A Scaling Algorithm to Equilibrate Both Rows and Columns Norms in Matrices¹

Daniel Ruiz²

ABSTRACT

We present an iterative procedure which asymptotically scales the infinity norm of both rows and columns in a matrix to 1. This scaling strategy exhibits some optimality properties and additionally preserves symmetry. The algorithm also shows fast linear convergence with an asymptotic rate of 1/2.

We discuss possible extensions of such an algorithm when considering the one-norm or the two norm of the rows and columns of the given matrix, and give the proof of its convergence when the matrix pattern satisfies some common properties.

Keywords: sparse matrices, equilibration, max-norm, doubly stochastic.

¹Current reports available by anonymous ftp to ftp.numerical.rl.ac.uk in directory pub/reports. This report is in file drRAL2001034.ps.gz. Report also available through URL http://www.numerical.rl.ac.uk/reports/reports.html. Also published as ENSEEIHT-IRIT Technical Report RT/APO/01/4. Report also available through URL http://www.enseeiht.fr/lima/apo/PUBLIS/list.html.

²Daniel.Ruiz@enseeiht.fr, Ecole Nationale Supérieure d'Electrotechnique, d'Electronique, d'Informatique, et d'Hydraulique de Toulouse, Institut de Recherche en Informatique de Toulouse, 2 rue Camichel, 31071 Toulouse Cedex, France.

Computational Science and Engineering Department Atlas Centre Rutherford Appleton Laboratory Oxon OX11 0QX September 10, 2001

Contents

1	Introduction	1
2	The algorithm	2
3	Fast linear convergence and properties	3
4	Some comparisons with the symmetric scaling algorithm of Bunch	6
5	Extensions to other norms	8
6	Conclusions	17

1 Introduction

Scaling or equilibration of data in linear systems of equations is a topic of great importance that has already been the subject of many scientific publications, with many different developments depending on the properties one wants to obtain after scaling. It has given rise to several well known algorithms (see Duff, Erisman, and Reid (1986), Schneider and Zenios (1990), for instance). Scaling consists in pre- and post-multiplying our original matrix by two diagonal matrices, \mathbf{D}_1 and \mathbf{D}_2 , respectively. If we denote by $\widehat{\mathbf{A}}$ the scaled matrix

$$\widehat{\mathbf{A}} = \mathbf{D_1} \mathbf{A} \mathbf{D_2} \ ,$$

we then solve the equation

$$\widehat{\mathbf{A}}\mathbf{\hat{x}} = \mathbf{\hat{b}}$$
,

where
$$\hat{\mathbf{x}} = \mathbf{D_2^{-1}}\mathbf{x}$$
 and $\hat{\mathbf{b}} = \mathbf{D_1}\mathbf{b}$.

Classical scalings are the well known row and column scaling. For row scaling, each row in the original matrix is divided by the norm of the row. Different norms, such as the infinity-norm or the 1-norm, may be considered, depending on the strategy one wishes to develop. Column scaling is identical to row scaling, except that it considers the columns of the original matrix. A more general purpose scaling method is the one used in the HSL 2000 routine MC29, which aims to make the nonzeros of the scaled matrix close to one by minimizing the sum of the squares of the logarithms of the moduli of the nonzeros (see Curtis and Reid (1972)). MC29 reduces this sum in a global sense and therefore should be useful on a wide range of sparse matrices. Any combination of these scalings is also a possibility. Scaling can also be combined with permutations (see Duff and Koster (1999) and the HSL 2000 routine MC64). The matrix is first permuted so that the product of absolute values of entries in on the diagonal of the permuted matrix is maximized (other measures such as maximizing the minimum element are also options). Then the matrix is scaled so that the diagonal entries are one and the off-diagonals are less than or equal to one. This then provides a useful tool for a good pivoting strategy for sparse direct solvers, as well as for building good preconditioners for an iterative method.

In the 1960's, Bauer (1963), Bauer (1969) and van der Sluis (1969), in particular, showed some optimal properties in terms of conditions numbers for scaled matrices with all rows or all columns of equal norm of 1.

The purpose of this article is to propose an iterative algorithm that will scale a matrix so that it reaches asymptotically a state with all rows as well as all columns with infinity-norm equal to one. This algorithm is introduced in detail in Section 2. The convergence towards the stationary state mentioned above is at least linear, with an asymptotic rate of convergence of $\frac{1}{2}$, and this is clearly demonstrated and illustrated in Section 3. From the theory developed by Bauer (1963) and van der Sluis (1969), we also indicate in Section 4 the particular properties that this algorithm yields for the scaled matrices and, in particular, we highlight the case of symmetric matrices since the algorithm "naturally" preserves such numerical structures. In that respect, we also mention the routine MC30 in the HSL (2000) library, which is a variant of the above MC29 routine for symmetric matrices.

Finally, we try in Section 5 to extend the algorithm to the case of other norms. Following the discussion in Parlett and Landis (1982), we establish under which hypothesis the algorithm is also convergent in the case of the one-norm, and we comment on the generalisation of these results with respect to what was stated in Parlett and Landis (1982). Concluding remarks as well as some additional extensions are briefly discussed in Section 6.

2 The algorithm

Consider a general $m \times n$ real matrix A, and denote by $\mathbf{r}_i = \mathbf{a}_{i\cdot}^T \in \mathbb{R}^{n\times 1}$, $i = 1, \dots, m$, the row-vectors from A and by $\mathbf{c}_j = \mathbf{a}_{\cdot j} \in \mathbb{R}^{n\times 1}$, $j = 1, \dots, n$, the column-vectors from A. Denote by \mathbf{D}_R and \mathbf{D}_C the $m \times m$ and $n \times n$ diagonal matrices given by:

$$\mathbf{D}_{R} = \operatorname{diag}(\sqrt{\|\mathbf{r}_{i}\|_{\infty}})_{i=1,\dots,m} \text{ and } \mathbf{D}_{C} = \operatorname{diag}(\sqrt{\|\mathbf{c}_{j}\|_{\infty}})_{j=1,\dots,n}$$
 (2.1)

where $\|.\|_{\infty}$ stands for the infinity-norm of a real vector (that is the maximum entry in absolute value, and also sometimes called the max norm). If a row (or colum) in A has all entries equal to zero, we replace the diagonal entry in D_R (or D_C respectively) by 1. In the following, we will assume that this does not happen, considering that such cases are fictitious in the sense that zero rows or columns should be taken away and the system reduced.

We then scale matrix A on both sides, forming the scaled matrix \widehat{A} in the following way

$$\widehat{\mathbf{A}} = \mathbf{D}_{\mathbf{R}}^{-1} \mathbf{A} \mathbf{D}_{\mathbf{C}}^{-1} . \tag{2.2}$$

Now, the idea of the algorithm we propose is to iterate on that process, viz.

Algorithm 2.1 (Simultaneous row and column iterative scaling)

$$\begin{split} \widehat{\mathbf{A}}^{(\mathbf{0})} &= \mathbf{A}, \quad \mathbf{D}_1^{(0)} = \mathbf{I}_m, \quad \text{and } \mathbf{D}_2^{(0)} = \mathbf{I}_n \\ \text{for } k = 0, 1, 2, \dots, \text{ until convergence do :} \\ \mathbf{D}_R &= \operatorname{diag}(\sqrt{\|\mathbf{r}_i^{(k)}\|_{\infty}})_{i=1,\dots,m}, \quad \text{and } \mathbf{D}_C = \operatorname{diag}(\sqrt{\|\mathbf{c}_j^{(k)}\|_{\infty}})_{j=1,\dots,n} \\ \widehat{\mathbf{A}}^{(\mathbf{k}+\mathbf{1})} &= \mathbf{D}_{\mathbf{R}}^{-1} \widehat{\mathbf{A}}^{(\mathbf{k})} \mathbf{D}_{\mathbf{C}}^{-1} \\ \mathbf{D}_1^{(k+1)} &= \mathbf{D}_1^{(k)} \ \mathbf{D}_R^{-1}, \quad \text{and } \mathbf{D}_2^{(k+1)} = \mathbf{D}_2^{(k)} \ \mathbf{D}_C^{-1} \end{split}$$

Convergence is obtained when

$$\max_{1 \le i \le m} \left\{ |(1 - \|\mathbf{r}_i^{(k)}\|_{\infty})| \right\} \le \varepsilon \text{ and } \max_{1 \le j \le n} \left\{ |(1 - \|\mathbf{c}_j^{(k)}\|_{\infty})| \right\} \le \varepsilon \tag{2.3}$$

for a given value of $\varepsilon > 0$. The properties of this algorithm, as well as its rate of convergence, are discussed in the following section.

