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RESEARCH MEMORANDUM



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SAMEH'S PARALLEL EIGENVALUE ALGORITHM
REVISITED

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SUMMARY

We give an improved version of Sameh's parallel norm-reducing eigenvalue algorithm. The use of so-called Euclidean parameters of nonunitary shears simplifies the formulae in the related minimization problem. Our main result is that with $n/2$ parallel processors almost diagonalization of an $n \times n$ non normal matrix is reached in $\mathcal{O}(n \log n)$ iterations. Each iteration needs $\mathcal{O}(n)$ steps; with $n^2/2$ processors one needs $\mathcal{O}(\log n)$ steps per iteration.

CONTENTS

1. Introduction
2. Unimodular shear transformations
3. Parallel identical norm-reducing shears
4. The preconditioned parallel shears method
5. Implementational aspects of the algorithm
6. References

1. INTRODUCTION

In 1962 Eberlein [2] proposed a Jacobi-like norm-reducing method for the eigenproblem of nonnormal matrices. Since that epochmaking article several authors [1,6,7,9,12,13,14,15] analysed, modified and improved that algorithm. In [11] Sameh developed, on base of Eberlein's procedure a Jacobi-like method for a parallel computer. The aim of this paper is to put forward a unified approach for Jacobi-like norm-reducing transformations and to apply that approach to elucidate and improve Sameh's method.

In Jacobi-like norm-reducing procedures shear matrices $W_{\ell,m}$ are used in similarity transformations in order to reduce the Euclidean norm of the current matrix: $A' = W_{\ell,m}^{-1} A W_{\ell,m}$. With successive executions of these transformations one aims to reach an almost normal matrix that can be (almost) diagonalized with unitary transformations. This solves approximately the eigenproblem.

The unimodular shear $W_{\ell,m}$ differs from the unit matrix I_n in the (ℓ,m) -plane. For convenience let be

$$\hat{W}_{\ell,m} = \begin{pmatrix} p & q \\ r & s \end{pmatrix} \in \mathbb{R}^{2 \times 2}, \quad ps - qr = 1,$$

to be called the (ℓ,m) -restriction of $W_{\ell,m}$. Since the Euclidean norm is invariant under orthogonal transformations, the optimal norm-reducing shear $W_{\ell,m}$ is determined except for an orthogonal factor, say $Q_{\ell,m}$. Matrices $S, P \in \mathbb{R}^{n \times n}$ will be called row-congruent if $S = PQ$ for some orthogonal matrix Q , notation $S \sim P$. It is easy to see that S and P are row-congruent iff $SS^T = PP^T$. Now for shear $W_{\ell,m}$ holds

$$\hat{W}_{\ell,m} \hat{W}_{\ell,m}^T = \begin{pmatrix} p^2 + q^2 & pr + qs \\ pr + qs & r^2 + s^2 \end{pmatrix} = \begin{pmatrix} x & z \\ z & y \end{pmatrix}.$$

The quantities

$$x = x(W_{\ell,m}) = p^2 + q^2, \quad y = y(W_{\ell,m}) = r^2 + s^2, \quad z = z(W_{\ell,m}) = pr + qs$$

will be called the Euclidean parameters of $W_{\ell,m}$ [7]. So row-congruent shears with the same pivot pair share their Euclidean parameters and effectuate the same Euclidean norm of the transformed matrix:

$$V_{\ell,m} \sim W_{\ell,m} \Leftrightarrow \|V_{\ell,m}^{-1} A V_{\ell,m}\|_E = \|W_{\ell,m}^{-1} A W_{\ell,m}\|_E.$$

We assume $W_{\ell,m}$ to be unimodular so

$$x, y > 0, \quad xy - z^2 = 1$$

The subset

$$H = \{(x, y, z) \in \mathbb{R}^3 \mid xy - z^2 = 1, x, y > 0\}$$

is the positive sheet of the elliptic hyperboloid $xy - z^2 = 1$.

Section 2 describes the sequential optimal norm-reducing process and is preparatory for the other sections. In the second section we present the calculation that proves the existence of a quadratic function

$\|W_{\ell,m}^{-1} A W_{\ell,m}\|_E^2 = f(x, y, z; A) = \alpha x + \beta y + 2\gamma z + (-\lambda x + \mu y + \nu z)^2 + \text{const.}$, x, y, z being the Euclidean parameters of unimodular shear $W_{\ell,m}$ and $\alpha, \beta, \gamma, \lambda, \mu, \nu$ are constants derived from A . In case p, q, r, s of $W_{\ell,m}$ are complex numbers, then the Euclidean parameters of $W_{\ell,m}$ are

$$x = |p|^2 + |q|^2, \quad y = |r|^2 + |s|^2, \quad z = p\bar{r} + q\bar{s}.$$

These quantities are the non-trivial elements of $W_{\ell,m} W_{\ell,m}^*$. The unifying effect of the Euclidean parameters for the description of $\|W_{\ell,m}^{-1} A W_{\ell,m}\|$ can be seen in table 1. Each row gives the parametrization used by that author.

$\hat{W}_{\ell m}$	(x, y, z)	
$\begin{pmatrix} e^{-i\beta} \cos w & -e^{i\alpha} \sin w \\ e^{-i\alpha} \sin w & e^{i\beta} \cos w \end{pmatrix}, w = u+iv$	$x=y=\cosh 2v$ $z=-e^{i(\alpha-\beta)} \sin 2v$	Eberlein [2]
$\begin{pmatrix} \cosh v & -ie^{i\alpha} \sinh v \\ ie^{-i\alpha} \sinh v & \cosh v \end{pmatrix}$	$x=y=\cosh 2v$ $z=-ie^{i\alpha} \sinh 2v$	Ruhe [9]
$\begin{pmatrix} \cos \alpha & \sin \alpha \\ -\sin \alpha & \cos \alpha \end{pmatrix} \begin{pmatrix} \cosh v & \sinh v \\ \sinh v & \cosh v \end{pmatrix}$	$x=\cosh 2v+\sin 2\alpha \sinh 2v$ $y=\cosh 2v-\sin 2\alpha \sinh 2v$ $z=\cos 2\alpha \sinh 2v$	Eberlein, Boothroyd [4] Sameh [11]
$\begin{pmatrix} \cos \alpha & \sin \alpha \\ -\sin \alpha & \cos \alpha \end{pmatrix} \begin{pmatrix} 1 & b \\ 0 & 1 \end{pmatrix}$	$x=1+b^2 \cos^2 \alpha + b \sin 2\alpha$ $y=1+b^2 \sin^2 \alpha + b \sin 2\alpha$ $z=b \cos 2\alpha - b^2 \sin^2 \alpha$	Voevodin [15] Veselic [13]
$\begin{pmatrix} \cosh v & \sinh v \\ \sinh v & \cosh v \end{pmatrix}$	$x=y=\cosh 2v$ $z=\sinh 2v$	Dollinger [1]

Table 1. Norm-reducing shears and their Euclidean parameters

The simplicity of function f on H enables the computation of the row congruent unimodular shears $\hat{W}_{\ell, m}$ that minimize $\|\hat{W}_{\ell, m}^{-1} A \hat{W}_{\ell, m}\|_E$. With a well chosen pivot-strategy $\{(\ell_k, m_k)\}$ the optimal norm-reducing shears \hat{W}_{ℓ_k, m_k} , $k \in \mathbb{N}$, generate a sequence $\{A_k\}$, where $A_1 = A$ and $A_{k+1} = \hat{W}_{\ell_k, m_k}^{-1} A_k \hat{W}_{\ell_k, m_k}$ such that this sequence converges to the set of normal matrices, i.e.

$$C(A_k) := A_k^T A_k - A_k A_k^T \rightarrow 0, (k \rightarrow \infty).$$

The matrix $C(A_k)$ is called the commutator of A_k and measures the nonnormality of A_k [3,5].

