# Dimension Reduction via Colour Refinement

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**Abstract**

Colour refinement is a basic algorithmic routine for graph isomorphism testing, appearing as a subroutine in almost all practical isomorphism solvers. It partitions the vertices of a graph into "colour classes" in such a way that all vertices in the same colour class have the same number of neighbours in every colour class. Tinhofer [27], Ramana, Scheinerman, and Ullman [23] and Godsil [13] established a tight correspondence between colour refinement and fractional automorphisms of graphs.

We introduce versions of colour refinement for weighted directed graphs, for matrices, and for linear programs and extend existing quasilinear algorithms for computing the colour classes. Then we generalise the correspondence between colour refinement and fractional automorphisms and fractional isomorphisms, giving a new proof that is much simpler than the known proofs even in the setting of unweighted undirected graphs.

We apply our results to reduce the dimensions of linear programs. Specifically, we show that any given linear program $L$ can efficiently be transformed into a (potentially) smaller linear program $L'$ whose number of variables and constraints is the number of colour classes of the colour refinement algorithm. (When applied to a linear program, colour refinement yields partitions both of the constraints and of the variables.) The transformation is such that we can easily (by a linear mapping) transform both feasible and optimal solutions back and forth between the two LPs. We demonstrate empirically that colour refinement can indeed greatly reduce the cost of solving linear programs. A precursor of the method proposed here has been applied successfully by the second and third author (jointly with Ahmadi) to inference problems in machine learning [20].

## 1 Introduction

Colour refinement (a.k.a. "naive vertex classification" or "colour passing") is a basic algorithmic routine for graph isomorphism testing. It iteratively partitions, or colours, the vertices of a graph according to an iterated degree sequence: initially, all vertices get the same colour, and then in each round of the iteration two vertices that so far have the same colour get different colours if for some colour $c$ they have a different number of neighbours of colour $c$. The iteration stops if in some step the partition remains unchanged; the resulting partition is known as the *coarsest equitable partition* of the graph. By refining the partition asynchronously using Hopcroft's strategy of "processing the smaller half" (for DFA-minimisation [14]), the coarsest equitable partition of a graph can be computed very efficiently, in time $O((n + m) \log n)$ [10, 21] (also see [3] for a matching lower bound).

When applied in the context of graph isomorphism testing, the goal of colour refinement is to partition the vertices of a graph as finely as possible, ideally one would like to compute the partition of the vertices into the orbits of the automorphism group of the graph. In this paper, our goal is to partition the vertices as coarsely as possible. We observe that by applying a generalisation of colour refinement (to be outlined soon) to a linear program $L$ and then "factoring" $L$ through the "equitable partition" of the variables and constraints, we obtain a smaller linear program $L'$ equivalent to $L$, in the sense that feasible and optimal solutions can be transferred back and forth between $L$ and $L'$ via simple linear mappings.

Hence we can use colour refinement as a simple and efficient preprocessing routine for linear programming, transforming a given linear program into an equivalent one in a lower dimensional space and with fewer constraints.

This has interesting applications in coding theory, statistical design and graph theory, for example, when computing maximum cardinality binary error correcting codes, edge colourings, minimum dominating sets in Hamming graphs, and Steiner-triple systems — as we will illustrate in the present paper — but also in machine learning when computing, say, the value function of a Markov decision problem or performing inference in graphical models, see e.g. [20]. Actually, many problems arising in a wide variety of other fields such as semantic web, network communication, computer vision, and robotics can actually be modelled using graphical models. Moreover, we often face inference problems with symmetries in the graphical model that are not exploited by classical inference approaches such as loopy belief propagation. Instead, symmetry-aware approaches, see e.g. [25, 16, 1, 9], run (a modified) loopy belief propagation on the quotient model of the (fractional) automorphisms of the graphical model and have been proven successful in several applications such as link prediction, social network analysis, satisfiability and boolean model counting problems.

### *Colour Refinement on Matrices and Weighted Graphs*

Consider a matrix $A \in \mathbb{R}^{V \times W}$.[1] We iteratively compute partitions $\mathcal{P}_i$ and $\mathcal{Q}_i$ of the rows and columns of $A$, that is, of the sets $V$ and $W$. We let $\mathcal{P}_0 = \{V\}$ and $\mathcal{Q}_0 = \{W\}$ be the trivial partitions. To define $\mathcal{P}_{i+1}$, we put two rows $v, v'$ in the same class if they are in the same class of $\mathcal{P}_i$ and if for all classes $Q$ of $\mathcal{Q}_i$,

$$\sum_{w \in Q} A_{vw} = \sum_{w \in Q} A_{v'w}. \tag{1.1}$$

Similarly, to define $\mathcal{Q}_{i+1}$, we put two columns $w, w'$ in the same class if they are in the same class of $\mathcal{Q}_i$ and if for all classes $P$ of $\mathcal{P}_i$,

$$\sum_{v \in P} A_{vw} = \sum_{v \in P} A_{vw'}. \tag{1.2}$$

Clearly, for some $i \leqslant m+n$ we have $(\mathcal{P}_i, \mathcal{Q}_i) = (\mathcal{P}_{i+1}, \mathcal{Q}_{i+1}) = (\mathcal{P}_j, \mathcal{Q}_j)$ for all $j \geqslant i$. We call $(\mathcal{P}_\infty, \mathcal{Q}_\infty) := (\mathcal{P}_i, \mathcal{Q}_i)$ the *coarsest equitable partition* of $A$. Here and in the following, we often refer to a pair $(\mathcal{P}, \mathcal{Q})$ of partitions of $V, W$, respectively, as a *partition of* $A \in \mathbb{R}^{V \times W}$. We call a partition $(\mathcal{P}, \mathcal{Q})$ of $A$ an *equitable partition* of $A$ if for all $P \in \mathcal{P}$, $Q \in \mathcal{Q}$ and all $v, v' \in P$, $w, w' \in Q$, equations (1.1) and (1.2) hold. It is easy to see that every equitable partition $(\mathcal{P}, \mathcal{Q})$ refines $(\mathcal{P}_\infty, \mathcal{Q}_\infty)$ and thus that $(\mathcal{P}_\infty, \mathcal{Q}_\infty)$ is indeed the coarsest equitable partition.

To see that this is a direct generalisation of colour refinement on graphs, suppose that $A$ is a 0-1-matrix, and view it as the adjacency matrix of a bipartite graph $B_A$ with vertex set $V(B_A) = V \cup W$ and edge set $E(B_A) = \{vw \mid A_{vw} \neq 0\}$. Then the coarsest equitable partition of $A$ is equal to the partition of $V(B_A)$ obtained by running colour refinement on $B_A$ starting from the partition $\{V, W\}$. More generally, we may associate a weighted bipartite graph with every matrix, where the edge weights correspond to the matrix entries. Hence our colour refinement procedure for matrices may be viewed as a generalisation of colour refinement to weighted bipartite graphs. We will also consider a version for arbitrary weighted directed graphs.

[1] We find it convenient to index the rows and columns of our matrices by elements of finite sets $V, W$, respectively, which we assume to be disjoint. $\mathbb{R}^{V \times W}$ denotes the set of matrices with real entries and row and column indices from $V$, $W$, respectively. The order of the rows and columns of a matrix is irrelevant for us. We denote the entries of a matrix $A \in \mathbb{R}^{V \times W}$ by $A_{vw}$.

The key result that enables us to apply colour refinement to linear programming is a generalisation of a beautiful result due to Tinhofer [27], Ramana, Scheinerman, and Ullman [23] and Godsil [13] that connects the equitable partitions of a graph with its *fractional automorphisms*. We generalise this theorem to matrices. Our notion of fractional automorphism of a matrix $A \in \mathbb{R}^{V \times W}$ is based on the view that an *automorphism* of a matrix is a pair of permutations of the rows and columns that leaves the matrix invariant, or equivalently, a pair $(P, Q) \in \mathbb{R}^{V \times V} \times \mathbb{R}^{W \times W}$ of permutation matrices such that $PA = AQ$. A *fractional automorphism* of $A$ is a pair $(X, Y) \in \mathbb{R}^{V \times V} \times \mathbb{R}^{W \times W}$ of doubly stochastic matrices such that

$$XA = AY. \tag{1.3}$$

To state the theorem, we need two more definitions. For every partition $\mathcal{R}$ of a set $U$, we let $\overline{\mathcal{R}}$ be the $U \times U$-matrix with entries $\overline{\mathcal{R}}_{uu'} = 1/|R|$ for $u, u' \in U$ contained in the same class $R \in \mathcal{R}$ and $\overline{\mathcal{R}}_{uu'} = 0$ for $u, u' \in U$ contained in distinct classses of $\mathcal{R}$. The *components* of a matrix $Z \in \mathbb{R}^{U \times U}$ are the vertex sets of the strongly connected components of the digraph $D_Z$ with vertex set $V(D_Z) = U$ and edge set $E(D_Z) = \{uu' \in U^2 \mid Z_{uu'} \neq 0\}$, and by $\overline{Z}$ we denote the partition of $U$ into the components of $Z$.