3 Fast linear convergence and properties

The first property of the algorithm we would like to highlight, because it has been one of the main reasons for the construction of this iterative scaling procedure, is that it preserves symmetry. Indeed, if the given matrix \mathbf{A} is symmetric, then the diagonal matrices \mathbf{D}_R and \mathbf{D}_C in (2.1) are equal and, consequently, matrix $\widehat{\mathbf{A}}$ in (2.2) is still symmetric, as is the case for the matrices $\widehat{\mathbf{A}}^{(\mathbf{k})}$ at any iteration in Algorithm 2.1. This is not the case for most scaling algorithms which alternately scale rows followed by columns or vice-versa.

For instance, in the case of unsymmetric matrices, one may consider the use of the Sinkhorn and Knopp (1967) iteration with infinity-norm (in place of the one-norm as in the Sinkhorn-Knopp method). This method simply normalizes alternately all rows and columns in A, and iterates on that process until convergence, although in the case of the infinity-norm, this is obtained after one single step. Because of its simplicity, this method is very appealing, but notice however that the Sinkhorn-Knopp iteration may provide very different results when applied to A or to A^T . As opposed to that, and this is linked to the first comment above, Algorithm 2.1 does provide exactly the same results when applied to A or A^T in the sense that the scaled matrix obtained on A^T is the transpose of that obtained on A. We have quoted the Sinkhorn and Knopp (1967) method in particular because it has been originally proposed by the authors to provide so called "doubly stochastic" matrices, that is positive matrices with all rows and columns of one-norm equal to 1, and we shall come back to this issue with respect to Algorithm 2.1 in the next section.

The particular case when the matrix A has all its rows and columns with infinity-norm equal to one is clearly a fixed point for the iterations in Algorithm 2.1. Also, if A is a square matrix in which the absolute value of each diagonal element is greater than or equal to the absolute value of any other entry in the corresponding row and column, then it can easily be seen that the algorithm converges in one iteration, with a resulting scaled matrix $\widehat{A}^{(1)}$ with all ones on the diagonal.

Concerning the rate of convergence of Algorithm 2.1 in the more general case, we shall now verify that the algorithm converges in all cases towards the above mentioned stationary point with an asymptotic linear rate of $\frac{1}{2}$.

The first point in the demonstration of this is to notice that, after the first iteration of the algorithm, all the entries in $\widehat{\mathbf{A}}^{(1)}$ are less than or equal to one in absolute value. This is very easy to see, since all entries a_{ij} in \mathbf{A} are divided by the square roots of two numbers, $\|\mathbf{r}_i^{(k)}\|_{\infty}$ and $\|\mathbf{c}_j^{(k)}\|_{\infty}$ respectively, each one of them being greater than or equal to $|a_{ij}|$ itself.

Then, for any subsequent iteration $(k \geq 1)$, if we consider the infinity-norm of any row $\mathbf{r}_i^{(k)}$ or column $\mathbf{c}_j^{(k)}$, and if we denote by $a_{ij_0}^{(k)}$ the entry in row i for which the equality $|a_{ij_0}^{(k)}| = \|\mathbf{r}_i^{(k)}\|_{\infty}$ holds, and by $a_{ioj}^{(k)}$ the entry in column j such that $|a_{ioj}^{(k)}| = \|\mathbf{c}_j^{(k)}\|_{\infty}$ respectively, we can easily verify that both entries $a_{ij_0}^{(k+1)}$ and $a_{ioj}^{(k+1)}$ in the scaled matrix $\widehat{\mathbf{A}}^{(\mathbf{k}+1)}$ are greater in absolute value than the square root of the

corresponding value at iteration k, and are still less than one. Indeed, we can write

$$1 \ge |a_{ij_0}^{(k+1)}| = \frac{|a_{ij_0}^{(k)}|}{\sqrt{\|\mathbf{r}_i^{(k)}\|_{\infty}}\sqrt{\|\mathbf{c}_{j_0}^{(k)}\|_{\infty}}} = \frac{\sqrt{|a_{ij_0}^{(k)}|}}{\sqrt{\|\mathbf{c}_{j_0}^{(k)}\|_{\infty}}} \ge \sqrt{|a_{ij_0}^{(k)}|}$$

since $|a_{ij_0}^{(k)}| = \|\mathbf{r}_i^{(k)}\|_{\infty}$ and $\|\mathbf{c}_{j_0}^{(k)}\|_{\infty} \le 1$ for any $k \ge 1$. A similar short demonstration enables us to show that

 $\sqrt{|a_{i_0j}^{(k)}|} \le |a_{i_0j}^{(k+1)}| \le 1$,

for any $k \geq 1$. From this, we can finally write that the iterations in Algorithm 2.1 provide scaled matrices $\widehat{\mathbf{A}}^{(\mathbf{k})}$, $k = 1, 2, \ldots$, with the following properties

$$\forall k \ge 1, \ 1 \le i \le m, \ \sqrt{\|\mathbf{r}_i^{(k)}\|_{\infty}} \le |a_{ij_0}^{(k+1)}| \le \|\mathbf{r}_i^{(k+1)}\|_{\infty} \le 1,$$
 (3.1)

and

$$\forall k \ge 1, \ 1 \le j \le n, \ \sqrt{\|\mathbf{c}_j^{(k)}\|_{\infty}} \le |a_{i_0j}^{(k+1)}| \le \|\mathbf{c}_j^{(k+1)}\|_{\infty} \le 1,$$
 (3.2)

which shows that both row and column norms must converge to 1. To conclude our demonstration, we just need to see that

$$1 - \|\mathbf{r}_{i}^{(k+1)}\|_{\infty} = \frac{1 - \|\mathbf{r}_{i}^{(k+1)}\|_{\infty}^{2}}{1 + \|\mathbf{r}_{i}^{(k+1)}\|_{\infty}} \le \frac{1 - \|\mathbf{r}_{i}^{(k)}\|_{\infty}}{1 + \|\mathbf{r}_{i}^{(k+1)}\|_{\infty}},$$

similar results holding for any of the columns norms, and which fulfils the proof of the linear convergence of Algorithm 2.1 with an asymptotic rate of $\frac{1}{2}$.

To conclude this section, we would like to come back to a few remarks made by Duff, Erisman, and Reid (1986, pages 86–87) about scaling, and which Algorithm 2.1 seems to address "*naturally*" well. As mentioned by the authors,

...equilibration, where diagonal matrices D_1 and D_2 are selected so that D_1AD_2 has the largest entry in each row and column of the same magnitude, unfortunately allows D_1 and D_2 to vary widely.

They also introduced a small 2×2 example

$$\mathbf{A} = \begin{pmatrix} 1.00 & 2420 \\ 1.00 & 1.58 \end{pmatrix},\tag{3.3}$$

and closed the discussion with the following comments:

If the unscaled matrix (3.3) had been caused by a badly scaled first equation, then simple row scaling would be a proper choice. If it had been caused by choosing units for variable x_2 that are 10^3 times too large, then column scaling would be the proper choice.