Just as well in Sameh's Jacobi-like algorithm the formula for the norm-reduction becomes simple with the Euclidean parametrization of the parallel performed transformations.

In section 3 we describe the construction of an optimal parallel transformation. The convergence to normality by preconditioned norm-reducing

parallel shears is discussed in section 4. The preconditioning transformation $Q_j^T A_j Q_j = A'_j$, $j = 1, 2, \dots$, where Q_j is a direct sum of orthogonal shears, annihilates the elements $c_{2\ell-1, 2\ell}$, $\ell = 1, \dots, n/2$, of $C(A_j)$. This pretreatment before the optimal norm-reducing transformation

$A''_j = W_j^{-1} A'_j W_j$, where W_j is a direct sum of $n/2$ identical shears, achieves the norm-reduction to be large enough for convergence to normality,

$C(A''_j) \rightarrow 0$ ($j \rightarrow \infty$).

Section 5 gives implementational details of the process.

2. UNIMODULAR SHEAR TRANSFORMATIONS

Let $A = (a_{ij})$ be a real $n \times n$ matrix and $W_{\ell, m}$ a unimodular shear. Let be $\begin{pmatrix} P & Q \\ R & S \end{pmatrix}$ the (ℓ, m) -restriction of $W_{\ell, m}$, (x, y, z) the Euclidean parameters of $W_{\ell, m}$, i.e.

$$x = p^2 + q^2, \quad y = r^2 + s^2, \quad z = pr + qs,$$

with

$$x, y > 0 \quad \text{and} \quad xy - z^2 = 1.$$

With easy but tedious calculations we obtain

THEOREM 2.1. [7]. If $W_{\ell, m}$ is a unimodular shear with Euclidean parameters (x, y, z) , then

$$\|W_{\ell, m}^{-1} A W_{\ell, m}\|_E^2 = f(x, y, z; A) + \sigma + e \quad (2.1)$$

where

$$f(x, y, z; A) = \alpha x + \beta y + \gamma z + (-\lambda x + \mu y + z)^2 + \sigma + e \quad (2.2)$$

with

$$\begin{aligned} \alpha &= \sum_{i=1}^n (a_{i\ell}^2 + a_{im}^2), & \lambda &= a_{m\ell} \\ \beta &= \sum_{i=1}^n (a_{\ell i}^2 + a_{im}^2), & \mu &= a_{\ell m} \\ \gamma &= \sum_{i=1}^n (a_{i\ell} a_{im} - a_{\ell i} a_{mi}), & \nu &= a_{\ell\ell} - a_{mm} \\ \sigma &= \sum_{i, j=1}^n a_{ij}^2, & e &= (a_{\ell\ell} + a_{mm})^2 - 2(a_{\ell\ell} a_{mm} - a_{\ell m} a_{m\ell}) \end{aligned} \quad (2.3)$$

(Σ' means summation except for ℓ, m).

□

With the Lagrange function

$$L(x, y, z, \rho) = f(x, y, z; A) - \rho(xy - z^2 - 1)$$

one derives that the Lagrange multiplier ρ together with

$$\tau := \tau(x, y, z) := -\lambda x + \mu y + \nu z \quad (2.4)$$

has to satisfy the equations

$$\rho^2 + E\tau^2 - 2D\tau - F = 0$$

$$(\rho + E)\tau - D = 0$$

where

$$D = \alpha\mu - \beta\lambda - \gamma\nu, \quad F = \alpha\beta - \gamma^2.$$

THEOREM 2.2. [5]. If D and F are not both equal to zero, then

$$\min\{f(x, y, z; A) \mid (x, y, z) \in H\} = f(\mathfrak{x}, \mathfrak{y}, \mathfrak{z}),$$

where

$$\mathfrak{x} = \frac{2\mu D + \beta(\rho + E)}{\rho(\rho + E)}, \quad \mathfrak{y} = \frac{-2\lambda D + \alpha(\rho + E)}{\rho(\rho + E)}, \quad \mathfrak{z} = \frac{-\nu D - \gamma(\rho + E)}{\rho(\rho + E)}$$

Here ρ is the unique root of the quartic equation

$$(\rho + E)^2(\rho^2 - F) - D^2(2\rho + E) = 0$$

for which root holds $\rho > \min(0, E)$. □

An accurate investigation of the minimization problem gives that the infimum of f on the unbounded subset H of \mathbb{R}^3 is not assumed when $D = 0 \wedge F = 0 \wedge (\alpha + \beta \neq 0 \vee (E = 0 \wedge \lambda \neq \mu))$. Then the intersection of the planes $\alpha x + \beta y + 2\gamma z = 0$ and $-\lambda x + \mu y + \nu z = 0$ is in the tangent cone

$xy - z^2 = 0$ of H .

With the new variables

$$w = (x-y)/2, \quad t = t(w, z) = (x+y)/2 = \sqrt{1+w^2+z^2}$$

we get

$$\|W_{\ell, m}^{-1} A W_{\ell, m}\|_E^2 = (\alpha+\beta)t + (\alpha-\beta)w + 2\gamma z + ((\mu-\lambda)t - (\mu+\lambda)w + uz)^2 + \sigma + e =: g(w, z; A) \quad (2.5)$$

The relation between the commutator of A and the partial derivatives of g is given in

THEOREM 2.3. [7, 10]. If $C(A) = (c_{ij})$ and $\|W_{\ell, m}^{-1} A W_{\ell, m}\|_E^2 = g(w, z; A)$, where $w = (x-y)/2$, then

$$\frac{\partial g}{\partial w}(0, 0) = c_{\ell\ell} - c_{mm}, \quad \frac{\partial g}{\partial z}(0, 0) = 2c_{\ell m}. \quad (2.6)$$

Moreover

$$\|W_{\ell, m}^{-1} A W_{\ell, m}\|_E^2 = \min\{g(w, z; A) \mid (w, z) \in \mathbb{R}^2\}$$

iff

$$\tilde{c}_{\ell\ell} - \tilde{c}_{mm} = \tilde{c}_{\ell m} = 0,$$

where

$$(\tilde{c}_{ij}) = C(W_{\ell, m}^{-1} A W_{\ell, m}). \quad \square$$

Without proof we mention

THEOREM 2.4. [7]. Let the sequence $\{A_k\}$, starting from $A_0 = A$ be constructed recursively by

$$A_k = W_{\ell_k, m_k}^{-1} A_{k-1} W_{\ell_k, m_k}, \quad k = 1, 2, \dots$$

where (ℓ_k, m_k) is the pivotpair selected according to rule

$$(c_{\ell_k, \ell_k}^{(A_k)} - c_{m_k, m_k}^{(A_k)})^2 + 4c_{\ell_k, m_k}^2(A_k) \geq \frac{4}{n(n-1)} \|C(A_k)\|_E^2 \quad (2.7)$$

and W_{ℓ_k, m_k} reduces the Euclidean norm in an optimal way.