**Theorem 1.1.** *Let $A \in \mathbb{R}^{V \times W}$.*

*(1) If $(\mathcal{P}, \mathcal{Q})$ is an equitable partition of $A$ then $(\overline{\mathcal{P}}, \overline{\mathcal{Q}})$ is a fractional automorphism.*

*(2) If $(X, Y)$ is a fractional automorphism of $A$, then $(\overline{X}, \overline{Y})$ is an equitable partition.*

We will show that the known results [27, 23, 13] relating fractional automorphisms and fractional isomorphisms of graphs with equitable partitions all follow directly from Theorem 1.1. Our proof of the theorem is elementary and simple, arguably much simpler than the known proofs of the special case of the theorem for graphs.

Adopting Paige and Tarjan's [21] algorithm for computing the coarsest equitable partition of a graph, we obtain an algorithm that, given a sparse representation of a matrix $A$, computes the coarsest equitable partition of $A$ in time $O((n + m) \log n)$, where $n = |V| + |W|$ and $m$ is the total bitlength of all nonzero entries of $A$ (so that the input size is $O(n + m)$).

*Application to Linear Programming*

Consider a linear program $L = L(A, b, c)$ in standard form:

$$\begin{gathered} \min c \cdot x \\ \text{subject to } Ax = b,\ x \geqslant 0, \end{gathered} \tag{1.4}$$

where $A \in \mathbb{R}^{V \times W}$, $b \in \mathbb{R}^{V}$, and $c \in \mathbb{R}^{W}$. An *equitable partition of $L$* is an equitable partition $(\mathcal{P}, \mathcal{Q})$ of $A$ such that $b$ is $\mathcal{P}$-invariant, that is, $b_v = b_{v'}$ for all $v, v' \in P \in \mathcal{P}$, and similarly, $c$ is $\mathcal{Q}$-invariant. We call the pair $(|\mathcal{P}|, |\mathcal{Q}|)$ the *dimension* of $(\mathcal{P}, \mathcal{Q})$.

**Theorem 1.2.** *Let $L$ be the linear program* (1.4)*, and let $(p, q)$ be the dimension of the coarsest equitable partition of $L$. Then there are matrices $\widehat{X} \in \mathbb{R}^{[p] \times V}$, $\check{Y} \in \mathbb{R}^{W \times [q]}$, and $\widehat{Y} \in \mathbb{R}^{[q] \times W}$ such that the following holds.*

*Let $A' = \widehat{X} A \check{Y} \in \mathbb{R}^{[p] \times [q]}$ and $b' = \widehat{X} b$ and $c' = \widehat{Y}^t c$, and let $L' = L(A', b', c')$ be defined as in* (1.4)*. Then the linear mapping $x \mapsto \widehat{Y} x$ maps the space of feasible solutions to $L$ to the space of feasible solutions to $L'$ and preserves optimality, and conversely, the linear mapping $x' \mapsto \check{Y} x'$ maps the space of feasible solutions to $L'$ to the space of feasible solutions to $L$ and preserves optimality.*

*Furthermore, sparse representations of the matrices $\widehat{X}, \check{Y}, \widehat{Y}$ can be computed from a sparse representation of $L$ in time $O((n + m) \log n)$, where $n = |V| + |W|$ and $m$ is the total bitlength of all nonzero entries of $A$.*

The matrices $\widehat{X}, \check{Y}, \widehat{Y}$ in the theorem are the suitably scaled and possibly transposed incidence matrices of the coarsest equitable partition of $L$. Thus essentially, we factor the LP $L$ by the coarsest equitable partition. Via fractional automorphisms, our reduction may be viewed as a form of "symmetry reduction". Compared to other forms of symmetry reduction using automorphisms of the matrix instead of fractional automorphisms, our method has two advantages. (1) Since we are not looking for full symmetries, we potentially have fewer equivalence classes and thus a better reduction. (2) As colour refinement is fast, the reduced LP can be computed very efficiently, much more efficiently than with methods based on computing automorphisms. This has been confirmed by our computational evaluation on a number of benchmark LPs with symmetries present. Actually, the time spent in total on solving the LPs — reducing an LP and solving the reduced LP — is often an order of magnitude smaller than using automorphisms or no symmetry reduction at all.

*Related Work*

Using automorphisms to speed-up solving optimisation problems has attracted a lot of attention in the literature (e.g. [17, 22, 7, 11]). The most relevant for the present work are those focusing on integer and linear programming. For ILPs, methods typically focus on pruning the search space to eliminate symmetric solutions, see e.g. [19] for a survey). In linear programming, however, one takes advantage of convexity and projects the LP into the fixed space of its symmetry group [6]. The projections we investigate in the present paper are similar in spirit. Until recently, discussions were mostly concentrated on the case where the symmetry group of the ILP/LP consists of permutations, e.g. [5]. In such cases the problem of computing the symmetry group of the LP can be reduced to computing the coloured automorphisms of a "coefficient" graph connected with the linear program, see e.g. [4, 19]. Moreover, the reduction of the LP in this case essentially consists of mapping variables to their orbits. As we will see, our approach subsumes this method, as we replace the orbits with a coarser equivalence relation which, in contrast to the orbits, is computable in quasilinear time. Going beyond permutations, [6] extends the scope of symmetry, showing that any invertible linear map, which preserves the feasible region and objective of the LP may be used to speed-up solving. While this setting offers more compression, the symmetry detection problem becomes even more difficult [8]. Finally, the second and fourth author (together with Ahmadi) observed that equitable partitions can compress LPs, as they preserve message-passing computations within the log-barrier method [20]. The present paper builds upon that observation, giving a rigorous theory of dimension reduction using colour-refinement, and connecting to existing symmetry approaches through the notion of fractional automorphisms. Moreover, we show that the resulting theory yields a more general notion of fractional automorphism that ties in nicely with the linear-algebra framework and potentially leads to even better reductions than the purely combinatorial approach of [20].

## 2 Preliminaries

We use a standard notation for graphs and digraphs. We write edges without parentheses: $vw$ denotes the edge $\{v, w\}$ in a graph $G$ and the edge $(v, w)$ in a digraph $D$. In graph $G$, we let $N^G(v)$ denote the set of neighbours of vertex $v$, and in a digraph $D$ we let $N_+^D(v)$ and $N_-^D(v)$ denote, respectively, the sets of out-neighbours and in-neighbours of $v$.

We already introduced our basic notation for matrices. A matrix $X \in \mathbb{R}^{V \times W}$ is *stochastic* if it is nonnegative and $\sum_{w \in W} X_{vw} = 1$ for all $v \in V$. It is *doubly stochastic* if both $X$ and its transpose $X^t$ are stochastic.

A *convex combination* of numbers $a_i$ is a sum $\sum_i \lambda_i a_i$ where $\lambda_i \geqslant 0$ for all $i$ and $\sum_i \lambda_i = 1$. If $\lambda_i > 0$ for all $i$, we call the convex combination *positive*. We need the following simple (and well-known) lemma about convex combinations.