What we wish to stress here is that, if there happens to be a badly scaled row (or column) in the unscaled matrix A then, despite the fact that the algorithm scales both sides of the matrix simultaneously, it naturally recovers the situation and ends up with an "appropriate" choice with regards to the comments above. To illustrate that, let us just consider the following small example with a badly scaled row

$$\mathbf{A} = \left(\begin{array}{cc} \alpha & \alpha \\ 1 & 1 \end{array}\right). \tag{3.4}$$

If $\alpha \ll 1$ in (3.4), then iteration k ($k \ge 1$) of the algorithm provides the following matrices:

$$\mathbf{D}_{1}^{(k)} = \begin{pmatrix} \alpha^{-(1-\frac{1}{2^{k}})} & 0\\ 0 & 1 \end{pmatrix}, \ \widehat{\mathbf{A}}^{(\mathbf{k})} = \begin{pmatrix} \alpha^{\frac{1}{2^{k}}} & \alpha^{\frac{1}{2^{k}}}\\ 1 & 1 \end{pmatrix}, \ \mathbf{D}_{2}^{(\mathbf{k})} = \mathbf{I}_{2},$$

converging to the situation where $\widehat{\mathbf{A}}$ is the matrix with all ones, \mathbf{D}_1 has its first diagonal entry equal to α^{-1} , and \mathbf{D}_2 stays the identity matrix. If $\alpha \gg 1$ in (3.4), then the first iteration yields

$$\mathbf{D}_{1}^{(1)} = \begin{pmatrix} \alpha^{-\frac{1}{2}} & 0 \\ 0 & 1 \end{pmatrix}, \ \widehat{\mathbf{A}}^{(1)} = \begin{pmatrix} 1 & 1 \\ \alpha^{-\frac{1}{2}} & \alpha^{-\frac{1}{2}} \end{pmatrix}, \ \mathbf{D}_{2}^{(1)} = \alpha^{-\frac{1}{2}} \mathbf{I}_{2},$$

and subsequent iterations ($k \ge 2$) will then give

$$\mathbf{D}_{1}^{(1)} = \begin{pmatrix} \alpha^{-\frac{1}{2}} & 0 \\ 0 & \alpha^{\frac{1}{2}(1 - \frac{1}{2^{k-1}})} \end{pmatrix}, \ \widehat{\mathbf{A}}^{(1)} = \begin{pmatrix} 1 & 1 \\ \alpha^{-\frac{1}{2^{k}}} & \alpha^{-\frac{1}{2^{k}}} \end{pmatrix}, \ \mathbf{D}_{2}^{(\mathbf{k})} = \alpha^{-\frac{1}{2}} \mathbf{I}_{2},$$

with an asymptotic situation very similar to the previous one except that the scalar factor $\alpha^{-\frac{1}{2}}$ appears in the column scaling matrix. Similar reasoning on a matrix with a badly scaled column would bring us to the same type of conclusions with an appropriate column scaling instead. The above two examples also show that we cannot expect (apart from some particular cases) to prove faster convergence than the linear rate of $\frac{1}{2}$. Finally, if we apply Algorithm 2.1 to the 2×2 example (3.3) from Duff, Erisman, and Reid (1986), convergence is achieved in 2 iterations, with the following matrices

$$\mathbf{D}_{1}^{(2)} = \left(\begin{array}{cc} .0203 & 0 \\ 0 & .8919 \end{array} \right), \ \widehat{\mathbf{A}}^{(2)} = \left(\begin{array}{cc} .0228 & 1 \\ 1 & .0286 \end{array} \right), \ \mathbf{D}_{2}^{(2)} = \left(\begin{array}{cc} 1.1212 & 0 \\ 0 & .0203 \end{array} \right).$$

The 2-norm condition number of A is 2421.6 and that of the scaled matrix $\widehat{A}^{(2)}$ is now of 1.0528. We also notice that the algorithm has distributed part of the bad scaling of this matrix into both the row and the column scaling matrices D_1 and D_2 , ending up with a situation where the scaled matrix can easily be permuted into a strongly diagonally dominant matrix. This is a very favourable situation for a good pivoting strategy in Gaussian elimination, for instance, if we refer to the motivations for scaling in Duff, Erisman, and Reid (1986).

4 Some comparisons with the symmetric scaling algorithm of Bunch

We have stressed, at the beginning of Section 3, that Algorithm 2.1 is well suited for symmetric scaling of symmetric matrices. Bunch (1971) also developed a symmetric scaling algorithm for equilibration in the infinity-norm. He additionally gave detailed explanations, by means of a small 2×2 example, about the fact that there was no assurance at all that his symmetric scaling algorithm would be optimal in minimising the infinity-norm condition number of the scaled matrix over all possible choices of positive diagonal scaling matrix. Uniqueness is not even guaranteed, except under certain conditions as recalled by the author. Our aim, in the following text, is to exploit the same 2×2 example to compare and discuss the main differences between Algorithm 2.1 and the one of Bunch (1971) in the case of symmetric matrices.

Bunch (1971, Section 7) mentions that his symmetric scaling algorithm can increase the condition number, but also highlights the fact that it is not always possible to reduce it with equilibration in the infinity-norm. To illustrate this point, he discussed the case of a simple 2×2 example where

$$\mathbf{A} = \left(\begin{array}{cc} a & b \\ b & c \end{array} \right), \quad \mathbf{D} = \left(\begin{array}{cc} d & 0 \\ 0 & e \end{array} \right),$$

with $a, b, c \neq 0$, d, e > 0, and $\det \mathbf{A} \neq 0$. The condition number in the infinity-norm can be easily computed in this case, giving:

$$\kappa_{\infty}(\mathbf{A}) = \|\mathbf{A}\|_{\infty} \|\mathbf{A}^{-1}\|_{\infty} = \frac{\{|b| + \max(|a|, |c|)\}^2}{|ac - b^2|},$$

and

$$\kappa_{\infty}(\mathbf{DAD}) = \frac{\{|b| + \max(|a|d/e, |c|e/d)\}^2}{|ac - b^2|},$$

with a minimum of

$$\min_{d,e>0} \kappa_{\infty}(\mathbf{DAD}) = \frac{\left\{|b| + \sqrt{|ac|}\right\}^2}{|ac - b^2|},$$

achieved with

$$\mathbf{D} = \lambda \begin{pmatrix} \sqrt{|c|} & 0 \\ 0 & \sqrt{|a|} \end{pmatrix}, \quad (\lambda > 0).$$

The scaled matrix then becomes

$$\widehat{\mathbf{A}} = \lambda^2 \begin{pmatrix} a|c| & b\sqrt{|ac|} \\ b\sqrt{|ac|} & c|a| \end{pmatrix},$$

and we can see that there always exists a scaling matrix \mathbf{D} such that $\widehat{\mathbf{A}}$ is equilibrated and with minimal condition number κ_{∞} . Depending whether $|ac| > b^2$ or not, one can indeed fix λ to set to ± 1 the largest entries in $\widehat{\mathbf{A}}$ above.

The algorithm of Bunch (1971) scales in fact the lower triangular part of A, one row at a time, starting with the first element a_{11} . In the case of this 2×2 example, it first gives

$$\mathbf{D}^{(1)} = \begin{pmatrix} \frac{1}{\sqrt{|a|}} & 0\\ 0 & 1 \end{pmatrix}, \ \widehat{\mathbf{A}}^{(1)} = \begin{pmatrix} \operatorname{sgn}(a) & \frac{b}{\sqrt{|a|}}\\ \frac{b}{\sqrt{|a|}} & c \end{pmatrix},$$

and then, depending which is the maximum of the two elements $|b|/\sqrt{|a|}$ and $\sqrt{|c|}$, gives the two following solutions:

$$\widehat{\mathbf{A}} = \begin{pmatrix} \operatorname{sgn}(a) & \frac{b}{\sqrt{|ac|}} \\ \frac{b}{\sqrt{|ac|}} & \operatorname{sgn}(c) \end{pmatrix}, \ \mathbf{D} = \begin{pmatrix} \frac{1}{\sqrt{|a|}} & 0 \\ 0 & \frac{1}{\sqrt{|c|}} \end{pmatrix}, \ \text{if } |\mathbf{ac}| > \mathbf{b^2}, \tag{4.1}$$

and

$$\widehat{\mathbf{A}} = \begin{pmatrix} \operatorname{sgn}(a) & \operatorname{sgn}(b) \\ \operatorname{sgn}(b) & \frac{c|a|}{b^2} \end{pmatrix}, \ \mathbf{D} = \begin{pmatrix} \frac{1}{\sqrt{|a|}} & 0 \\ 0 & \frac{\sqrt{|a|}}{|b|} \end{pmatrix}, \ \text{if } |\mathbf{ac}| \le \mathbf{b^2}.$$
 (4.2)