Then

$$\|A_k\|_E^2 - \|A_{k+1}\|_E^2 \geq \frac{1}{3n(n-1)} \frac{\|C(A_k)\|_E^2}{\|A\|_E^2} \quad (2.8)$$

and

$$C(A_k) \rightarrow 0 \quad (k \rightarrow \infty).$$

□

For the sequel it is important to note that in the proof of this theorem a suboptimal shear V_{ℓ_k, m_k} is constructed. This suboptimal V_{ℓ_k, m_k} already suffices to reduce the norm as in (2.8). V_{ℓ_k, m_k} is the product of two shears $Q_{\ell_k, m_k}^D D_{\ell_k, m_k} \cdot Q_{\ell_k, m_k}$ is an orthogonal shear that annihilates element c_{ℓ_k, m_k} of the commutator and D_{ℓ_k, m_k} is a diagonal shear with Euclidean parameters $(x_k, x_k^{-1}, 0)$. Since $\frac{\partial g}{\partial z}(0, 0; Q_{\ell_k, m_k}^T A_{k-1} Q_{\ell_k, m_k}) = 0$, we take z , the third Euclidean parameter of D_{ℓ_k, m_k} , equal to zero. A Newton iteration in the minimization of $x \rightarrow f(x, x^{-1}, 0; Q_{\ell_k, m_k}^T A_{k-1} Q_{\ell_k, m_k})$ gives x_k for D_{ℓ_k, m_k} . This suboptimal V_{ℓ_k, m_k} already gives norm-reduction (2.8). The conclusion $C(A_k) \rightarrow 0$ follows from the Eberlein inequality [3,5]:

$$\|A\|_E^2 - \sum_{i=1}^n |\lambda_i|^2 \geq \frac{1}{6} \|C(A)\|_E^2 / \|A\|_E^2.$$

3. PARALLEL IDENTICAL NORMREDUCING SHEARS

Let the matrix A be real and of even order $n = 2k$. Then it can be partitioned as follows

$$A = \begin{pmatrix} A_{11} & A_{12} & \dots & A_{1k} \\ A_{21} & A_{22} & \dots & A_{2k} \\ \vdots & \vdots & & \vdots \\ A_{k1} & A_{k2} & \dots & A_{kk} \end{pmatrix}$$

where each submatrix is given by

$$A_{\ell,m} = \begin{pmatrix} a_{2\ell-1,2m-1} & a_{2\ell-1,2m} \\ a_{2\ell,2m-1} & a_{2\ell,2m} \end{pmatrix}, \quad \ell, m = 1, \dots, k.$$

For convenience define

$$\begin{aligned} \lambda_{\ell,m} &:= a_{2\ell,2m-1}, \quad \mu_{\ell,m} := a_{2\ell-1,2m}, \quad \alpha_{\ell,m} := a_{2\ell-1,2m-1}, \\ \beta_{\ell,m} &:= a_{2\ell,2m}, \quad \nu_{\ell,m} := \alpha_{\ell,m} - \beta_{\ell,m}, \quad \ell, m = 1, \dots, k. \end{aligned} \quad (3.1)$$

Let

$$A' = W^{-1}AW,$$

where

$$W = \text{diag}(S_1, S_2, \dots, S_k)$$

and

$$S_i = \begin{pmatrix} p_i & q_i \\ r_i & s_i \end{pmatrix}, \quad p_i s_i - q_i r_i = 1, \quad i = 1, \dots, k. \quad (3.2)$$

As before $x_i := p_i^2 + q_i^2$, $y_i := r_i^2 + s_i^2$, $z_i := p_i r_i + q_i s_i$, $i = 1, \dots, k$: they are the Euclidean parameters of S_i , so $x_i y_i - z_i^2 = 1$.

Then

$$A'_{\ell m} = S_\ell^{-1} A_{\ell m} S_m = \begin{pmatrix} \alpha'_{\ell m} & \mu'_{\ell m} \\ \lambda'_{\ell m} & \beta'_{\ell m} \end{pmatrix}, \quad \ell, m = 1, \dots, k.$$

or, equivalently

$$\begin{pmatrix} \alpha'_{\ell, m} \\ \mu'_{\ell, m} \\ \lambda'_{\ell, m} \\ \beta'_{\ell, m} \end{pmatrix} = S_\ell^{-1} \otimes S_m \begin{pmatrix} \alpha_{\ell, m} \\ \mu_{\ell, m} \\ \lambda_{\ell, m} \\ \beta_{\ell, m} \end{pmatrix}$$

Trivially one finds

THEOREM 3.1. For each pair (ℓ, m) , $\ell, m = 1, \dots, k$, $\|A'_{\ell, m}\|_E^2$ is a bilinear function of the Euclidean parameters (x_ℓ, y_ℓ, z_ℓ) of S_ℓ and (x_m, y_m, z_m) of S_m :

$$\|S_\ell^{-1} A_{\ell, m} S_m\|_E^2 = (x_\ell, y_\ell, z_\ell) \begin{pmatrix} \lambda_{\ell, m}^2 & \beta_{\ell, m}^2 & 2\lambda_{\ell, m} \beta_{\ell, m} \\ \alpha_{\ell, m}^2 & \mu_{\ell, m}^2 & 2\alpha_{\ell, m} \mu_{\ell, m} \\ -2\alpha_{\ell, m} \lambda_{\ell, m} & -2\beta_{\ell, m} \mu_{\ell, m} & -2(\alpha_{\ell, m} \beta_{\ell, m} + \lambda_{\ell, m} \mu_{\ell, m}) \end{pmatrix} \begin{pmatrix} x_m \\ y_m \\ z_m \end{pmatrix} \quad \square$$

Completely analogous to theorem 2.3 we get

THEOREM 3.2. For each $i \in \{1, \dots, k\}$ let be

$$w_i := (x_i - y_i)/2, \quad t_i := (x_i + y_i)/2 = (1 + w_i^2 + z_i^2)^{\frac{1}{2}}.$$