**Lemma 2.1.** *Let $D$ be a strongly connected digraph. Let $f : V(D) \to \mathbb{R}$, such that for every $v \in V(D)$, the* *number $f(v)$ is a positive convex combination of all $f(w)$ for $w \in N_+(v)$. Then $f$ is constant.*

*Proof.* Suppose for contradiction that $f$ satisfies the assumptions, but is not constant. Let $v \in V(D)$ be a vertex with maximum value $f(v)$ and $w \in V(D)$ such that $f(w) < f(v)$. Let $P$ be a path from $v$ to $w$. Then $P$ contains an edge $v'w'$ such that $f(v) = f(v') > f(w')$. By the maximality of $f(v)$, for all $w'' \in N_+(v')$ it holds that $f(v') \geqslant f(w'')$, and this contradicts $f(v')$ being a positive convex combination of the $f(w'')$ for $w'' \in N_+(v')$. $\square$

All our results hold for rational and real matrices and vectors. For the algorithms, we assume the input matrices and vectors to be rational. To analyse the algorithms, we use a standard RAM model.

## 3 Fractional Automorphisms and Equitable Partitions

Let $V, W$ be disjoint sets and $A \in \mathbb{R}^{V \times W}$. For every subset $P \subseteq V, Q \subseteq W$, we let

$$F_A(P,Q) = \sum_{(v,w) \in P \times Q} A_{vw}. \tag{3.1}$$

If we interpret $A$ as a weighted bipartite graph (as described in the introduction), then $F_A(P,Q)$ is the total weight of the edges from $P$ to $Q$. If $A$ is a 0-1-matrix, this is simply the number of edges from $P$ to $Q$. We omit the subscript $A$ in $F_A$ if $A$ is clear from the context, which it will almost always be, and we write $F(v,Q)$, $F(P,w)$ instead of $F(\{v\},Q)$, $F(P,\{w\})$. Rephrasing conditions (1.1) and (1.2) from the introduction, we note that a partition $(\mathcal{P}, \mathcal{Q})$ of $A$ is *equitable* if it satisfies the following two conditions for all $P \in \mathcal{P}, Q \in \mathcal{Q}$:

$$F(v,Q) = F(v',Q) \qquad \text{for all } v, v' \in P, \tag{3.2}$$
$$F(P,w) = F(P,w') \qquad \text{for all } w, w' \in Q. \tag{3.3}$$

An important observation that we frequently use is that for a doubly stochastic matrix $Z \in \mathbb{R}^{U \times U}$ the components, that is, the strongly connected components of the digraph $D_Z$ with vertex set $V(D_Z) = U$ and edge set $E(D_Z) = \{uu' \mid Z_{uu'} \neq 0\}$, coincide with the connected components of the undirected graph $G_Z$ with vertex set $V(G_Z) = U$ and edge set $E(G_Z) = \{uu' \mid u \neq u', Z_{uu'} \neq 0 \text{ or } Z_{u'u} \neq 0\}$. (In terms of the matrices this means that a doubly stochastic matrix in upper triangular block form is actually in diagonal block form.)

*Proof of Theorem 1.1.* To prove (1), let $(\mathcal{P}, \mathcal{Q})$ be an equitable partition of $A$. Let $v \in V, w \in W$, and let $P \in \mathcal{P}$ and $Q \in \mathcal{Q}$ be the classes of $v$ and $w$, respectively. Then

$$(\overline{\mathcal{P}}A)_{vw} = \sum_{v' \in P} \frac{1}{|P|} \cdot A_{v'w} = \frac{1}{|P|} \cdot F(P,w) \overset{(a)}{=} \frac{1}{|Q|} \cdot F(v,Q) = \sum_{w' \in Q} A_{vw'} \cdot \frac{1}{|Q|} = (A\overline{\mathcal{Q}})_{vw} \tag{3.4}$$

Equality $(a)$ can be established by a double-counting argument: we have $F(P,Q) = \sum_{v' \in P} F(v',Q) = |P| \cdot F(v,Q)$ by (3.2) and $F(P,Q) = \sum_{w' \in Q} F(P,w') = |Q| \cdot F(P,w)$ by (3.3).

To prove (2), let $(X,Y)$ be a fractional automorphism of $A$. Let $P \in \overline{X}$ and $Q \in \overline{Y}$. We first prove (3.2). For every $v \in P$, we have

$$\begin{aligned} F(v,Q) &= \sum_{w' \in Q} A_{vw'} \overset{(b1)}{=} \sum_{w' \in Q} A_{vw'} \sum_{w \in Q} Y_{w'w} = \sum_{w \in Q} \sum_{w' \in Q} A_{vw'} Y_{w'w} \\ &\overset{(b2)}{=} \sum_{w \in Q} \sum_{v' \in P} X_{vv'} A_{v'w} = \sum_{v' \in P} X_{vv'} \underbrace{\sum_{w \in Q} A_{v'w}}_{=F(v',Q)} \overset{(b3)}{=} \sum_{v' \in N_+^{D_X}(v)} X_{vv'} \cdot F(v',Q), \end{aligned} \tag{3.5}$$

Equation $(b1)$ holds because $\sum_{w \in W} Y_{w'w} = 1$ and $Y_{w'w} = 0$ for $w' \in Q, w \notin Q$. Here we use that $Q$, which by definition is a strongly connected component of the digraph $D_Y$, is also a connected component of the undirected graph $G_Y$. Equation $(b2)$ holds by $XA = AY$ and $Y_{w'w} = 0$ for $w' \notin Q, w \in Q$ and $X_{vv'} = 0$ for $v \in P, v' \notin P$. Equation $(b3)$ holds, because $N_+^{D_X}(v) \subseteq P$ and $X_{vv'} \neq 0 \iff v' \in N_+^{D_X}(v)$. As the matrix $X$ is stochastic, this also implies that $F(v, Q)$ is a positive convex combination of the $F(v', Q)$ for $v' \in N_+^{D_X}(v)$. As $P$ is the vertex set of a strongly connected component of $D_X$, by Lemma 2.1, it follows that $F(v, Q) = F(v', Q)$ for all $v, v' \in P$. This proves (3.2).

(3.3) can be proved similarly. □

While the proof of (1) is fairly straightforward, the proof of (2) is harder to penetrate. The following alternative reasoning may make it a bit clearer. Suppose first that the matrix $X$ has the following form: for every component $P$ of $X$, all entries $X_{vv'}$ for $v, v' \in P$ are equal and nonzero. We call such a matrix $X$ *homogeneous*. Actually, as $X$ is doubly stochastic, in the homogeneous case we must have $X_{vv'} = 1/|P|$ for all $v, v' \in P$. Suppose furthermore that $Y$ is homogeneous as well, that is, for all components $Q$ and all $w, w' \in Q$ we have $Y_{ww'} = 1/|Q|$. In this case, we can just revert the simple calculation that proved assertion (1): Let $P \in \overline{X}$, $Q \in \overline{Y}$. Choose an arbitrary $w \in Q$. Then, for all $v \in P$ we have

$$F(v, Q) = |Q| \cdot (AY)_{vw} \overset{(c)}{=} |Q| \cdot (XA)_{vw} = \frac{|Q|}{|P|} F(P, w).$$

Here $(c)$ holds by $XA = AY$. As the right-hand side $\frac{|Q|}{|P|} F(P, w)$ does not depend on $v$, this implies (3.2). (3.3) can be proved similarly.

Now let $(X, Y)$ be an arbitrary fractional automorphism of $A$. Without loss of generality, we may assume that all diagonal entries of $X$ and $Y$ are nonzero; if they are not, we take the matrices $X' = (1/2)X + (1/2)I_m$ and $Y' = (1/2)Y + (1/2)I_n$, which also form a fractional automorphism. Now the crucial observation is that the sequences $X^k$ and $Y^k$, for $k \to \infty$, converge to homogeneous matrices. To see this, view them as Markov chains and let them converge to their stationary distribution. By assuming the diagonal entries to be nonzero, we have avoided periodicity, and as the matrices are doubly stochastic, there are no transient states. For every $k$ the pair $(X^k, Y^k)$ is still a fractional automorphism of $A$. Thus the homogeneous limit matrices $(X^\infty, Y^\infty)$ also form a fractional automorphism, and moreover, they have the same components as $X, Y$. Now we can apply the simple argument for homogeneous matrices, and we are done.

### *3.1 Square Matrices and Weighted Digraphs*

So far, we have interpreted matrices as weighted bipartite graphs, and we have obtained a generalisation of Godsil's theorem about the connection between fractional automorphisms and equitable partitions for bipartite graphs. In this section, we turn to arbitrary graphs. We have to extend our theory to square matrices and automorphisms that permute rows and columns simultaneously.