Now, when applying Algorithm 2.1 to this 2×2 symmetric matrix, we must consider 6 different cases:

- 1. |a| > |b| > 0 and |c| > |b| > 0. In this case, the algorithm converges in one iteration as already explained in the beginning of this section, giving the same solution (4.1) as the Bunch algorithm (because |ac| is obviously bigger than b^2), which corresponds to the optimal scaling discussed above.
- 2. |a|>|b|>0, 0<|c|<|b|, and $|ac|\le b^2$. In this case, Algorithm 2.1 generates an asymptotically convergent sequence, giving at iteration $k\ge 2$

$$\widehat{\mathbf{A}}^{(\mathbf{k})} = \begin{pmatrix} \operatorname{sgn}(a) & \operatorname{sgn}(b) \left| \frac{b}{a} \right|^{\frac{1}{2k}} \\ \operatorname{sgn}(b) \left| \frac{b}{a} \right|^{\frac{1}{2k}} & \frac{c}{|b|} \left| \frac{a}{b} \right|^{(1 - \frac{1}{2k - 1})} \end{pmatrix}, \ \mathbf{D}^{(\mathbf{k})} = \begin{pmatrix} \frac{1}{\sqrt{|a|}} & 0 \\ 0 & \frac{1}{\sqrt{|b|}} \left| \frac{a}{b} \right|^{\frac{1}{2}(1 - \frac{1}{2k - 1})} \end{pmatrix},$$

and converging to the situation (4.2), which again corresponds to the answer the Bunch algorithm would give in this case. The scaled matrix is not the optimal one. Its condition number is $\kappa_{\infty}(\widehat{\mathbf{A}}) = 4\mathbf{b^2}/|\mathbf{b^2} - \mathbf{ac}|$, since $|ac| \leq b^2$, and is smaller than the condition number of \mathbf{A} , $\kappa_{\infty}(\mathbf{A}) = (|b| + |a|)^2/|b^2 - ac|$, because |a| > |b| > |c|.

3. |a| > |b| > 0, 0 < |c| < |b|, and $|ac| > b^2$. In this case, we are sure that there exists an iteration k_0 such that

$$\left| \frac{b}{a} \right|^{\frac{1}{2^{k_0}}} < \left| \frac{c}{b} \right| \left| \frac{a}{b} \right|^{\left(1 - \frac{1}{2^{k_0 - 1}}\right)}$$

and Algorithm 2.1 will then terminate at iteration $k_0 + 1$ with exactly the same solution as in (4.1). This corresponds again to the optimal scaling and is also provided by the Bunch algorithm.

- 4. The cases where |c| > |b| > |a| > 0, with $|ac| \le b^2$ or $|ac| > b^2$, imply very similar discussions to the two previous cases. The only difference is for the asymptotic solution in the case $|ac| \le b^2$, for which the two elements on the diagonal of $\widehat{\mathbf{A}}$ in (4.2) are interchanged (and their signs set appropriately), and differs from the solution provided by the Bunch algorithm which is still exactly the same as in (4.2). At any rate, the condition numbers of the two solutions are equal and less than that of matrix $\widehat{\mathbf{A}}$.
- 5. Finally, in the case |b| > |a| > 0 and |b| > |c| > 0, Algorithm 2.1 converges in one iteration and simply gives

$$\widehat{\mathbf{A}} = \begin{pmatrix} \frac{a}{|b|} & \operatorname{sgn}(b) \\ \operatorname{sgn}(b) & \frac{c}{|b|} \end{pmatrix}, \ \mathbf{D} = \begin{pmatrix} \frac{1}{\sqrt{|b|}} & 0 \\ 0 & \frac{1}{\sqrt{|b|}} \end{pmatrix}, \tag{4.3}$$

which does not correspond to the optimal scaling but still does not increase the condition number. In this case, the Bunch algorithm still gives the same solution as in (4.2), because |ac| is obviously smaller than b^2 , but there the resulting condition number is necessarily increased.

We observe that Algorithm 2.1 provides, in half the cases, a scaling with optimal condition number and that, in all cases, it does not increase the condition number of the original matrix, as opposed to the Bunch algorithm which can do so (see case number 5 above). One of the major differences between Algorithm 2.1 and the Bunch algorithm is that the latter always forces the first element \hat{a}_{11} in the scaled matrix to be equal to ± 1 (see Bunch (1971, page 572)). Because of that, the Bunch algorithm is sensitive to a priori symmetric permutations applied to A that may change the first element on the diagonal. In that respect, and this is easy to see, Algorithm 2.1 is totally independent of any permutations on A, in the sense that the resulting scaling on the permuted matrix would correspond to the permutation of the scaling matrices obtained on the original matrix.

However, the algorithm of Bunch (1971) ensures termination in n steps, n being the size of the symmetric matrix, whereas Algorithm 2.1 is only guaranteed, even in the symmetric case (see the second case discussed just above), to converge asymptotically to an equilibrated solution in the infinity-norm, with fast linear convergence nevertheless. A final comment, just worth mentioning, is that Algorithm 2.1 also has a natural parallelism, whereas the Bunch algorithm is more intrinsically sequential.

5 Extensions to other norms

A natural idea would be to change the norm used in Algorithm 2.1, and to try for instance the two-norm or the one-norm because of the optimal properties they induce

(see van der Sluis (1969), Parlett and Landis (1982)), and still expect convergence towards an equilibrated situation with all rows and columns of norm 1 in the corresponding norm. We shall see, in the remainder of this section, that this will usually, but not always, work and we investigate the potential and limitations of such extensions.

The idea of equilibrating a matrix with both rows and columns of one-norm equal to 1 in not new, and has been the subject of constant efforts since the 1960's, and even before. Sinkhorn and Knopp (1967) have studied a method for scaling square nonnegative matrices to **doubly stochastic** form, that is a nonnegative matrix with all rows and columns of equal one-norm. Sinkhorn (1964) originally showed that: Any positive square matrix of order n is diagonally equivalent to a unique doubly stochastic matrix of order n, and the diagonal matrices which take part in the equivalence are unique up to scalar factors. Very recently, Borobia and Cantó (1998) gave a different proof for the existence part of Sinkhorn's theorem with some elementary geometric interpretations.

The above result was further extended to the case of nonnegative nonzero matrices as follows. A square $n \times n$ nonnegative matrix $\mathbf{A} \geq 0$ is said to have *support* if there exists a permutation σ such that $a_{i,\sigma(i)} > 0$, $1 \leq i \leq n$. Note that matrices not having support are matrices for which no *full transversal* can be found (see Duff, Erisman, and Reid (1986, page 107)), that is a column permutation – or equivalently, a row permutation – making the diagonal zero-free, and are thus *structurally singular*. A matrix \mathbf{A} is said to have *total support* if every positive entry in \mathbf{A} can be permuted onto a positive diagonal with a column permutation. A nonnegative nonzero square matrix \mathbf{A} of size n > 1 is said to be *fully indecomposable* if there does not exist permutation matrices \mathbf{P} and \mathbf{Q} such that \mathbf{PAQ} is of the form

$$\left(\begin{array}{cc} \mathbf{A}_{11} & \mathbf{A}_{12} \\ 0 & \mathbf{A}_{22} \end{array}\right),\,$$

with A_{11} and A_{22} being square matrices. Duff, Erisman, and Reid (1986, Chapter 6) also use the term "bi-irreducible" for such a property. Sinkhorn and Knopp (1967) established that their balancing algorithm, which simply iterates on normalizing all rows and columns in the matrix A alternately, converges to a doubly stochastic limit \widehat{A} if and only if the matrix A has support. The doubly stochastic limit \widehat{A} can be represented as D_1AD_2 (meaning that A and \widehat{A} are diagonally equivalent) if and only if A has total support and, if the support of A is not total, then there must be a positive entry in A converging to A0. Additionally, Sinkhorn and Knopp (1967) proved that the diagonal matrices A1 and A2, when they exist, are unique up to some scalar factors if and only if the matrix A1 is fully indecomposable. Brualdi, Parter, and Schneider (1966) independently showed the same diagonal equivalence between A1 and a doubly stochastic matrix when A1 is a direct sum of fully indecomposable matrices, and according to Soules (1991), Mirsky and Perfect (1965) showed that a matrix A1 has total support if and only if there exist permutation matrices A2 and A3 direct sum of fully indecomposable matrices.