Then is $\|W^{-1} A W\|_E^2$ is a bilinear function of (t_i, w_i, z_i) , $i = 1, \dots, k$ and as such a function $g(\underline{w}, \underline{z})$, where $\underline{w} = (w_1, \dots, w_k)$, $\underline{z} = (z_1, \dots, z_k)$. Moreover

$$\frac{\partial g}{\partial w_i}(0, 0) = c_{2i-1, 2i-1} - c_{2i, 2i}, \quad \frac{\partial g}{\partial z_i}(0, 0) = 2c_{2i-1, 2i},$$

where $(c_{ij}) = A^T A - AA^T$. □

The complexity of the unconstrained minimization of $g(\underline{w}, \underline{z})$ forces the restriction to a simpler minimization problem with fewer variables. Therefore we consider, following Sameh [11],

$$W = \text{diag}(S_1, S_2, \dots, S_k),$$

with $S_i = S = \begin{pmatrix} p & q \\ r & s \end{pmatrix}$, $ps - qr = 1$, $i = 1, \dots, k$, to be called a parallel identical shear. The computation of $W^{-1}AW$ is readily adapted to parallel computation. As in the foregoing let be

$$x = p^2 + q^2, \quad y = r^2 + s^2, \quad z = pr + qs,$$

the Euclidean parameters of S . Analogous to theorem 2.1 we formulate for this parallel shear transformation

THEOREM 3.3. If W is a k -fold direct sum of shears $S = S_1 = \dots = S_k$ with Euclidean parameters (x, y, z) then

$$\|W^{-1}AW\|_E^2 = \sum_{\ell, m=1}^k (-\lambda_{\ell, m} x + \mu_{\ell, m} y + \nu_{\ell, m} z)^2 / (xy - z^2) + \kappa. \quad (3.3)$$

The quantities $\lambda_{\ell, m}$, $\mu_{\ell, m}$, $\nu_{\ell, m}$ are defined in (3.1) and

$$\kappa = \sum_{\ell, m=1}^k ((\text{tr}(A_{\ell, m}))^2 - 2 \det(A_{\ell, m})). \quad (3.4)$$

PROOF. Let be

$$A'_{\ell, m} = S^{-1}AS = \begin{pmatrix} \alpha'_{\ell, m} & \mu'_{\ell, m} \\ \lambda'_{\ell, m} & \beta'_{\ell, m} \end{pmatrix}, \quad \nu'_{\ell, m} = \alpha'_{\ell, m} - \beta'_{\ell, m}.$$

Then

$$\|A'_{\ell, m}\|_E^2 = (\mu'_{\ell, m} - \lambda'_{\ell, m})^2 + (\text{tr}(A'_{\ell, m}))^2 - 2 \det(A'_{\ell, m})$$

$$= (\mu'_{\ell,m} - \lambda'_{\ell,m})^2 + (\text{tr}(A_{\ell,m}))^2 - 2 \det(A_{\ell,m}).$$

Since $(ps - qr)^2 = xy - z^2$ and

$$\mu'_{\ell,m} = s^2 \mu_{\ell,m} - q^2 \lambda_{\ell,m} + qs u_{\ell,m}$$

$$\lambda'_{\ell,m} = p^2 \lambda_{\ell,m} - r^2 \mu_{\ell,m} + pr u_{\ell,m}$$

we have

$$(\mu'_{\ell,m} - \lambda'_{\ell,m})^2 = (-\lambda_{\ell,m} x + \mu_{\ell,m} y + u_{\ell,m} z)^2.$$

This proves (3.3). □

Since $\|W^{-1}AW\|_E^2$ is an homogeneous function of the Euclidean parameters of the nonsingular shear S , without loss of generality we may assume $xy - z^2 = 1$ with $x, y > 0$.

To avoid cumbersome formulae we introduce the following notation

$$\begin{cases} \underline{b}_1 := -(\lambda_{11}, \lambda_{12}, \dots, \lambda_{1k}, \lambda_{21}, \dots, \lambda_{kk}) \in \mathbb{R}^{k^2}, \\ \underline{b}_2 := (\mu_{11}, \mu_{12}, \dots, \mu_{1k}, \mu_{21}, \dots, \mu_{kk}) \in \mathbb{R}^{k^2}, \\ \underline{b}_3 := (u_{11}, u_{12}, \dots, u_{1k}, u_{21}, \dots, u_{kk}) \in \mathbb{R}^{k^2}, \end{cases} \quad (3.5)$$

$$B := B(A) := (\underline{b}_1, \underline{b}_2, \underline{b}_3) \in \mathbb{R}^{k^2 \times 3}, \quad p := (p_1, p_2, p_3)^T := (x, y, z)^T,$$

$$H = \begin{pmatrix} 0 & \frac{1}{2} & 0 \\ \frac{1}{2} & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}. \quad (3.6)$$

As a simple consequence of theorem 3.1 we get

THEOREM 3.4. If W is a unimodular parallel identical shear with Euclidean parameters $p = (x, y, z)$, then

$$\|W^{-1}AW\|_E^2 = \|Bp\|^2 + \kappa,$$

where κ as given in (3.4) and B in (3.6). The Euclidean parameters satisfy the restriction

$$\underline{p}^T H \underline{p} = 1, \quad p_1 > 0. \quad \square$$

The minimization of $\|B\underline{p}\|$ subject to $\underline{p}^T H \underline{p} = 1$ leads to a generalized eigenproblem. We first present a method for solving this minimization problem in case $\text{rank}(B) = 3$.

THEOREM 3.5. Let be $\text{rank}(B) = 3$ and $B = QR$, with $Q^T Q = I$ and $R \in \mathbb{R}^{3 \times 3}$ uppertriangular. Let be $\underline{p} = (x, y, z)^T$ the vector of the Euclidean parameters of S in $W = \text{diag}(S, S, \dots, S)$ that minimizes $\|W^{-1}A\underline{p}\|_E$. Then $R\underline{p}$ is an eigenvector corresponding with the unique positive eigenvalue of $R^{-T}HR^{-1}$.

PROOF. The function $f(\underline{p}; A) = \|B\underline{p}\|^2$ assumes a minimum on H . For if $M = \|R(1, 1, 0)^T\|$, and $V := \{\underline{p} \in \mathbb{R}^3 \mid \|\underline{p}\| \leq M\|R^{-1}\|\} \cap H$, then $\|B\underline{p}\| > M$ if $\underline{p} \in H \setminus V$. Continuity and compactness arguments prove the existence of a minimum. The stationarity conditions of the Lagrange function $L(\underline{p}, \rho) = \|B\underline{p}\|^2 - \rho(\underline{p}^T H \underline{p} - 1)$ are $\underline{p}^T H \underline{p} = 1$ and

$$(B^T B - \rho H)\underline{p} = 0.$$

Hence

$$(R^{-T}HR^{-1} - \rho^{-1}I)R\underline{p} = 0;$$

so ρ is an eigenvalue of $R^{-T}HR^{-1}$. The eigenvalue ρ^{-1} corresponding with $R\underline{p}$ is positive as follows from convex programming arguments. \square

Now we investigate the minimization of f on H in the particular cases that $\text{rank}(B) < 3$.