Let $A \in \mathbb{R}^{V \times V}$ be a square matrix. A *2-sided equitable partition* of $A$ is a partition $\mathcal{P}$ of $V$ such that for all $P \in \mathcal{P}$ and $v, v' \in P$ we have

$$F(v, P) = F(v', P) \qquad \text{and} \qquad F(P, v) = F(P, v'). \tag{3.6}$$

Here $F = F_A$ is defined as before in (3.1).

A *2-sided fractional automorphism* of $A$ is a doubly stochastic matrix $X \in \mathbb{R}^{V \times V}$ such that

$$XA = AX \qquad \text{and} \qquad X^t A = AX^t. \tag{3.7}$$

**Corollary 3.1.** *Let $A \in \mathbb{R}^{V \times V}$ be a square matrix.*

*(1) If $\mathcal{P}$ is a 2-sided equitable partition of $A$ then $\overline{\mathcal{P}}$ is a 2-sided fractional automorphism.*

*(2) If $X$ is a 2-sided fractional automorphism of $A$, then $\overline{X}$ is a 2-sided equitable partition.*

*Proof.* (1) If $\mathcal{P}$ is a 2-sided equitable partition of $A$, then $(\mathcal{P}, \mathcal{P})$ is an equitable partition. Hence by Theorem 1.1, $(\overline{\mathcal{P}}, \overline{\mathcal{P}})$ is a fractional automorphism, and as $\overline{\mathcal{P}}$ is symmetric, it follows that it is a 2-sided fractional automorphism.

(2) If $X$ is a 2-sided fractional automorphism of $A$, then $(X, X)$ is a fractional isomorphism of $A$. Hence $(\overline{X}, \overline{X})$ is an equitable partition of $A$, and this implies that $\overline{X}$ is a 2-sided equitable partition. □

For symmetric matrices $A$, the situation is particularly nice, because the two conditions in (3.7) are equivalent and can be replaced by either one. Hence we obtain the following corollary, which generalises Godsil's theorem from [13] to weighted graphs.

**Corollary 3.2.** *Let $A \in \mathbb{R}^{V\times V}$ be a symmetric matrix and $X \in \mathbb{R}^{V\times V}$ a doubly stochastic matrix such that $XA = AX$. Then $\overline{X}$ is a 2-sided equitable partition of $A$.*

### *3.2 Fractional Isomorphisms*

In this section, we want to relate different matrices by "fractional isomorphisms". As this is only a side topic in this paper, we only define fractional isomorphisms for matrices of the same dimensions and leave it to future work to find a useful generalisation to pairs of matrices of different dimensions. The main purpose of this section is to point out that Theorem 1.1 implies the known results [23, 27] relating fractional isomorphisms and equitable partitions and generalises them to matrices and weighted digraphs.

Let $A \in \mathbb{R}^{V\times W}$ and $A' \in \mathbb{R}^{V'\times W'}$, where we assume $V, V', W, W'$ to be mutually disjoint. A *fractional isomorphism* from $A$ to $A'$ is a pair $(X, Y) \in \mathbb{R}^{V'\times V} \times \mathbb{R}^{W'\times W}$ of doubly stochastic matrices such that

$$XA = A'Y \tag{3.8}$$

$$X^tA' = AY^t. \tag{3.9}$$

Note that a fractional isomorphism can only exist if $|V| = |V'|$ and $|W| = |W'|$, because doubly stochastic matrices are always square. We are mainly interested in the question whether there is a fractional isomorphism between $A$ and $A'$. If there is, we call $A$ and $A'$ *fractionally isomorphic* (we write $A \cong^* A'$). Again, there is a connection with colour refinement and equitable partitions.

Let us review the situation for undirected graphs. Let $G, G'$ be undirected graphs with vertex sets $V, V'$, respectively, and let $A \in \mathbb{R}^{V\times V}$ and $A' \in \mathbb{R}^{V'\times V'}$ be their adjacency matrices. To use colour refinement as an isomorphism test, it is run on the disjoint union $G^*$ of $G$ and $G'$. We say that colour refinement *distinguishes* $G$ and $G'$ if there is some class $P$ of the coarsest equitable partition of $G^*$ such that $|P \cap V| \neq |P \cap V'|$. Tinhofer [27] proved that there is a fractional isomorphism $(X, X)$ from $A$ to $A'$ (a "2-sided" fractional isomorphism) if and only if colour refinement does not distinguish $G$ and $G'$.

Now consider arbitrary matrices $A \in \mathbb{R}^{V\times W}$ and $A' \in \mathbb{R}^{V'\times W'}$ again. Let $V^* = V \cup V'$ and $W^* = W \cup W'$ and

$$A^* = \begin{pmatrix} A & 0 \\ 0 & A' \end{pmatrix} \in \mathbb{R}^{V^*\times W^*}$$

This matrix is sometimes called the *direct sum* of $A$ and $A'$. If $A$ and $A'$ are adjacency matrices of graphs $G$ and $G'$, then $A^*$ is the adjacency matrix of the disjoint union of these two graphs. In the following, whenever we consider a partition $(\mathcal{P}^*, \mathcal{Q}^*)$ of $A^*$, we denote the elements of $\mathcal{P}^*$ by $P^*$ and those of $\mathcal{Q}^*$ by $Q^*$. For every $P^* \in \mathcal{P}^*$, we let $P = P^* \cap V$ and $P' = P^* \cap V'$. Similarly, for every $Q^* \in \mathcal{Q}^*$, we let $Q = Q^* \cap W$ and $Q' = Q^* \cap W'$.

We say that *colour refinement does not distinguish* $A$ and $A'$ if there is an equitable partition $(\mathcal{P}^*, \mathcal{Q}^*)$ of $A^*$ such that

$$|P| = |P'| \qquad \text{for all } P^* \in \mathcal{P}^*, \tag{3.10}$$
$$|Q| = |Q'| \qquad \text{for all } Q^* \in \mathcal{Q}^*. \tag{3.11}$$

Instead of an arbitrary equitable partition $(\mathcal{P}^*, \mathcal{Q}^*)$ of $A^*$, we can as well take the coarsest equitable partition $(\mathcal{P}^*_\infty, \mathcal{Q}^*_\infty)$ of $A^*$, because if $(\mathcal{P}^*, \mathcal{Q}^*)$ satisfies (3.10) and (3.11) then $(\mathcal{P}^*_\infty, \mathcal{Q}^*_\infty)$ does as well.

With every partition $(\mathcal{P}^*, \mathcal{Q}^*)$ of $A^*$ we associate matrices $\overline{\overline{\mathcal{P}^*}} \in \mathbb{R}^{V' \times V}$ and $\overline{\overline{\mathcal{Q}^*}} \in \mathbb{R}^{W' \times W}$ defined by

$$\overline{\overline{\mathcal{P}^*}}_{v'v} = \begin{cases} \dfrac{1}{|P|} & \text{if } v', v \in P^* \text{ for some } P^* \in \mathcal{P}^*, \\ 0 & \text{otherwise} \end{cases}$$

for $v' \in V', v \in V$, and

$$\overline{\overline{\mathcal{Q}^*}}_{w'w} = \begin{cases} \dfrac{1}{|Q|} & \text{if } w', w \in Q^* \text{ for some } Q^* \in \mathcal{Q}^*, \\ 0 & \text{otherwise} \end{cases}$$

for $w' \in W', w \in W$.

Conversely, for every matrix $X \in \mathbb{R}^{V' \times V}$ we let $\overline{\overline{X}}$ be the partition of $V^* = V \cup V'$ into the vertex sets of the connected components of the bipartite graph $B_X$ (with vertex set $V^*$ and edges $v'v$ for all $v' \in V', v \in V$ with $X_{v'v} \neq 0$; viewed as an undirected graph). For every matrix $Y \in \mathbb{R}^{W' \times W}$ we define the partition $\overline{\overline{Y}}$ of $W^*$ similarly.