Different contributions have also been made in the study of convergence of the Sinkhorn-Knopp method under various hypothesis. Sinkhorn (1967) proved geometric convergence for positive starting matrices, and Soules (1991) extended the result to matrices with total support. Finally, Achilles (1993) has established the converse of the above, that is that geometric convergence of the Sinkhorn-Knopp method implies total support for the nonnegative starting matrix **A**.

Parlett and Landis (1982) describe three new iterative scaling algorithms, with experimental evidence of better average and worst-case convergence behaviour than the Sinkhorn-Knopp method for at least one of the three. They also gave a generalized version of the convergence theorem of Sinkhorn and Knopp (1967), including a characterisation of scaling algorithms that will converge to a doubly stochastic situation when the starting matrix A has support. Such algorithms are called by Parlett and Landis "diagonal product increasing (DPI)" algorithms, and we shall comment on this characterisation in the end of this section since our algorithm also verifies the DPI hypothesis stated by Parlett and Landis (1982). It must be mentioned beforehand that the discussion in the rest of this section follows very closely that of Parlett and Landis (1982), with a few slight differences worth mentioning.

We now state our main result, which concerns the convergence of Algorithm 2.1 with the one-norm in place of the infinity one and, to do so, we will use the same notation as in Parlett and Landis (1982). Algorithm 2.1 produces a sequence of iteration matrices diagonally equivalent to the starting matrix $\mathbf{A} = \mathbf{A}^{(0)}$:

$$\mathbf{A}^{(k)} = \left(a_{ij}^{(k)}\right) = \mathbf{D}^{(k)} \mathbf{A} \mathbf{E}^{(k)}, \quad k = 1, 2, \dots,$$

$$\mathbf{D}^{(k)} = \operatorname{diag}\left(d_1^{(k)}, \dots, d_n^{(k)}\right),$$

$$\mathbf{E}^{(k)} = \operatorname{diag}\left(e_1^{(k)}, \dots, e_n^{(k)}\right),$$
(5.1)

(so, for example, $a_{ij}^{(k)} = d_i^{(k)} a_{ij} e_j^{(k)}$) and we set $\mathbf{D}^{(0)} = \mathbf{E}^{(0)} = \mathbf{I}$. We denote by $r_i^{(k)}$, $i = 1, \ldots, n$, and $c_j^{(k)}$, $j = 1, \ldots, n$, the one-norm of rows and columns respectively, thus:

$$r_i^{(k)} = \sum_{j=1}^n |a_{ij}^{(k)}|,$$

$$c_j^{(k)} = \sum_{i=1}^n |a_{ij}^{(k)}|.$$
(5.2)

We also assume for simplicity that $\mathbf{A} \geq 0$, since scaling \mathbf{A} or $|\mathbf{A}|$ will be the same. Under this simplification, the one-norm of rows and columns reduces to row and column sums respectively, $r_i^{(k)} = \sum_{j=1}^n a_{ij}^{(k)}$ and $c_j^{(k)} = \sum_{i=1}^n a_{ij}^{(k)}$, and to generalize our results to any matrix, one just needs to extend the definition of a "doubly stochastic matrix" so that the absolute value of the matrix under consideration is doubly stochastic in the usual sense.

THEOREM 5.1 Given the sequence (5.1) of diagonal equivalents for A, in which

$$a_{ij}^{(k+1)} = \frac{a_{ij}^{(k)}}{\sqrt{r_i^{(k)}}\sqrt{c_j^{(k)}}}, \quad 1 \le i, j \le n,$$

with $r_i^{(k)}$ and $c_j^{(k)}$ given by (5.2):

- 1. If **A** has support, then $\mathbf{S} = \lim_{k \to \infty} \mathbf{A}^{(k)}$ exists and is doubly stochastic.
- 2. If A has total support, then both $D = \lim_{k\to\infty} D^{(k)}$ and $E = \lim_{k\to\infty} E^{(k)}$ exist and S = DAE.

Proof of point (1) in Theorem 5.1: We recall from Parlett and Landis (1982) the arithmetic-geometric mean inequality which states that, if $x_i \geq 0$ for $i = 1, \ldots, n$ then

$$\prod_{i=1}^{n} x_i \le \left(\sum_{i=1}^{n} \frac{x_i}{n}\right)^n,\tag{5.3}$$

with equality holding if and only if $x_1 = x_2 = \ldots = x_n$.

Now, using (5.3), we can write for all k

$$\prod_{i=1}^{n} r_i^{(k+1)} \le \left(\frac{1}{n} \sum_{i=1}^{n} r_i^{(k+1)}\right)^n = \left(\frac{1}{n} \sum_{1 \le i, j \le n} \frac{a_{ij}^{(k)}}{\sqrt{r_i^{(k)}} \sqrt{c_j^{(k)}}}\right)^n,$$

with the same inequality for $\prod_{j=1}^{n} c_{j}^{(k+1)}$ since

$$\sum_{i=1}^{n} r_i^{(k+1)} = \sum_{j=1}^{n} c_j^{(k+1)} = \sum_{1 \le i, j \le n} a_{ij}^{(k+1)}.$$

Additionally, using the Cauchy-Schwarz inequality on the dot-product of the two n^2 -vectors $\mathbf{v} = (\sqrt{a_{ij}^{(k)}}/\sqrt{r_i^{(k)}})_{1 \leq i,j \leq n}$ and $\mathbf{w} = (\sqrt{a_{ij}^{(k)}}/\sqrt{c_j^{(k)}})_{1 \leq i,j \leq n}$, we can write that

$$\sum_{1 \le i, j \le n} \frac{a_{ij}^{(k)}}{\sqrt{r_i^{(k)}} \sqrt{c_j^{(k)}}} \le \sqrt{\sum_{1 \le i, j \le n} \frac{a_{ij}^{(k)}}{r_i^{(k)}}} \sqrt{\sum_{1 \le i, j \le n} \frac{a_{ij}^{(k)}}{c_j^{(k)}}} = \sqrt{n} \sqrt{n},$$

and thus, for all $k \ge 0$, we have

$$\prod_{i=1}^{n} r_i^{(k+1)} \le \left(\frac{1}{n} \sum_{i=1}^{n} r_i^{(k+1)}\right)^n \le 1 \text{ and } \prod_{j=1}^{n} c_j^{(k+1)} \le \left(\frac{1}{n} \sum_{j=1}^{n} c_j^{(k+1)}\right)^n \le 1.$$
 (5.4)

Finally, if we introduce

$$s_k = \prod_{i=1}^n d_i^{(k)} e_i^{(k)}, \quad k = 1, 2, \dots$$

we easily see that

$$\frac{s_k}{s_{k+1}} = \prod_{i=1}^n \sqrt{r_i^{(k)} c_i^{(k)}} \le 1,\tag{5.5}$$

which shows that the sequence $(s_k)_{k=1,2,...}$ is monotonically increasing (unless all row and column sums are equal).