THEOREM 3.6. Let be $\text{rank}(B) = 1$ and $\text{range}(B^T) = \text{span}(t_1, t_2, t_3)^T$. Then

$$(i) \quad \min\{\|B\underline{p}\| \mid \underline{p} \in H\} = 0, \quad t_3^2 - 4t_1 t_2 > 0,$$

$$(ii) \quad \min\{\|B\underline{p}\| \mid \underline{p} \in H\} > 0, \quad 4t_1 t_2 - t_3^2 > 0,$$

$$(iii) \quad \inf\{\|Bp\| \mid p \in H\} = 0 \quad , \quad t_3^2 - 4t_1t_2 = 0 ,$$

this infimum is not assumed for finite $p \in H$.

PROOF. Evidently $\|Bp\| = c t_1 p_1 + t_2 p_2 + t_3 p_3$ for some $c \geq 0$.

(i) The equation $t_1 p_1 + t_2 p_2 + t_3 p_3 = 0$ determines a solution curve Γ on H . The parametric form of Γ is

$$p(\lambda) = (\lambda, \lambda^{-1}, 0)^T \quad , \quad t_1 = t_2 = 0$$

$$p(\lambda) = (-t_3 \lambda / t_1, -t_1(1+\lambda^2)/(t_3 \lambda), \lambda)^T \quad , \quad t_1 t_3 \neq 0 \quad , \quad t_2 = 0 \quad (, \quad p_1 > 0)$$

$$p(\lambda) = (-t_2(1+\lambda^2)/(t_3 \lambda), -t_3 \lambda / t_2, \lambda)^T \quad , \quad t_2 t_3 \neq 0 \quad , \quad t_1 = 0 \quad (p_1 > 0)$$

$$p(\lambda) = (\frac{1}{2}(-t_3 \lambda \pm D) / t_1, \frac{1}{2}(-t_3 \lambda \mp D) / t_2, \lambda)^T \quad , \quad D = (t_3^2 - 4t_1 t_2) \lambda^2 - 4t_1 t_2 \geq 0 \quad , \quad t_1 t_2 \neq 0$$

In each of the cases obviously one of the two branches of Γ is on H .

(ii) The positive minimum on H is assumed for

$$p = (4t_1 t_2 - t_3^2)^{-\frac{1}{2}} t_1 / |t_1| (2t_1, 2t_2, -t_3)^T$$

(iii) Let be $t_1, t_2 > 0$. The plane $t_1 p_1 + t_2 p_2 + t_3 p_3 = 0$ contacts the cone $\{p \mid p_1 p_2 = p_3^2, p_1 > 0\}$ along the line $L : p(\lambda) = \lambda(2t_2, 2t_1, -t_3)^T$, $\lambda > 0$. It follows that $\|Bp\| > 0$ on H , for $L \cap H = \emptyset$.

Now we describe a curve Γ on H of which L is in the asymptote:

$$\Gamma : p = \frac{1}{2} \mu (t_1 + t_2)^{-1} (2t_2, 2t_1, -t_3) + \frac{1}{2} \mu^{-1} (t_1 + t_2)^{-1} (2t_1, 2t_2, t_3), \quad \mu > 0.$$

On this curve we find, using the fact that $4t_1 t_2 = t_3^2$
 $t_1 p_1 + t_2 p_2 + t_3 p_3 = (t_1 + t_2) / \mu \rightarrow 0$ for $\mu \rightarrow \infty$. The infimum 0 of $\|Bp\|$ on H is not assumed. \square

In a similar way one derives the next theorem for the case that $\text{rank}(B) = 2$.

THEOREM 3.7. Let be $\text{rank}(B) = 2$ and $N(B) = \text{span}(t_1, t_2, t_3)^T$. Then

$$\min\{\|Bp\| \mid p \in H\} = 0 \quad , \quad t_1 t_2 < t_3^2$$

$$\min\{\|Bp\| \mid p \in H\} > 0, \quad t_1 t_2 < t_3^2$$

$$\inf\{\|Bp\| \mid p \in H\} = 0, \quad t_1 t_2 = t_3^2,$$

this infimum is not assumed for finite p .

REMARK. $C := \{\underline{t} \in \mathbb{R}^3 \mid t_1 \geq 0, 4t_1 t_2 \geq t_3^2\}$ is the positive dual cone of $K := \{p \in \mathbb{R}^3 \mid p_1 \geq 0, p_1 p_2 \geq p_3^2\}$, i.e. $C = K^0 := \{\underline{t} \in \mathbb{R}^3 \mid (\underline{t}, p) \geq 0, \forall p \in K\}$. For if $t_1 p_1 = 0$, then $\underline{t} \in C$ and $p \in K$ implies $\underline{t} \in K^0$. If $t_1 p_1 \neq 0$ then from $\underline{t} \in C$ and $p \in K$ follows $(\underline{t}, p) = (2t_1 p_1 + t_3 p_3)^2 / (4t_1 p_1) \geq 0$. Hence $C \subset K^0$.

Reversely, if $(\underline{t}, p) \geq 0$ for each $p \in K$ with $p_2 > 0$ then $t_2 p_2 \geq -t_3 p_3 - t_1 p_3^2 / p_2$, i.e. $t_2 p_2^2 + t_3 p_2 p_3 + t_1 p_3^2 \geq 0$ for each $p \in K$ with $p_2 > 0$. This implies $\underline{t} \in C$. If $(\underline{t}, p) \geq 0$ for $p \in K$ with $p_2 = 0$ then evidently $K^0 \subset C$. \square

At the ending of this section we demonstrate that minimization of $\|W^{-1}AW\|_E^2$, considered as a function of the Euclidean parameters of the unimodular S in $W = \text{diag}(S, S, \dots, S)$, effectuates the annihilation of a part of $C(W^{-1}AW)$.

Preparatory we introduce new variables, t and w :

$$x = t + w, \quad y = t - w \quad (3.7)$$

Since $xy - z^2 = 1$, $x, y > 0$ on H , $t = t(w, z) = (1 + w^2 + z^2)^{\frac{1}{2}}$.