**Corollary 3.3.** *Let $A \in \mathbb{R}^{V \times W}$ and $A' \in \mathbb{R}^{V' \times W'}$. With the notation above, the following holds.*

*(1) If $(\mathcal{P}^*, \mathcal{Q}^*)$ is an equitable partition of $A^*$ satisfying* (3.10) *and* (3.11)*, then $(\overline{\overline{\mathcal{P}^*}}, \overline{\overline{\mathcal{Q}^*}})$ is a fractional isomorphism from $A$ to $A'$.*

*(2) If $X, Y$ is a fractional isomorphism from $A$ to $A'$, then $(\overline{\overline{X}}, \overline{\overline{Y}})$ is an equitable partition of $A^*$ satisfying* (3.10) *and* (3.11).

*Proof.* To prove (1), note first that $\overline{\overline{\mathcal{P}^*}}$ and $\overline{\overline{\mathcal{Q}^*}}$ are doubly stochastic by (3.10) and (3.11), respectively. To prove (3.2), let $v' \in V'$ and $w \in W$, and let $P^* \in \mathcal{P}^*$, $Q^* \in \mathcal{Q}^*$ such that $v' \in P' \subseteq P^*$ and $w \in Q \subseteq Q^*$. Then

$$(\overline{\overline{\mathcal{P}^*}}A)_{v'w} = \sum_{v \in P} \frac{1}{|P|} A_{vw} \overset{(e)}{=} 2 \sum_{v^* \in P^*} \frac{1}{|P^*|} A^*_{vw} = 2(\overline{\mathcal{P}^*}A^*)_{v'w},$$

where equality $(e)$ holds because $A^*_{v'w} = 0$ for all $v' \in P'$ and $|P^*| = 2|P|$ by (3.10). Similarly, $(A'\overline{\overline{\mathcal{Q}^*}})_{v'w} = 2(A^*\overline{\mathcal{Q}^*})_{v'w}$. Since $(\mathcal{P}^*, \mathcal{Q}^*)$ is equitable, by Theorem 1.1, we have $\overline{\mathcal{P}^*}A^* = A^*\overline{\mathcal{Q}^*}$, and (3.8) follows. (3.9) can be proved similarly.

To prove (2), we let

$$X^* = \begin{pmatrix} 0 & X^t \\ X & 0 \end{pmatrix} \quad \text{and} \quad Y^* = \begin{pmatrix} 0 & Y^t \\ Y & 0 \end{pmatrix}$$

Then $(X^*, Y^*)$ is a fractional automorphism of $A^*$. Thus by Theorem 1.1, $(\overline{X^*}, \overline{Y^*})$ is an equitable partition of $A^*$. Moreover, $D_{X^*} = B_X$, and thus $\overline{X^*} = \overline{\overline{X}}$, and similarly $D_{Y^*} = B_Y$ and thus $\overline{Y^*} = \overline{\overline{Y}}$. As $X$ is doubly stochastic, we have $|P| = \sum_{v \in P} \sum_{v' \in P'} X_{v'v} = \sum_{v' \in P'} \sum_{v \in P} X_{v'v} = |P'|$ and similarly $|Q| = |Q'|$. □

**Corollary 3.4.** *Let $A \in \mathbb{R}^{V \times W}$ and $A' \in \mathbb{R}^{V' \times W'}$. Then $A$ and $A'$ are fractionally isomorphic if and only if colour refinement does not distinguish $A$ and $A'$.*

Similarly to Section 3.1, for square matrices $A \in \mathbb{R}^{V \times V}$ and $A' \in \mathbb{R}^{V' \times V'}$, we define a *2-sided fractional isomorphism* to be a matrix $X \in \mathbb{R}^{V \times V}$ such that $(X, X)$ is a fractional isomorphism from $A$ to $A'$.

**Corollary 3.5.** *Let $A \in \mathbb{R}^{V \times V}$ and $A' \in \mathbb{R}^{V' \times V'}$.*

*(1) If $\mathcal{P}^*$ is a 2-sided equitable partition of $A^*$ such that $|P| = |P'|$ for all $P^* \in \mathcal{P}^*$, then $\overline{\overline{\mathcal{P}^*}}$ is a 2-sided fractional isomorphism from $A$ to $A'$.*

*(2) If $X$ is a 2-sided fractional isomorphism from $A$ to $A'$, then $\overline{\overline{X}}$ is an equitable partition of $A^*$ such that $|P| = |P'|$ for all $P^* \in \overline{\overline{X}}$.*

Again, the conditions simplify for symmetric matrices: if $A$ and $A'$ are symmetric, then a doubly stochastic matrix $X$ is a 2-sided fractional isomorphism from $A$ to $A'$ if $XA = A'X$.

## 4 Colour Refinement in Quasilinear Time

Throughout this section, we consider matrices $A \in \mathbb{R}^{V \times W}$ and let $n := |V| + |W|$ and $m$ the total bitlength of all nonzero entries of $A$. To describe the algorithm, we view $A$ as a weighted bipartite graph with vertex set $V \cup W$ and edges with nonzero weights representing the nonzero matrix entries. For every vertex $u \in V \cup W$ and every set $P \subseteq V \cup W$ of vertices, we let $F(u, P)$ be the sum of the weights of the edges incident with $u$. That is, $F(v, P) = \sum_{w \in W \cap P} A_{vw}$ for $v \in V$ and $F(w, P) = \sum_{v \in V \cap P} A_{vw}$ for $w \in W$. Moreover, for every subset $P \subseteq V \cup W$, we let $m_P$ be the total bitlength of the weight of all edges incident with a vertex in $P$. For a vertex $u$, we write $m_u$ instead of $m_{\{u\}}$. Note that $m = \sum_{u \in V \cup W} m_u$.

We consider the problem of computing the coarsest equitable partition of $A$. A naive implementation of the iterative refinement procedure described in the introduction would yield a running time that is (at least) quadratic: in the worst case, we need $n$ refinement rounds, and each round takes time $O(n + m)$.

A significant improvement can be achieved if the refinement steps are carried out asynchronously, using a strategy that goes back to Hopcroft's algorithm for minimising deterministic finite automata [14]. The idea is as follows. The algorithm maintains partitions $\mathcal{P}$ of $V \cup W$. We call the classes of $\mathcal{P}$ *colours*. Initially, $\mathcal{P} = \{V, W\}$. Furthermore, the algorithm keeps a stack $S$ that holds some colours that we still want to use for refinement in the future. Initially, $S$ holds $V, W$ (in either order). In each refinement step, the algorithm pops a colour $Q$ from the stack. We call $Q$ the *refining colour* of this refinement step. For all $v \in V$ we compute the value $F(v, Q)$. Then for each colour $P$ in the current partition that has at least one neighbour in $Q$, we partition $P$ into new classes $P_1, \ldots, P_k$ according to the values $F(v, Q)$. Then we replace $P$ by $P_1, \ldots, P_k$ in the partition $\mathcal{P}$. Moreover, we add all classes among $P_1, \ldots, P_k$ *except for the largest* to the stack $S$. If we use the right data structures, we can carry out such a refinement step with refining colour $Q$ in time $O(|Q| + m_Q)$. Compared to the standard, unweighted version of colour refinement, the weights add some complication when it comes to computing the partition $P_1, \ldots, P_k$ of $P$. We can handle this by standard vector partitioning techniques, running in time linear in the total bitlength of the weights involved. By not adding the largest among the classes $P_1, \ldots, P_k$ to the stack, we achieve that every vertex $u$ appears at most $\log n$ times in a refining colour $Q$. Whenever $u$ appears in the refining colour, it contributes $O(1 + m_v)$ to the cost of that refinement step. Thus the overall cost is $\sum_{u \in V \cup W} O(1 + m_v) \log n = O((n + m) \log n)$. We refer the reader to [3, 21] for details on the algorithm (for the unweighted case) and its analysis.

**Theorem 4.1.** *There is an algorithm that, given a sparse representation of a matrix $A$, computes the coarsest equitable partition of $A$ in time $O((n + m) \log n)$.*

## 5 Reducing the Dimension of a Linear Program

Recall that for a matrix $A \in \mathbb{R}^{V\times W}$ and vectors $b \in \mathbb{R}^V$, $c \in \mathbb{R}^W$.we let $L(A, b, c)$ be the linear program

$$\min c \cdot x$$
$$\text{subject to } Ax = b,\ x \geqslant 0$$

(in *standard form*). Moreover, we let $D(A, b, c)$ be the linear program

$$\max c \cdot x$$
$$\text{subject to } Ax \leqslant b$$

(in *dual form*).