Since A has support, there exists a permutation σ such that $a_{i,\sigma(i)} > 0$, $1 \le i \le n$. Let $a = \min_{1 \le i \le n} (a_{i,\sigma(i)})$. Then, for all $k \ge 1$,

$$\sum_{i=1}^{n} d_i^{(k)} e_{\sigma(i)}^{(k)} a \le \sum_{i=1}^{n} d_i^{(k)} e_{\sigma(i)}^{(k)} a_{i,\sigma(i)} = \sum_{i=1}^{n} a_{i,\sigma(i)}^{(k)} \le n,$$

the last inequality being simply due to the fact that, after the first iteration, all the entries in matrix $A^{(k)}$ are less than or equal to 1. Then, by the arithmetic-geometric mean inequality (5.3),

$$s_k = \prod_{i=1}^n d_i^{(k)} e_i^{(k)} \le a^{-n}, \ k = 1, 2, \dots$$

and the monotonically increasing sequence $(s_k)_{k=1,2,...}$ is bounded. Therefore

$$\lim_{k \to \infty} s_k = L > 0$$

exists, and

$$\lim_{k \to \infty} \frac{s_k}{s_{k+1}} = 1. \tag{5.6}$$

Using (5.3) and (5.4), we can write

$$\frac{s_k}{s_{k+1}} = \prod_{i=1}^n \sqrt{r_i^{(k)} c_i^{(k)}} \le \left\{ \sum_{i=1}^n \frac{1}{2n} \left(r_i^{(k)} + c_i^{(k)} \right) \right\}^n \le 1,$$

and because of (5.6) we can conclude both that

$$\lim_{k \to \infty} \prod_{i=1}^{n} r_i^{(k)} c_i^{(k)} = 1 \text{ and } \lim_{k \to \infty} \sum_{i=1}^{n} \frac{1}{2n} \left(r_i^{(k)} + c_i^{(k)} \right) = 1.$$
 (5.7)

Now, since all the elements in $\mathbf{A}^{(k)}$ are less than 1 after the first iteration, we know that each of the two sequences $(r_i^{(k)})_{k=1,2,\dots}$ and $(c_j^{(k)})_{k=1,2,\dots}$, for all $1 \leq i,j \leq n$, are bounded (note that this is also implied by (5.4)). Let us introduce the sequence $(\mathbf{v}^{(k)})_{k=1,2,\dots}$ of the 2n-vectors

$$\mathbf{v}^{(k)} = (r_1^{(k)}, \dots, r_n^{(k)}, c_1^{(k)}, \dots, c_1^{(k)}),$$

which is also bounded in $I\!\!R^{2n}$ of finite dimension. Consider then any convergent subsequence $(\mathbf{v}^{(\hat{k})})_{\hat{k}}$ and denote by

$$x_i = \lim_{\hat{k} \to \infty} r_i^{(\hat{k})}, \ 1 \le i \le n,$$

and

$$y_j = \lim_{\hat{k} \to \infty} c_j^{(\hat{k})}, \ 1 \le j \le n.$$

From (5.7), we can write

$$\prod_{i=1}^{n} x_i y_i = \left\{ \sum_{i=1}^{n} \frac{1}{2n} (x_i + y_i) \right\}^{2n} = 1,$$

and since the arithmetic-geometric mean equality only holds if all the elements are equal, we easily see that $x_1 = \ldots = x_n = 1 = y_1 = \ldots = y_n$. Therefore any convergent subsequence of the bounded sequence $(\mathbf{v}^{(k)})_{k=1,2,...}$ in finite dimensional space must have the same limit (made with all ones), which implies that the sequence $(\mathbf{v}^{(k)})_{k=1,2,...}$ is necessarily convergent and that

$$\lim_{k \to \infty} r_i^{(k)} = 1 \text{ and } \lim_{k \to \infty} c_j^{(k)} = 1, \ 1 \le i, j \le n.$$
 (5.8)

Again, since all $a_{ij}^{(k)}$ are less than 1 after the first iteration, the sequence of matrices $(\mathbf{A}^{(k)})_{k=1,2,...}$ is also bounded in the finite dimensional space $\mathcal{M}_n(\mathbb{R})$. Let us consider any convergent subsequence $(\mathbf{A}^{(\hat{k})})_{\hat{k}}$ of $(\mathbf{A}^{(k)})_{k=1,2,...}$, and denote by

$$\mathbf{S} = \lim_{\hat{k} \to \infty} \mathbf{A}^{(\hat{k})}.$$

Then, paraphrasing the results in Parlett and Landis (1982) for the proof of their Corollary 1, we can state the following: because of (5.8), S is doubly stochastic and, since the set of $n \times n$ doubly stochastic matrices is the convex hull of the set of $n \times n$ permutation matrices (see Birkhoff (1946)), S must thus have total support. Therefore, $s_{ij} = \lim_{\hat{k} \to \infty} a_{ij}^{(\hat{k})} = 0$ whenever $a_{ij} > 0$ cannot be permuted onto a positive diagonal. Now, consider the matrix $\widehat{\mathbf{A}}$ in which all entries $a_{ij} > 0$ in \mathbf{A} that cannot be permuted onto a positive diagonal have been set to zero, the others remaining the same. From the previous remark, it is clear that $S = \lim_{\hat{k} \to \infty} A^{(\hat{k})}$ is also equal to

$$\mathbf{S} = \lim_{\hat{k} \to \infty} \mathbf{D}^{(\hat{k})} \widehat{\mathbf{A}} \mathbf{E}^{(\hat{\mathbf{k}})}.$$

Additionally, from the proof in Parlett and Landis (1982, pages 67-68) of THEOREM 1, point (2), which simply exploits properties (5.3), (5.4), (5.5), and the fact that any nonzero element in A can be permuted onto a positive diagonal, since by construction A has total support, we know that there exists a strictly positive constant γ such that, for each nonzero entry a_{ij} in **A**, we have:

$$\forall k \ge 1, \ d_i^{(k)} e_j^{(k)} \ge \gamma > 0.$$
 (5.9)

We mention, however, a very little difference in (5.4) and the hypothesis exploited by Parlett and Landis, which comes from the fact that they were considering "scaled algorithms" in general, thus imposing the property

(P3)
$$\mu_k = \frac{1}{n} \sum_{i=1}^n r_i^{(k+1)} = 1,$$

which in our case holds just as an inequality in (5.4). However, since they only use property (P3) as an upper bound in some parts of their demonstration, the inequality (5.4) is sufficient and all conclusions remain the same. Note also that result (5.9) is valid for the entire sequence and not just the subsequence indexed by k. Consequently, for each nonzero entry a_{ij} in $\widehat{\mathbf{A}}$, we can write:

$$\lim_{\hat{k} \to \infty} d_i^{(\hat{k})} e_j^{(\hat{k})} = \frac{s_{ij}}{a_{ij}} > 0.$$

Then, applying LEMMA 2 in Parlett and Landis (1982) (which is itself paraphrased from Sinkhorn and Knopp (1967, page 345)) we know that there exist positive sequences $(x_i^{(\hat{k})})_{\hat{k}}$ and $(y_i^{(\hat{k})})_{\hat{k}}$ with positive limits such that

$$d_i^{(\hat{k})} e_j^{(\hat{k})} = x_i^{(\hat{k})} y_j^{(\hat{k})}, \quad \forall a_{ij} > 0 \text{ in } \widehat{\mathbf{A}}, \text{ and } \forall (\hat{\mathbf{k}}).$$

Then, taking

$$\mathbf{X}^{(\hat{k})} = \operatorname{diag}\left(x_1^{(\hat{k})}, \dots, x_n^{(\hat{k})}\right),$$

$$\mathbf{Y}^{(\hat{k})} = \operatorname{diag}\left(y_1^{(\hat{k})}, \dots, y_n^{(\hat{k})}\right),$$

$$\mathbf{X} = \lim_{\hat{k} \to \infty} \mathbf{X}^{(\hat{k})} \text{ and } \mathbf{Y} = \lim_{\hat{k} \to \infty} \mathbf{Y}^{(\hat{k})},$$

we have

$$\mathbf{S} = \lim_{\hat{k} \to \infty} \mathbf{D}^{(\hat{k})} \widehat{\mathbf{A}} \mathbf{E}^{(\hat{\mathbf{k}})} = \lim_{\hat{\mathbf{k}} \to \infty} \mathbf{X}^{(\hat{\mathbf{k}})} \widehat{\mathbf{A}} \mathbf{Y}^{(\hat{\mathbf{k}})} = \mathbf{X} \widehat{\mathbf{A}} \mathbf{Y},$$

showing that $\widehat{\mathbf{A}}$ is diagonally equivalent to \mathbf{S} . Now, consider any other convergent subsequence in $(\mathbf{A}^{(k)})_{k=1,2,\dots}$. For the same reasons as above, its limits will also be doubly stochastic and diagonally equivalent to $\widehat{\mathbf{A}}$, and since doubly stochastic equivalents are unique (see Sinkhorn and Knopp (1969)), the two limits must be the same. Therefore, we can conclude that $\lim_{k\to\infty} \mathbf{A}^{(k)}$ exists and is doubly stochastic, which fulfils the proof of point (1).