With the variables w and z we find a new expression $g(w, z; A)$ for $\|W^{-1}AW\|_E^2$.

$$g(w, z; A) = \|(b_{-1} + b_{-2})t + (b_{-1} - b_{-2})w + b_{-3}z\|^2 + \kappa, \quad w, z \in \mathbb{R} \quad (3.8)$$

THEOREM 3.8. Let be $C' = (c'_{ij}) = C(W^{-1}AW)$, where W is the direct sum of k unimodular shears. If $t = (x+y)/2$, $w = (w-y)/2$ then

$$\sum_{\ell=1}^k \begin{pmatrix} c'_{2\ell-1, 2\ell-1} & -c'_{2\ell, 2\ell} \\ & 2c'_{2\ell-1, 2\ell} \end{pmatrix} = \begin{pmatrix} \frac{1}{2}(p^2 + s^2 - q^2 - r^2) & pr - qs \\ pq - rs & ps + qr \end{pmatrix} \begin{pmatrix} g_w(w, z; A) \\ g_z(w, z; A) \end{pmatrix} \quad (3.9)$$

For the elements of C' holds $\sum_{\ell=1}^k (c'_{2\ell-1, 2\ell-1} - c'_{2\ell, 2\ell}) = \sum_{\ell=1}^k c'_{2\ell-1, 2\ell} = 0$
iff g is stationary.

PROOF. Since $\sum_{i=1}^n c'_{i1} = 0$,

$$\begin{aligned} \sum_{\ell=1}^k (c'_{2\ell-1, 2\ell-1} - c'_{2\ell, 2\ell}) &= 2 \sum_{\ell=1}^k c'_{2\ell-1, 2\ell-1} = 2 \sum_{\ell, m=1}^k ((\lambda'_{\ell m})^2 - (\mu'_{\ell m})^2) \quad (3.10) \\ &= 2 \sum_{\ell, m=1}^k ((\mu_{\ell m} - \lambda_{\ell m})^{t-(\mu_{\ell m} + \lambda_{\ell m})w + \nu_{\ell m} z}) ((q^2 - p^2)\lambda_{\ell m} + (r^2 - s^2)\mu_{\ell m} + (pr + qs)\nu_{\ell m}), \end{aligned}$$

where

$$\lambda'_{\ell m} = a'_{2\ell, 2m-1}, \quad \mu'_{\ell m} = a'_{2\ell-1, 2m}, \quad \ell, m = 1, \dots, k.$$

Similarly

$$\begin{aligned} \sum_{\ell=1}^m c'_{2\ell-1, 2\ell} &= \sum_{\ell, m=1}^k \nu'_{\ell m} (\mu'_{\ell m} - \lambda'_{\ell m}) \quad (3.11) \\ &= \sum_{\ell, m=1}^k ((\mu_{\ell m} - \lambda_{\ell m})^{t-(\mu_{\ell m} + \lambda_{\ell m})w + \nu_{\ell m} z}) (-2pq \lambda_{\ell m} + 2rs \mu_{\ell m} + (ps - qr)\nu_{\ell m}) \end{aligned}$$

with

$$\nu'_{\ell m} = a'_{2\ell-1, 2m-1} - a'_{2\ell, 2m}, \quad \ell, m = 1, \dots, k.$$

Further, as follows from (3.8)

$$\begin{aligned} \frac{\partial g}{\partial w}(w, z; A) &= 2 \sum_{\ell, m=1}^k ((\mu_{\ell m} - \lambda_{\ell m})^{t-(\mu_{\ell m} + \lambda_{\ell m})w + \nu_{\ell m} z}) ((\mu_{\ell m} - \lambda_{\ell m}) \frac{w}{t} - (\mu_{\ell m} + \lambda_{\ell m})) \\ \frac{\partial g}{\partial z}(w, z; A) &= 2 \sum_{\ell, m=1}^k ((\mu_{\ell m} - \lambda_{\ell m})^{t-(\mu_{\ell m} + \lambda_{\ell m})w + \nu_{\ell m} z}) ((\mu_{\ell m} - \lambda_{\ell m}) \frac{z}{t} + \nu_{\ell m}). \end{aligned}$$

With simple but tedious calculations one verifies (3.9). Since

$$\frac{1}{2} (p^2+s^2-q^2-r^2)(ps+qr)-(pq-rs)(pr-qs) = \frac{1}{2} (ps-qr)(p^2+q^2+r^2+s^2) = t \geq 1,$$

we conclude $\sum_{\ell=1}^k (c'_{2\ell-1,2\ell-1} - c'_{2\ell,2\ell}) = \sum_{\ell=1}^k c'_{2\ell-1,2\ell} = 0$ iff $g_w = g_z = 0$. \square

THEOREM 3.9. If $C(A) = (c_{ij})$, then

$$\begin{pmatrix} k \\ \sum_{\ell=1}^k (c_{2\ell-1,2\ell-1} - c_{2\ell,2\ell}) \\ \\ k \\ 2 \sum_{\ell=1}^k c_{2\ell-1,2\ell} \end{pmatrix} = \begin{pmatrix} g_w(0,0;A) \\ \\ \\ g_z(0,0;A) \end{pmatrix} \quad (3.12)$$

PROOF. Substitute $p = s = 1, q = r = 0$ in (3.9). \square

4. THE PRECONDITIONED PARALLEL SHEARS METHOD

This section describes the norm-reducing transformation

$$A' = W^{-1} Q^T A Q W = W^{-1} (Q^T A Q) W \quad (4.1)$$

where

$$Q = \text{diag}(Q_1, \dots, Q_k), \quad W = \text{diag}(S, \dots, S), \quad (4.2)$$

with

$$Q_\ell = \begin{pmatrix} \cos \phi_\ell & \sin \phi_\ell \\ -\sin \phi_\ell & \cos \phi_\ell \end{pmatrix}, \quad \frac{\pi}{2} < \phi_\ell \leq \frac{\pi}{2}, \quad \ell = 1, \dots, k. \quad (4.3)$$

and

$$S = \begin{pmatrix} p & q \\ r & s \end{pmatrix}, \quad ps - qr = 1. \quad (4.4)$$

As in Sameh's algorithm [11] the preconditioning orthogonal matrix Q is chosen such that $\text{grad } g(0,0;Q A Q)$ has maximal length. On base of theorem 3.9 one derives

THEOREM 4.1. Let be $Q = \text{diag}(Q_1, \dots, Q_k)$, with Q_ℓ , $\ell = 1, \dots, k$, as given in (4.3) and let be

$$\underline{v}_\ell(A) = \underline{v}_\ell = \begin{pmatrix} c_{2\ell-1,2\ell-1} - c_{2\ell,2\ell} \\ 2c_{2\ell-1,2\ell} \end{pmatrix}, \quad \ell = 1, \dots, k. \quad (4.5)$$

Then the maximum length of $\text{grad } g(0,0;Q A Q)$ with respect to Q equals

$\sum_{\ell=1}^k \|\underline{v}_\ell\|$ and is assumed for

$$\begin{pmatrix} \cos 2\phi_\ell \\ -\sin 2\phi_\ell \end{pmatrix} = \begin{cases} (1,0)^T & , \text{ if } \underline{v}_\ell = \underline{0} \\ \|\underline{v}_\ell\|^{-1} \underline{v}_\ell & , \text{ if } \underline{v}_\ell \neq \underline{0} \end{cases}, \quad |\phi_\ell| \leq \frac{\pi}{4}. \quad (4.6)$$

with this $Q : g_z(0,0;Q^T A Q) = 0$.