**Lemma 5.1 (Reduction Lemma).** *Let $A \in \mathbb{R}^{V\times W}$, $b \in \mathbb{R}^V$, $c \in \mathbb{R}^W$, and $L = L(A, b, c)$. Let $X = \check{X}\widehat{X} \in \mathbb{R}^{V\times V}$, where $\check{X} \in \mathbb{R}^{V\times T}$, $\widehat{X} \in \mathbb{R}^{T\times W}$, and $Y = \check{Y}\widehat{Y} \in \mathbb{R}^{W\times W}$, where $\check{Y} \in \mathbb{R}^{W\times U}$, $\widehat{Y} \in \mathbb{R}^{U\times W}$, such that:*

*(R.1) $XA = AY$;*

*(R.2) $Xb = b$ and $c^tY = c^t$;*

*(R.3) $\check{Y}, \widehat{Y}$ are nonnegative.*

*Let $A' = \widehat{X}A\check{Y} \in \mathbb{R}^{T\times U}$, $b' = \widehat{X}b \in \mathbb{R}^T$, and $c' = (c^t\check{Y})^t \in \mathbb{R}^U$, and let $L' = L(A', b, c')$. Then*

*(1) if $x$ is a feasible solution to $L$, then $\widehat{Y}x$ is a feasible solution to $L'$;*

*(2) if $x'$ is a feasible solution to $L'$, then $Y\check{Y}x'$ is a feasible solution to $L$;*

*(3) if $x$ is an optimal solution to $L$ then $\widehat{Y}x$ is an optimal solution to $L'$;*

*(4) if $x'$ is an optimal solution to $L'$ then $Y\check{Y}x'$ is an optimal solution to $L$.*

*Proof.* To prove (1), let $x$ be a feasible solution to $L$ and $x' = \widehat{Y}x$. Then $x' \geqslant 0$, because $\widehat{Y}$ is nonnegative. Moreover, $A'x' = \widehat{X}A\check{Y}\widehat{Y}x = \widehat{X}AYx = \widehat{X}XAx = \widehat{X}Xb = \widehat{X}b = b'$.

To prove (2), let $x'$ be a feasible solution to $L'$ and $x = Y\check{Y}x'$. Then $x \geqslant 0$ because $Y\check{Y}$ is nonnegative. Moreover, $Ax = AY\check{Y}x' = XA\check{Y}x' = \check{X}A'x' = \check{X}b' = Xb = b$.

To prove (3), let $x$ be an optimal solution to $L$, and let $x' = \widehat{Y}x$. By (1), $x'$ is a feasible solution to $L'$. Let $y'$ be another feasible solution to $L'$. Then by (2), $y = Y\check{Y}y'$ is a feasible solution to $L$. Thus $c^ty \geqslant c^tx$, which implies $(c')^ty' = c^t\check{Y}y' = c^tY\check{Y}y' = c^ty \geqslant c^tx = c^tYx = c^t\check{Y}\widehat{Y}x = (c')^tx'$.

To prove (4), let $x'$ be an optimal solution to $L'$. Let $x = Y\check{Y}x'$. By (2), $x$ is a feasible solution to $L$. Let $y \in \mathbb{R}^n$ be another feasible solution to $L$. Then by (1), $y' = \widehat{Y}y$ is a feasible solution to $L'$, and thus $(c')^ty' \geqslant (c')^tx'$. Hence $c^ty = c^tYy = c^t\check{Y}\widehat{Y}y = (c')^ty' \geqslant (c')^tx' = c^t\check{Y}x' = c^tY\check{Y}x' = c^tx$. □

There is also a version of the Reduction Lemma for LPs in dual form.

**Lemma 5.2 (Reduction Lemma, Dual Version).** *Let $A, b, c, X, \check{X}, \widehat{X}, Y, \check{Y}, \widehat{Y}, A', b', c'$ be as in the Reduction Lemma 5.1, and suppose that conditions (R.1) and (R.2) and the following condition are satisfied.*

**(R.3d)** *$\check{X}$, $\widehat{X}$ are nonnegative.*

*Then assertion (i)–(iv) hold for $L = D(A, b, c)$ and $L' = D(A', b', c')$.*

The proof is a straightforward modification of the proof for the standard form.

For the reduction lemma to be useful, we would like the dimensions $(|T|, |U|)$ of the reduced LP $L'$ to be significantly smaller than those of $L$. Furthermore, we need an efficient algorithm for computing the matrices

$X$, $Y$ and their decompositions $\check{X}\hat{X}$ and $\check{Y}\hat{Y}$. While in general we cannot guarantee that the dimensions can be reduced at all — often they can, but certainly not always — colour refinement gives us an efficient way to find the reduction matrices.

Recall (from the introduction) that an *equitable partition* of $L = L(A, b, c)$ is an equitable partition $(\mathcal{P}, \mathcal{Q})$ of $A$ such that $b$ is $\mathcal{P}$-invariant and $c$ is $\mathcal{Q}$-invariant. For each partition $\mathcal{P}$ of $V$ we define matrices $\check{\mathcal{P}} \in \mathbb{R}^{V\times\mathcal{P}}$ and $\hat{\mathcal{P}} \in \mathbb{R}^{\mathcal{P}\times V}$ as follows. $\check{\mathcal{P}}$ is the incidence matrix of $\mathcal{P}$, that is, $\check{\mathcal{P}}_{vP} = 1$ if $v \in P$ and $\check{\mathcal{P}}_{vP} = 0$ otherwise. $\hat{\mathcal{P}}$ is the transpose of $\check{\mathcal{P}}$ scaled to a stochastic matrix, that is, $\hat{\mathcal{P}}_{Pv} = 1/|P|$ if $v \in P$ and $\hat{\mathcal{P}}_{Pv} = 0$ otherwise. Observe that $\check{\mathcal{P}}\hat{\mathcal{P}} = \overline{\mathcal{P}}$, and $\hat{\mathcal{P}}\check{\mathcal{P}}$ is the $\mathcal{P} \times \mathcal{P}$-identity matrix. Similarly, for each partition $\mathcal{Q}$ of $W$ we define $\check{\mathcal{Q}} \in \mathbb{R}^{W\times\mathcal{Q}}$ to be the incidence matrix of $\mathcal{Q}$ and $\hat{\mathcal{Q}} \in \mathbb{R}^{\mathcal{Q}\times W}$ to be its transpose scaled to a stochastic matrix.

We are now ready to prove our second main result.

*Proof of Theorem 1.2.* Let $L = L(A, b, c)$, and let $(\mathcal{P}, \mathcal{Q})$ be the coarsest stable partition of $L$. Let $p := |\mathcal{P}|$ and $q := \mathcal{Q}$. Let $\check{X} \in \mathbb{R}^{V\times[p]}$ be $\check{\mathcal{P}}$ with columns renamed according to some fixed bijection between $\mathcal{P}$ and $[p]$, and let $\hat{X}, \check{Y}, \hat{Y}$ be similarly defined from $\hat{\mathcal{P}}, \check{\mathcal{Q}}, \hat{\mathcal{Q}}$. Then $X := \check{X}\hat{X} = \overline{\mathcal{P}}$ and $Y := \check{Y}\hat{Y} = \overline{\mathcal{Q}}$. Moreover, $\check{Y} = Y\check{Y}$ because $\hat{Y}\check{Y}$ is the $[q] \times [q]$ identity matrix.

By Theorem 1.1, $(X, Y)$ is a fractional isomorphism of $A$, and this implies condition (R.1) of the Reduction Lemma 5.1. Condition (R.2) holds because $b$ is $\mathcal{P}$-invariant and $c$ is $\mathcal{Q}$-invariant, and condition (R.3) is obviously satisfied as well. Thus Theorem 1.2 follows from the Reduction Lemma and Theorem 4.1. □

A version of Theorem 1.2 for linear programs in dual form can be derived from the dual version of the reduction lemma. Actually, the theorem can easily be generalised to arbitrary LPs.