Proof of point (2) in Theorem 5.1: As a direct consequence of the demonstration of point (1), we can state that, if **A** has total support, then $\mathbf{S} = \lim_{k \to \infty} \mathbf{A}^{(k)}$ is diagonally equivalent to **A**, since in this case $\mathbf{A} = \widehat{\mathbf{A}}$ in the previous discussion.

To prove that, under the same hypothesis, both $\mathbf{D} = \lim_{k \to \infty} \mathbf{D}^{(k)}$ and $\mathbf{E} = \lim_{k \to \infty} \mathbf{E}^{(k)}$ exist and $\mathbf{S} = \mathbf{D}\mathbf{A}\mathbf{E}$, we first make the assumption that \mathbf{A} not only has total support but is also fully indecomposable. In this case, \mathbf{A} is not only diagonally equivalent to the doubly stochastic limit $\mathbf{S} = \lim_{k \to \infty} \mathbf{A}^{(k)}$, but we also know from Sinkhorn and Knopp (1967) that the diagonal matrices which take place in this equivalence are unique up to a scalar factor.

Without loss of generality, we can consider that the matrix \mathbf{A} has a full diagonal, since \mathbf{A} has support and since Algorithm 2.1 is independent of any permutations on \mathbf{A} . Let us suppose now that one of the sequences $(d_i^{(k)})_{k=1,2,\dots}$ is unbounded for some i (the same could be done with one of the $(e_i^{(k)})_{k=1,2,\dots}$). In such a case, there exist a subsequence $(d_i^{(\hat{k})})_{\hat{k}}$ such that

$$\lim_{\hat{k} \to \infty} (d_i^{(\hat{k})})_{\hat{k}} = +\infty.$$

As the matrix is fully indecomposable, for any index j, $1 \le j \le n$, there exist a subset of nonzero entries in A

$$a_{ij_1}, a_{j_1j_2}, \dots, a_{j_{q-1}j_q}, a_{j_qj}$$

"connecting" index i to index j. Consequently, because of (5.9), we can show by using each of the nonzero intermediate entries $a_{j_pj_{p+1}}$ in the subset above as well

as each of the corresponding nonzero diagonal pivots, that there exist $\alpha_{ij} > 0$ and $\beta_{ij} > 0$ such that

$$\lim_{\hat{k}\to\infty} \frac{d_j^{(\hat{k})}}{d_i^{(\hat{k})}} = \alpha_{ij} \text{ and } \lim_{\hat{k}\to\infty} d_i^{(\hat{k})} e_j^{(\hat{k})} = \beta_{ij}.$$

Since this can be done for any index j, we can conclude that the subsequence $(\prod_{j=1}^n d_j^{(\hat{k})})_{\hat{k}}$ goes to infinity as $(d_i^{(\hat{k})})^n \prod_{j=1}^n \alpha_{ij}$ and that the subsequence $(\prod_{j=1}^n e_j^{(\hat{k})})_{\hat{k}}$ (which is strictly positive) goes to zero as $(d_i^{(\hat{k})})^{-n} \prod_{j=1}^n \beta_{ij}$, and the last conclusion is in contradiction with (5.4) which shows that both sequences $(\prod_{j=1}^n d_j^{(k)})_{k=1,2,\dots}$ and $(\prod_{j=1}^n e_j^{(k)})_{k=1,2,\dots}$ are monotonically increasing. Consequently, each of the sequences $(d_i^{(k)})_{k=1,2,\dots}$ and $(e_i^{(k)})_{k=1,2,\dots}$ are bounded.

Now, since the two sequences $(\mathbf{D}^{(k)})_{k=1,2,...}$ and $(\mathbf{E}^{(k)})_{k=1,2,...}$ are bounded in the finite dimensional space $\mathcal{D}_n(\mathbb{R})$, let us consider two convergent subsequences:

$$\left(\mathbf{D}^{(\hat{k})}, \mathbf{E}^{(\hat{k})}\right) \underset{\hat{k} \to +\infty}{\longrightarrow} \left(\mathbf{D}_1, \mathbf{E}_1\right),$$

and

$$\left(\mathbf{D}^{(\tilde{k})}, \mathbf{E}^{(\tilde{k})}\right) \xrightarrow[\tilde{k} \to +\infty]{} \left(\mathbf{D}_2, \mathbf{E}_2\right).$$

Obviously, $\mathbf{D}_1\mathbf{A}\mathbf{E}_1=\mathbf{S}=\mathbf{D}_2\mathbf{A}\mathbf{E}_2$, and thus, because of the unicity shown by Sinkhorn and Knopp (1967), there exists $\alpha>0$ such that $\mathbf{D}_1=\alpha\mathbf{D}_2$ and $\mathbf{E}_1=(1/\alpha)\mathbf{E}_2$. Then, as mentioned above, since both sequences $(\prod_{p=1}^n d_p^{(k)})_{k=1,2,\dots}$ and $(\prod_{p=1}^n e_p^{(k)})_{k=1,2,\dots}$ are monotonically increasing, it is clear that α must be equal to 1 and the two limits must be equal. Therefore, we can conclude that $\mathbf{D}=\lim_{k\to\infty}\mathbf{D}^{(k)}$ and $\mathbf{E}=\lim_{k\to\infty}\mathbf{E}^{(k)}$ exist and point (2) in Theorem 5.1 holds for fully indecomposable matrices.

Finally, we know from Mirsky and Perfect (1965) that matrices with total support can be permuted into a direct sum of fully indecomposable matrices. Now, since Algorithm 2.1 is independent of any permutation, we get the result from what precedes by applying it independently to each fully indecomposable matrix in such a direct sum. This fulfils the proof of point (2).

We would like to recall some of the results contained in Parlett and Landis (1982), which can also be collected from the proof of Theorem 5.1 above.

COROLLARY 5.1

1. If A is diagonally equivalent to a doubly stochastic matrix, S, then

$$\mathbf{S} = \lim_{k \to \infty} \mathbf{A}^{(k)}.$$

2. If **A** has support and is not diagonally equivalent to a doubly stochastic matrix, then for each pair of indices (i, j) such that a_{ij} cannot be permuted onto a positive diagonal by a column permutation,

$$\lim_{k \to \infty} a_{ij}^{(k)} = 0.$$

Parlett and Landis (1982), in their THEOREM 1, additionally gave some characterisations for iterative scaling algorithms that would converge to doubly stochastic situations when matrix $\bf A$ has support. Namely, they introduced three properties (P1), (P2), and (P3) which, when they hold for the iterates (5.1), enable one to prove convergence of the sequence $({\bf A}^{(k)})_{k=1,2,...}$ to a doubly stochastic limit. Property (P1) is simply equation (5.5), or equivalently that the sequence $(s_k)_{k=1,2,...}$ is monotonically increasing. Property (P2) implies that, under the hypothesis (5.6), both (5.8) and

$$\lim_{k \to \infty} d_i^{(k+1)} / d_i^{(k)} = \lim_{k \to \infty} e_j^{(k+1)} / e_j^{(k)} = 1, \quad 1 \le i, j \le n,$$
 (5.10)

hold. Property (P3) is simply to consider that the algorithm is scaled, with

(P3)
$$\mu_k = \frac{1}{n} \sum_{i=1}^n r_i^{(k+1)} = 1$$

at each iteration. In our case, this only holds as an inequality and, as we already mentioned, it is sufficient to complete the proof. It is important to note also that we did not need to establish the second set of conclusions (5.10) contained in (P2) to complete the proof of Theorem 5.1. This was the main reason why we wanted to rederive the proof of the convergence which, as one may easily see, can be extended to any algorithm that satisfies (P1), the first part of (P2), and just an inequality in (P3). Strictly speaking, (P3) is not even necessary and it is only sufficient to prove that all the elements $a_{ij}^{(k)}$ are bounded. However, the inequality in (P3) was necessary in our case to prove (5.8), and even if (P2) is a consequence of (P3), it has to be shown by some means.