PROOF. It follows from theorem 3.9 that

$$\text{grad } g(0,0;Q^T A Q) = \sum_{\ell=1}^k c'_{2\ell-1,2\ell-1} - c'_{2\ell,2\ell} - 2c'_{2\ell-1,2\ell}$$

where $(c'_{ij}) = C(Q^T A Q)$.

Since $C(Q^T A Q) = Q^T C(A) Q$ we find

$$\begin{pmatrix} c'_{2\ell-1,2\ell-1} \\ c'_{2\ell,2\ell} \\ c'_{2\ell-1,2\ell} \end{pmatrix} = \begin{pmatrix} \cos^2 \phi_\ell & \sin^2 \phi_\ell & -2 \cos \phi_\ell \sin \phi_\ell \\ \sin^2 \phi_\ell & \cos^2 \phi_\ell & 2 \cos \phi_\ell \sin \phi_\ell \\ \cos \phi_\ell \sin \phi_\ell & -\cos \phi_\ell \sin \phi_\ell & \cos^2 \phi_\ell - \sin^2 \phi_\ell \end{pmatrix} \begin{pmatrix} c_{2\ell-1,2\ell-1} \\ c_{2\ell,2\ell} \\ c_{2\ell-1,2\ell} \end{pmatrix}.$$

Consequently

$$\begin{pmatrix} c'_{2\ell-1,2\ell-1} - c'_{2\ell,2\ell} \\ 2c'_{2\ell-1,2\ell} \end{pmatrix} = \begin{pmatrix} \cos 2\phi_\ell & -\sin 2\phi_\ell \\ \sin 2\phi_\ell & \cos 2\phi_\ell \end{pmatrix} \begin{pmatrix} c_{2\ell-1,2\ell-1} - c_{2\ell,2\ell} \\ 2c_{2\ell-1,2\ell} \end{pmatrix},$$

i.e.

$$\underline{v}_{-2\ell}(Q_\ell^T A Q_\ell) = Q_\ell^{-2} \underline{v}_{-2\ell}(A), \quad \ell = 1, \dots, k. \quad (4.7)$$

Hence $\text{grad } g(0,0;Q^T A Q) = \sum_{\ell=1}^k Q_\ell^{-2} \underline{v}_{-2\ell}$. The Euclidean norm of $g(0,0;Q^T A Q)$ is maximal with respect to the rotation parameters ϕ_1, \dots, ϕ_k of Q_1, \dots, Q_k iff the vectors $Q_\ell^{-2} \underline{v}_{-2\ell}$, $\ell = 1, \dots, k$, have the same direction. With the orthogonal matrices $Q_\ell \in \mathbb{R}^{2 \times 2}$, $\ell = 1, \dots, k$, given by (4.6) we get

$Q_\ell^{-2} \underline{v}_{-2\ell} = \|\underline{v}_{-2\ell}\| (1,0)^T$. Thus $\text{grad } g(0,0;Q^T A Q) = \sum_{\ell=1}^k \|\underline{v}_{-2\ell}\| (1,0)^T$ and

$g_z(0,0;Q^T A Q) = 0$. □

REMARK. Except for the (permitted large) range $(-\frac{\pi}{2}, \frac{\pi}{2}]$ of the rotation angles ϕ_ℓ , $\ell = 1, \dots, k$, the matrix Q in theorem 4.1 effectuates Jacobi annihilations of $c_{2\ell-1,2\ell}$, $\ell = 1, \dots, k$.

THEOREM 4.2. Let be Q an orthogonal matrix as defined in (4.2), (4.3) and (4.6). Then there exists a diagonal matrix $W = \text{diag}(x^{\frac{1}{2}}, x^{-\frac{1}{2}}, \dots, x^{\frac{1}{2}}, x^{-\frac{1}{2}})$ such that

$$\|A\|_E^2 - \|W^{-1}Q^T A Q W\|_E^2 \geq \frac{1}{8} \|A\|_E^{-2} \sum_{\ell=1}^k \|v_{-\ell}\|^2, \quad (4.8)$$

where $v_{-\ell}$ as defined in (4.5).

PROOF. Let be $A' = O^T A Q$ and $B' = (b'_1, b'_2, b'_3) \in \mathbb{R}^{k^2 \times 3}$, according to (3.6). Let be $W = \text{diag}(S, \dots, S)$, where $(x, x^{-1}, 0)$ are the Euclidean parameters of the unimodular matrix S . Then it follows from theorem 3.2 that

$$\|W^{-1}A W\|_E^2 = \|x b'_1 + x^{-1} b'_2\|^2 + \text{constant}$$

1. If $\|b'_1\| \|b'_2\| \neq 0$ then $\|x b'_1 + x^{-1} b'_2\|$ is minimal for $x = (\|b'_1\| / \|b'_2\|)^{\frac{1}{2}}$.

With the Euclidean parameters $((\|b'_1\| / \|b'_2\|)^{\frac{1}{2}}, (\|b'_2\| / \|b'_1\|)^{\frac{1}{2}}, 0)$ the decrease of the Euclidean norm equals

$$\|A\|_E^2 - \|W^{-1}A'W\|_E^2 = \|A\|_E^2 - \|W^{-1}Q^T A Q W\|_E^2 = (\|b'_1\| - \|b'_2\|)^2.$$

Hence, as follows from (3.10),

$$\begin{aligned} \|b'_1\| - \|b'_2\| &= (\|b'_1\| + \|b'_2\|)^{-1} (\|b'_1\|^2 - \|b'_2\|^2) = \\ &= \frac{1}{2} (\|b'_1\| + \|b'_2\|)^{-1} g_w(0, 0; A'). \end{aligned}$$

Now $\|b'_1\| + \|b'_2\| \leq \sqrt{2}(\|b'_1\|^2 + \|b'_2\|^2)^{\frac{1}{2}} \leq \sqrt{2} \|A'\|_E = \sqrt{2} \|A\|_E$ and

$$g_w(0, 0; A') = \sum_{\ell=1}^k (c'_{2\ell-1, 2\ell-1} - c'_{2\ell, 2\ell}) = \sum_{\ell=1}^k \|v_{-\ell}\| (Q^T A Q) = \sum_{\ell=1}^k \|v_{-\ell}\| \|A\|$$

as can be seen from (4.7). Consequently

$$\|A\|_E^2 - \|W^{-1}Q^T A Q W\|_E^2 > \frac{1}{8} \|A\|_E^{-2} \left(\sum_{\ell=1}^k \|v_{-\ell}\| \right)^2 \geq \frac{1}{8} \|A\|_E^{-2} \sum_{\ell=1}^k \|v_{-\ell}\|^2.$$