Let us close this section by noting that Theorem 1.2 subsumes a method of symmetry reduction for LPs proposed by Bödi, Grundhöfer and Herr [5]. They define an *automorphism* of $L = L(A, b, c)$ to be a pair $(X, Y)$ of permutation matrices such that $XA = AY$ and $Xb = b$ and $c^tY = c^t$. Thus an automorphism is an integral fractional automorphism. Let $\mathrm{Aut}(L)$ denote the group of all automorphisms of $L$. Bödi et al. observe that for every feasible solution $x$ to $L$,

$$x' = \frac{1}{|\mathrm{Aut}(L)|} \sum_{(X,Y)\in\mathrm{Aut}(L)} Yx$$

is a feasible solution to $L$ as well, and if $x$ is an optimal solution then $x'$ is an optimal solution. They argue that $x'$ is in the intersection $E$ of the 1-eigenspaces of all matrices $Y$ such that $(X, Y) \in \mathrm{Aut}(L)$ for some $X$. If there are many automorphisms, the dimension of $E$ can be expected to be much smaller than $n$, and thus we can reduce the number of variables of the linear program by projecting to $E$.

Observe that the pair $(X, Y)$ of matrices defined by

$$X := \frac{1}{|\mathrm{Aut}(L)|} \sum_{(X',Y')\in\mathrm{Aut}(L)} X' \quad \text{and} \quad Y := \frac{1}{|\mathrm{Aut}(L)|} \sum_{(X',Y')\in\mathrm{Aut}(L)} Y' \tag{5.1}$$

is a fractional isomorphisms of $L$. Note that the dimension of the $E$ is equal to the rank of $Y$, which is at least the number $q$ of classes of $\mathcal{Q}$ in the coarsest equitable partition $(\mathcal{P}, \mathcal{Q})$ of $L$.

## 6 Computational Evaluation

Our intention here is to investigate the computational benefits of colour refinement for solving linear programs in the presence of symmetries. To this aim, we realised our colour refinement based on the Saucy [15], where the unweighted version is already implemented as a preprocessing heuristic for automorphism group computation. We modified the code to return the colour classes after preprocessing and not proceed with the

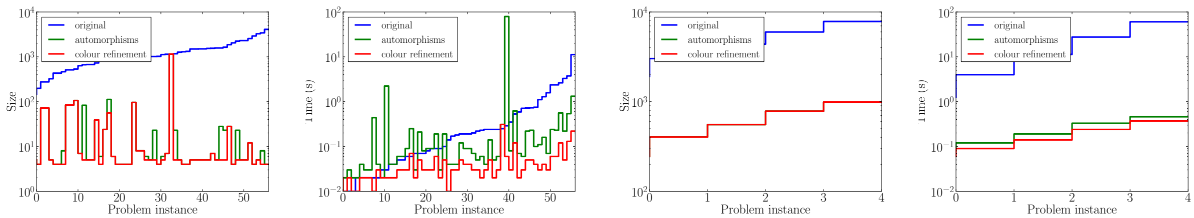


**Figure 6.1.** Computational results on the different linear programs (x-axis). From left to right: (a) The dimension (number of variables and constraints in log-scale) of the linear programs used for the evaluation. (b) The running times in (log-scaled) seconds (including the time for reduction) for solving the linear programs. Note that for clarity, the values in (a,b) are sorted according to the baseline independently for each figure. We refer the reader to the table in the appendix for the exact numbers. (c,d) Same figures for computing the value funtions of the grid Markov decision processes.

actual automorphism search. From the colour classes we computedthe reduced LPs according to Lemma 5.1. We used CVXOPT (`http://cvxopt.org/`) for solving the original and reduced linear programs. We report on the dimensions of the linear programs and on the running times when solving the original linear programs (without compression) as well as the reduced ones using colour refinement. We additionally compare the results to the approach of compressing by projecting into the fixed space of the automorphism group (which coincides with using the fractional automorphism induced by the orbit partition of the LP — also computed using Saucy). All experiments were conducted on a standard Linux desktop machine with a 3 GHz Intel Core2-Duo processor and 8GB RAM.

The linear programs chosen for the evaluation are relaxed versions of all the integer programs available at Francois Margot's website `http://wpweb2.tepper.cmu.edu/fmargot/lpsym.html`. They encode combinatorial optimisation problems with applications in coding theory, statistical design and graph theory such as computing maximum cardinality binary error correcting codes, edge colourings, minimum dominating sets in Hamming graphs, and Steiner-triple systems.

The results are summarised in Fig. 6.1(a,b). One can clearly see that colour refinement reduces the dimension of the linear programs at least as much as the orbit partition, in many cases — as expected — even more. Looking at the running times, this reduction also results in faster total computations, often an order of magnitude faster. Overall, solving all linear programs took 38 seconds without dimension reduction. Using the orbit partition to reduce the dimensions, running all experiments actually increased to 89 seconds, whereas using colour refinement it only took 2 seconds. Indeed, the higher complexity when using the orbit partition is due to few instances only but also illustrates the benefit of running a guaranteed quasilinear method for reducing the dimension of linear programs such as colour refinement.

Indeed, so far we considered relaxed integer programs. As an example for LPs that are not relaxed integer programs, we considered the computation of the value function of a Markov Decision Problem modeling decision making in situations where outcomes of actions are partly random. As shown in e.g. [18], the LP is $\max_{\boldsymbol{v}}\ \mathbf{1}^T\boldsymbol{v}, \quad \text{s.t.}\ \ v_i \leqslant c_i^k + \gamma \sum_j p_{ij}^k v_j$ , where $v_i$ is the value of state $i$, $c_i^k$ is the reward that the agent receives when carrying out action $k$ in $i$, and $p_{ij}^k$ is the probability of transferring from state $i$ to state $j$ by the action $k$. The MDP instance that we used is the well-known Gridworld, see e.g. [26]. Here, an agent navigates within a grid of $n \times n$ states. Every state has an associated reward $R(s)$. Typically there is one or several states with high rewards, considered the goals, whereas the other states have zero or negative associated rewards. We induced symmetries by putting a goal in every corner of the grid. The results for different grid sizes $n$ are summarised in Fig. 6.1(c,d) and confirm our previous results. Indeed, as expected, colour refinement and authormorphisms result in the same partitions but colour refinement is faster.

Finally, triggered by [20], we considered MAP inference in Markov logic networks (MLNs) [24] via the standard LP relaxation for MAP of the induced graphical model, see e.g. [12]. Specifically, we used Richardson and Domingos' smoker-friends MLN encoding that friends have similar smoking habits. The so-called Frucht (among 12 people) and McKay (among 8 people) graphs were used to encode the social network, i.e., who are friends. The induced LPs were of sizes 1710 resp. 729. Solving them took 0.35 resp. 0.05 seconds. Using orbit partitions, the sizes reduced to 1590 resp. 247. Reducing and solving them took 0.34 resp 0.02 seconds. Colour refinement, however, reduced the sizes to 46 resp 114. Reducing and solving the corresponding LPs took 0.02 seconds in both cases.

## 7 Conclusions

We develop a theory of fractional automorphisms and equitable partitions of matrices and show how it can be used to reduce the dimension of linear programs. The main point is that there is no need to compute full symmetries (that is, automorphisms) to do a symmetry reduction for linear programs, and equitable partition will do, and that colour refinement can compute the coarsest equitable partition very efficiently. We demonstrate experimentally that the gain of our method can be significant, also in comparison with other symmetry reduction methods.

In particular, we benefit from the fact that the colour refinement algorithm on which we rely is very efficient, running in quasilinear time. For really large scale applications, however, it would be desirable to implement the algorithm in a distributed fashion. We leave it for future work to find efficient and scalable ways of doing this. Somewhat related, but more speculative, we would like to point out a similarity between the colour refinement iteration and power iteration methods. To this end, note that if $(X, Y)$ is a fractional automorphism of a matrix $A$ then for all $k \geqslant 0$ we have $X^kA = AY^k$, and the sequences $X^k$ and $Y^k$ converge to homogeneous block matrices. Thus we would expect $X^{k+1}A \approx AY^k$. Maybe this can be the basis of an efficient "linear algebraic" algorithm for computing the coarsest stable partition.

Our method works well if colour refinement has few colour classes. A key to understanding when this happens might be Atserias and Maneva's [2] notion of local linear programs. In particular, for local linear programs we may have a substantial reduction for higher levels of the Sherali-Adams hierarchy.