Finally, the proof that each of the sequences $(d_i^{(k)})_{k=1,2,\dots}$ and $(e_j^{(k)})_{k=1,2,\dots}$ converges under the hypothesis that ${\bf A}$ has total support is not contained in Parlett and Landis (1982, Theorem 1), and relies on the added property induced by (5.4), which we may call (P4), and which says that both sequences $(\prod_{p=1}^n d_p^{(k)})_{k=1,2,\dots}$ and $(\prod_{p=1}^n e_p^{(k)})_{k=1,2,\dots}$ are monotonically increasing and also implies (P1). It also relies on the property (P5) that the iterates (5.1), are permutation independent, otherwise these results only hold a priori for fully indecomposable matrices. Now, looking carefully at the convergence proof above, it is clear that we can extend the results in Theorem 5.1 to all sequences (5.1) of diagonal equivalents for ${\bf A}$ satisfying the first part of (P2), the inequality in (P3), and (P4)+(P5) instead of (P1).

A last comment for the symmetric case. Considering the fact that Algorithm 2.1 preserves symmetry, we can state the following additional results:

COROLLARY 5.2

- 1. If A is symmetric and has support, then Algorithm 2.1 in the one-norm builds a sequence of symmetric scalings of A converging to a symmetric doubly stochastic limit.
- 2. If A is symmetric and has total support, then A is symmetrically equivalent to a symmetric doubly stochastic matrix S, and Algorithm 2.1 in the one-norm builds a convergent sequence of diagonal matrices $\mathbf{D}^{(k)}$ such that $\mathbf{S} = \lim_{k \to \infty} \mathbf{D}^{(k)} \mathbf{A} \mathbf{D}^{(k)}$.

We did not investigate the speed of convergence of Algorithm 2.1 in the case of the one-norm, and we have not yet performed enough experiments to add any pertinent comment on that. We can mention however that we have seen cases where Algorithm 2.1 outperforms the Sinkhorn-Knopp method by a factor of 10 or more, and cases where it is the opposite. We still need to investigate in detail what can be the reasons for such varying behaviour in Algorithm 2.1, in order to determine if it is possible to accelerate the convergence of Algorithm 2.1 in some way.

6 Conclusions

One particular issue concerns the extension of Algorithm 2.1 to any of the l_p norms, $1 \le p < \infty$. and in particular to the 2-norm as mentionned in the introduction. If the discussion in Rothblum, Schneider, and Schneider (1994) (see Section 8, page 13) was applied to Algorithm 2.1, then scaling a matrix with the l_p norm of each row and column is equivalent to applying Algorithm 2.1 in the one-norm to the pth Hadamard power of \mathbf{A} , that is the matrix whose ijth entry is $(a_{ij})^p$, and to take the Hadamard pth root of the resulting iterates. Therefore, all the convergence results shown in the previous section still hold with any of the l_p norms, $1 \le p < \infty$.

Extensions of Algorithm 2.1 to the scaling of multidimensional matrices (see Bapat (1982), Raghavan (1984), Franklin and Lorenz (1989), for instance) can also be done in a very simple manner. Consider for example a three dimensional nonnegative matrix $\mathbf{A} = (a_{ijk})$, and suppose that its one-dimensional marginals $x_i = \sum_j \sum_k a_{ijk}$, $y_j = \sum_i \sum_k a_{ijk}$, and $z_k = \sum_i \sum_j a_{ijk}$ are all positive, then the idea is to scale \mathbf{A} to $\widehat{\mathbf{A}}$ by setting

$$\hat{a}_{ijk} = \frac{a_{ijk}}{\sqrt[3]{x_i}\sqrt[3]{y_j}\sqrt[3]{z_k}}$$

for all i, j, k, and to iterate on that. Generalization to p-dimensional matrices can be done with the pth root of each of the p corresponding one-dimensional marginals. We must mention, however, that we did not investigate these extensions at all, and we cannot state whether they are convergent of not.

Acknowledgements. I would like to thank Nick Gould, Iain Duff, and Mario Arioli for careful proofreading of the article and the useful discussions that helped to improve the content of the article.

References

- E. ACHILLES, (1993), *Implications of Convergence Rates in Sinkhorn Balancing*, Linear Algebra and its Applications, **187**, 109–112.
- R. BAPAT, (1982), D_1AD_2 theorems for multidimensional matrices, Linear Algebra and its Applications, 48, 437–442.
- F. L. BAUER, (1963), Optimally scaled matrices, Numer. Math., 5, 73–87.

- F. L. BAUER, (1969), Remarks on optimally scaled matrices, Numer. Math., 13, 1–3.
- G. D. BIRKHOFF, (1946), *Tres Observaciones Sobre el Algebra Lineal*, Universidad Nacional de Tucuman Revista, Serie A, **5**, 147–151.
- A. BOROBIA AND R. CANTÓ, (1998), *Matrix Scaling: A Geometric Proof of Sinkhorn's Theorem*, Linear Algebra and its Applications, **268**, 1–8.
- R. A. Brualdi, S. V. Parter, and H. Schneider, (1966), *The diagonal equivalence of a nonnegative matrix to a stochastic matrix*, J. Math. Anal. Appl., **16**, 31–50.
- J. R. Bunch, (1971), Equilibration of Symmetric Matrices in the Max-Norm, J. ACM, 18, 566–572.
- A. R. Curtis and J. K. Reid, (1972), On the automatic scaling of matrices for Gaussian elimination, J. Inst. Maths. Applies., 10, 118–124.
- I. S. DUFF AND J. KOSTER, (1999), On algorithms for permuting large entries to the diagonal of a sparse matrix, Tech. Rep. RAL-TR-1999-030, Rutherford Appleton Laboratory. To appear in SIAM Journal on Matrix Analysis and Applications.
- I. S. DUFF, A. M. ERISMAN, AND J. K. REID, (1986), *Direct Methods for Sparse Matrices*, Oxford University Press, London.
- J. Franklin and J. Lorenz, (1989), *On the scaling of multidimensional matrices*, Linear Algebra and its Applications, **114/115**, 717–735.
- HSL, (2000), A collection of Fortran codes for large scale scientific computation. http://www.cse.clrc.ac.uk/Activity/HSL.
- L. MIRSKY AND L. PERFECT, (1965), *The distribution of positive elements in doubly stochastic matrices*, J. London Math. Soc., **40**, 689–698.
- B. N. PARLETT AND T. L. LANDIS, (1982), *Methods for Scaling to Double Stochastic Form*, Linear Algebra and its Applications, **48**, 53–79.
- T. E. S. RAGHAVAN, (1984), *On pairs of multidimensional matrices*, Linear Algebra and its Applications, **62**, 263–268.
- U. G. ROTHBLUM, H. SCHNEIDER, AND M. H. SCHNEIDER, (1994), Scaling matrices to prescribed row and column maxima, SIAM J. Matrix Anal. Appl., 15, 1–14.
- M. H. Schneider and S. Zenios, (1990), A comparative study of algorithms for matrix balancing, Operations Research, 38, 439–455.
- R. SINKHORN AND P. KNOPP, (1967), Concerning nonnegative matrices and doubly stochastic matrices, Pacific J. Math., 21, 343–348.

- R. SINKHORN AND P. KNOPP, (1969), *Problems concerning diagonal products in nonnegative matrices*, Trans. Amer. Math. Soc., **136**, 67–75.
- R. SINKHORN, (1964), A relationship between arbitrary positive matrices and doubly stochastic matrices, Ann. Math. Statist., **35**, 876–879.
- R. SINKHORN, (1967), Diagonal equivalence to matrices with prescribed row and column sums, Amer. Math. Monthly, **74**, 402–405.
- G. W. SOULES, (1991), *The rate of convergence of Sinkhorn balancing*, Linear Algebra and its Applications, **150**, 3–40. Proceedings of the First Conference of the International Linear Algebra Society (Provo, UT, 1989).
- A. VAN DER SLUIS, (1969), Condition Numbers and Equilibration of Matrices, Numer. Math., 14, 14–23.