 19 for the systems $\langle A, D\rangle$ and $\langle B, D'\rangle$ from Example 27 are of a very particular form. Indeed, using the fact that D and D' represent equitable partitions, the column vectors in these matrices can be shown to span the generalised controllable and observable space of $\langle A, D\rangle$ and $\langle B, D'\rangle$. As a consequence, one obtains that $P_A = \Pi \cdot \Pi^{\mathsf{t}}$, $P_V = \Pi' \cdot (\Pi')^{\mathsf{t}}$ and $S = \Pi \cdot (\Pi')^{\mathsf{t}}$, where $\Pi = D \cdot (D^{\mathsf{t}} \cdot D)^{-1/2}$ and $\Pi' = D' \cdot ((D')^{\mathsf{t}} \cdot D')^{-1/2}$. Hence, $\Pi \cdot (\Pi^{\mathsf{t}}) \cdot A \cdot \Pi \cdot (\Pi')^{\mathsf{t}} = \Pi \cdot (\Pi')^{\mathsf{t}} \cdot B \cdot \Pi' \cdot (\Pi')^{\mathsf{t}}$. A second crucial observation is that, in a similar way as shown in the proof of Theorem 4.1 in [24], one can verify that $\Pi \cdot \Pi^{\mathsf{t}}$ commutes with A and similarly, $\Pi' \cdot (\Pi')^{\mathsf{t}}$ commutes with B, due to equitability. Further manipulation then shows that P_A and P_B can be omitted, resulting in $A \cdot \Pi \cdot (\Pi')^{\mathsf{t}} = \Pi \cdot (\Pi')^{\mathsf{t}} \cdot B$. It now suffices to observe that for $S = \Pi \cdot (\Pi')^{\mathsf{t}}$, we have that $S_{vw} = \frac{1}{|V_k|}$ for the unique part V_k such that $i \in V_k$ and $j \in W_k$, and $S_{vw} = 0$ otherwise. It is now easy to verify that S satisfies the conditions stated in the Corollary. ◀

For digraphs, the existence of a stochastic matrix S such that $A_G \cdot S = S \cdot A_H$ and $A^{\mathsf{t}}_G \cdot S = S \cdot A^{\mathsf{t}}_H$ hold is known to correspond to $G \equiv_{\mathsf{C}^2} H$ [1, 25]. Hence, the previous Corollary implies that $G \equiv_{\mathsf{ML}(^*,\mathbb{1},\odot_v)} H$ if and only if $G \equiv_{\mathsf{C}^2} H$, just as for undirected graphs. We also remark that Corollary 28 can be shown by relying on known correspondences between fractional isomorphisms and equitable partitions of matrices [1, 25]. Nevertheless, proving it by relying on minimal realisations (Proposition 19) further illustrates the usefulness of our approach.

▶ Remark 29. We can obtain similar results for $\mathsf{ML}(\mathbb{1}, \mathbb{1}^{\mathsf{t}}, \odot_v)$-equivalence. In this case, we have to use standard linear systems described by $\langle A, C_c, D_r\rangle$ where C_c consists of transposed indicator vectors of a column-equitable partition of A and D_r consists of indicator vectors of a row-equitable partition of A. Note that C_c is not necessarily equal to the transpose of D_r. Then, given $\langle A, C_c, D_r\rangle$ and $\langle B, C'_c, D'_r\rangle$, a generalisation of Theorem 18 allows to obtain a relationship between A and B. We defer the precise analysis of $\mathsf{ML}(\mathbb{1}, \mathbb{1}^{\mathsf{t}}, \odot_v)$-equivalence to future work. ◀

7 Concluding remarks

While at first, it seemed daunting to understand the distinguishing power of MATLANG on general matrices, we showed that moving to this more general setting (compared to adjacency matrices of undirected graphs) makes the analysis more elegant. Of course, the right tools are needed, such as the connection with Specht's Theorem and mininal realisations of linear systems. Considering the general setting has as additional advantage that previous results can be seen as special cases. Although we focused on the setting where MATLANG expressions only take a single matrix as input, some of our results can be generalised. This is particularly true for cases relying on Specht's Theorem. It is less clear how to deal with multiple inputs by relying on linear systems theory.

In this work, we consider equivalence of matrices by sentences that allow an arbitrary number of applications of the supported operators. In practice, one would like to understand the impact of allowing, say only k matrix multiplications. Indeed, each operator application has a computational cost attached. Developing the right tools for analysing such a quantified setting is, we believe, an interesting line of research.

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