Another interesting open question is whether there exist "approximate versions" of colour refinement that can be used to solve (certain) linear programs approximately and can be implemented even more efficiently.

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## A Experimental Results

The following table shows the results of our first series of experiments with Margot's benchmark (see `http://wpweb2.tepper.cmu.edu/fmargot/lpsym.html`) in some more detail. The filenames refer to Margot's benchmark. We run three different solvers: Columns marked "N" refer to the original LP without any reduction. Columns marked "Op" refer to the LP reduced by the orbit partition, and columns marked "Cr" refer to the LP reduced by colour refinement. We list the total time for solving the the LPs, including the time for the reduction, the number of variables, and the number of constraints.

| | Solution time | | | Variables | | | Constraints | | |
|---|---|---|---|---|---|---|---|---|---|
| Filename | N | Op | Cr | N | Op | Cr | N | Op | Cr |
| O4_35.lp | 0.23 | 0.03 | 0.02 | 280 | 1 | 1 | 840 | 5 | 4 |
| bibd1152.lp | 0.71 | 0.21 | 0.04 | 462 | 1 | 1 | 1034 | 4 | 4 |
| bibd1154.lp | 0.72 | 0.22 | 0.04 | 462 | 1 | 1 | 1034 | 4 | 4 |
| bibd1331.lp | 0.22 | 0.05 | 0.01 | 286 | 1 | 1 | 728 | 4 | 4 |
| bibd1341.lp | 2.36 | 0.22 | 0.05 | 715 | 1 | 1 | 1586 | 4 | 4 |
| bibd1342.lp | 2.36 | 0.23 | 0.05 | 715 | 1 | 1 | 1586 | 4 | 4 |
| bibd1531.lp | 0.74 | 0.09 | 0.03 | 455 | 1 | 1 | 1120 | 4 | 4 |
| bibd738.lp | 0.0 | 0.0 | 0.01 | 35 | 1 | 1 | 112 | 4 | 4 |
| bibd933.lp | 0.01 | 0.01 | 0.0 | 84 | 1 | 1 | 240 | 4 | 4 |
| ca36243.lp | 0.01 | 0.02 | 0.01 | 64 | 1 | 1 | 368 | 3 | 3 |
| ca57245.lp | 0.05 | 0.08 | 0.02 | 128 | 1 | 1 | 816 | 3 | 3 |
| ca77247.lp | 0.06 | 0.07 | 0.02 | 128 | 1 | 1 | 816 | 3 | 3 |
| clique9.lp | 0.21 | 0.04 | 0.02 | 288 | 1 | 1 | 720 | 5 | 4 |
| cod105.lp | 11.18 | 1.31 | 0.21 | 1024 | 1 | 1 | 3072 | 3 | 3 |
| cod105r.lp | 2.62 | 0.55 | 0.11 | 638 | 3 | 3 | 1914 | 9 | 9 |
| cod83.lp | 0.19 | 0.06 | 0.02 | 256 | 1 | 1 | 768 | 3 | 3 |
| cod83r.lp | 0.16 | 0.03 | 0.02 | 219 | 6 | 6 | 657 | 18 | 18 |
| cod93.lp | 1.28 | 0.15 | 0.03 | 512 | 1 | 1 | 1536 | 3 | 3 |
| cod93r.lp | 1.1 | 0.1 | 0.02 | 466 | 7 | 7 | 1398 | 21 | 21 |
| codbt06.lp | 3.28 | 0.21 | 0.04 | 729 | 1 | 1 | 2187 | 3 | 3 |
| codbt24.lp | 0.34 | 0.07 | 0.02 | 324 | 1 | 1 | 972 | 3 | 3 |
| cov1053.lp | 0.18 | 0.11 | 0.04 | 252 | 1 | 1 | 679 | 5 | 5 |
| cov1054.lp | 0.23 | 0.13 | 0.04 | 252 | 1 | 1 | 889 | 6 | 6 |
| cov1054sb.lp | 0.24 | 0.3 | 0.3 | 252 | 252 | 252 | 898 | 898 | 898 |
| cov1075.lp | 0.05 | 0.24 | 0.06 | 120 | 1 | 1 | 877 | 7 | 7 |
| cov1076.lp | 0.06 | 0.2 | 0.04 | 120 | 1 | 1 | 835 | 7 | 7 |
| cov1174.lp | 0.52 | 0.61 | 0.11 | 330 | 1 | 1 | 1221 | 6 | 6 |
| cov954.lp | 0.04 | 0.05 | 0.02 | 126 | 1 | 1 | 507 | 6 | 6 |
| flosn52.lp | 0.17 | 0.03 | 0.02 | 234 | 4 | 1 | 780 | 19 | 4 |
| flosn60.lp | 0.23 | 0.04 | 0.01 | 270 | 4 | 1 | 900 | 19 | 4 |
| flosn84.lp | 0.58 | 0.06 | 0.01 | 378 | 4 | 1 | 1260 | 19 | 4 |
| jgt18.lp | 0.02 | 0.01 | 0.01 | 132 | 19 | 19 | 402 | 87 | 87 |
| jgt30.lp | 0.13 | 0.03 | 0.0 | 228 | 20 | 10 | 690 | 92 | 46 |
| mered.lp | 1.57 | 0.06 | 0.02 | 560 | 4 | 1 | 1680 | 19 | 4 |
| oa25332.lp | 0.18 | 0.08 | 0.03 | 243 | 1 | 1 | 1026 | 4 | 4 |
| oa25342.lp | 0.23 | 0.05 | 0.02 | 243 | 1 | 1 | 1296 | 4 | 4 |
| oa26332.lp | 3.74 | 0.53 | 0.12 | 729 | 1 | 1 | 2538 | 4 | 4 |
| oa36243.lp | 0.01 | 0.03 | 0.02 | 64 | 1 | 1 | 608 | 4 | 4 |
| oa56243.lp | 0.01 | 0.03 | 0.01 | 64 | 1 | 1 | 608 | 4 | 4 |
| oa57245.lp | 0.09 | 0.18 | 0.04 | 128 | 1 | 1 | 1376 | 4 | 4 |
| oa66234.lp | 0.01 | 0.02 | 0.01 | 64 | 16 | 16 | 212 | 56 | 56 |
| oa67233.lp | 0.03 | 0.03 | 0.01 | 128 | 20 | 20 | 384 | 64 | 64 |
| oa68233.lp | 0.18 | 0.08 | 0.03 | 256 | 24 | 24 | 698 | 72 | 72 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| oa76234.lp | 0.0 | 0.01 | 0.0 | 64 | 16 | 16 | 212 | 56 | 56 |
| oa77233.lp | 0.03 | 0.03 | 0.01 | 128 | 20 | 20 | 384 | 64 | 64 |
| oa77247.lp | 0.08 | 0.18 | 0.05 | 128 | 1 | 1 | 1376 | 4 | 4 |
| of5_14_7.lp | 0.06 | 0.02 | 0.01 | 175 | 15 | 1 | 490 | 68 | 4 |
| of7_18_9.lp | 0.7 | 0.05 | 0.02 | 441 | 5 | 1 | 1134 | 23 | 4 |
| ofsub9.lp | 0.08 | 0.02 | 0.01 | 203 | 7 | 7 | 527 | 32 | 32 |
| pa36243.lp | 0.0 | 0.02 | 0.01 | 64 | 1 | 1 | 368 | 3 | 3 |
| pa57245.lp | 0.07 | 0.08 | 0.02 | 128 | 1 | 1 | 816 | 3 | 3 |
| pa77247.lp | 0.08 | 0.08 | 0.02 | 128 | 1 | 1 | 816 | 3 | 3 |
| sts135.lp | 0.28 | 79.18 | 0.05 | 135 | 1 | 1 | 3285 | 7 | 3 |
| sts27.lp | 0.0 | 0.01 | 0.0 | 27 | 1 | 1 | 171 | 3 | 3 |
| sts45.lp | 0.01 | 0.43 | 0.0 | 45 | 1 | 1 | 420 | 7 | 3 |
| sts63.lp | 0.02 | 2.22 | 0.01 | 63 | 1 | 1 | 777 | 5 | 3 |
| sts81.lp | 0.04 | 0.05 | 0.02 | 81 | 1 | 1 | 1242 | 3 | 3 |