2. In case $\underline{b}'_1 \neq 0$ and $\underline{b}'_2 = 0$, choose x so small that, $x^2 < 1 - \frac{1}{8} \|A\|_E^{-2} \|\underline{b}'_1\|^2$. Then

$$\|A\|_E^2 - \|W^{-1}Q^T A Q W\|_E^2 = \|\underline{b}'_1\|^2 - x^2 \|\underline{b}'_1\|^2 \geq \frac{1}{8} \|A\|_E^{-2} \|\underline{b}'_1\|^4 \geq \frac{1}{8} \|A\|_E^{-2} \sum_{\ell=1}^k \|\underline{v}_\ell\|^2,$$

for

$$\|\underline{b}'_1\|^2 = \sum_{\ell=1}^k (c'_{2\ell-1, 2\ell-1} - c'_{2\ell, 2\ell}) = \sum_{\ell=1}^k \|\underline{v}_\ell\| (O^T A O) = \sum_{\ell=1}^k \|\underline{v}_\ell\|.$$

3. In case $\underline{b}'_1 = 0$ and $\underline{b}'_2 \neq 0$, similarly, choose x so large that

$$x^2 \geq (1 - \frac{1}{8} \|A\|_E^{-2} \|\underline{b}'_2\|^2)^{-1}. \text{ Once again (4.8) holds. } \square$$

The pivotstrategy which must guarantee that the Euclidean norm decreases in sufficient degree for convergence to normality [3,4] will be derived from lowerbound (4.8). Therefore we need

THEOREM 4.3. There exists a set of k disjunct index pairs (ℓ_j, m_j) with $\ell_j \neq m_j$, $j = 1, \dots, k$, such that

$$\sum_{j=1}^k ((c_{\ell_j, \ell_j} - c_{m_j, m_j})^2 + 4c_{\ell_j, m_j}^2) \geq \frac{4}{n-1} \|C(A)\|_E^2. \quad (4.9)$$

PROOF. We have

$$\sum_{\ell \neq m} (c_{\ell\ell} - c_{mm})^2 = 2(n-1) \sum_{\ell=1}^n c_{\ell\ell}^2 - 2 \sum_{\ell \neq m} c_{\ell\ell} c_{mm}.$$

But since $\sum_{\ell=1}^n c_{\ell\ell} = 0$, $(\sum_{\ell=1}^n c_{\ell\ell})^2 = \sum_{\ell=1}^n c_{\ell\ell}^2 + \sum_{\ell \neq m} c_{\ell\ell} c_{mm} = 0$.

Whence for $n \geq 2$

$$\sum_{\ell \neq m} (c_{\ell\ell} - c_{mm})^2 = 2n \sum_{\ell=1}^n c_{\ell\ell}^2 \geq 4 \sum_{\ell=1}^n c_{\ell\ell}^2$$

Consequently

$$\sum_{\ell \neq m} ((c_{\ell\ell} - c_{mm})^2 + 4c_{\ell m}^2) \geq 4 \|C(A)\|_E^2. \quad (4.10)$$

Let be Ω the collection of all sets ω of k distinct index pairs (ℓ_j, m_j) . The number of sets ω in Ω is $\frac{n!}{k!2^k}$, and each pair (ℓ, m) with $\ell \neq m$ occurs in $\frac{(n-2)!}{(k-1)!2^{k-1}}$ sets of Ω . Thus

$$\begin{aligned} \sum_{\omega \in \Omega} \sum_{(\ell, m) \in \omega} ((c_{\ell\ell} - c_{mm})^2 + 4c_{\ell m}^2) &= \sum_{\ell \neq m} \sum_{\omega \in \Omega} ((c_{\ell\ell} - c_{mm})^2 + 4c_{\ell m}^2) = \\ &= \frac{(n-2)!}{(k-1)!2^{k-1}} \sum_{\ell \neq m} ((c_{\ell\ell} - c_{mm})^2 + 4c_{\ell m}^2) \end{aligned}$$

Hence the mean of $\sum_{(\ell, m) \in \omega} ((c_{\ell\ell} - c_{mm})^2 + 4c_{\ell m}^2)$ over all $\omega \in \Omega$ equals

$$\left(\frac{n!}{k!2^k}\right)^{-1} \frac{(n-2)!}{(k-1)!2^{k-1}} \sum_{\ell \neq m} ((c_{\ell\ell} - c_{mm})^2 + 4c_{\ell m}^2) = (n-1)^{-1} \sum_{\ell \neq m} ((c_{\ell\ell} - c_{mm})^2 + 4c_{\ell m}^2).$$

This result, together with (4.10), proofs the theorem. \square

THEOREM 4.4. Let a sequence $\{A^j\}$ starting with $A^0 = A$, be constructed recursively by

$$A^j = (P^j Q^j \tilde{W}^j)^{-1} A^{j-1} P^j Q^j \tilde{W}^j, \quad j = 1, 2, \dots, \quad (4.11)$$

where in each step k disjunct index pairs $(\ell_1^{(j)}, m_1^{(j)}), \dots, (\ell_k^{(j)}, m_k^{(j)})$ are selected according to rule (4.9). P^j is a permutation with $P^j(\ell_1^{(j)}, m_1^{(j)}, \dots, \ell_k^{(j)}, m_k^{(j)}) = (1, 2, \dots, n-1, n)$, Q^j is a preconditioning orthogonal block diagonal matrix as described in (4.2), (4.3), (4.6) and $\tilde{W}^j = \text{diag}(x_j^{\frac{1}{2}}, x_j^{-\frac{1}{2}}, \dots, x_j^{\frac{1}{2}}, x_j^{-\frac{1}{2}})$ that reduces the Euclidean norm of $(P^j Q^j)^{-1} A^{j-1} P^j Q^j$ as described in theorem 4.2. Then $\{A^j\}$ converges to normality.

PROOF. $\{\|A^j\|_E\}$ decreases monotonically and is bounded below. Therefore

$$\delta_j := \|A^{j-1}\|_E^2 - \|A^j\|_E^2 \rightarrow 0 \quad (j \rightarrow \infty). \text{ Since by theorem 4.2 and theorem 4.4}$$

$$\delta_j \geq \frac{1}{8} \|A\|_E^{-2} \sum_{\ell=1}^k \|v((P^j Q^j)^{-1} A^{j-1} P^j Q^j)\|_E^2$$

$$\geq \frac{1}{2(n-1)} \|A\|_E^{-2} \|C((P^j Q^j)^{-1} A^{j-1} P^j Q^j)\|_E^2 = \frac{1}{2(n-1)} \|A\|_E^{-2} \|C(A^{j-1})\|_E^2,$$

we have $\lim_{j \rightarrow \infty} C(A^j) = 0$. □

THEOREM 4.5. Let $\{A^j\}$ be constructed recursively by

$$A^j = (P^j Q^j W^j)^{-1} A^{j-1} P^j Q^j W^j \quad (4.12)$$

with pivot strategy, P^j and Q^j as in theorem 4.4 but W^j an optimal parallel norm-reducing shear as described in the theorem 3.3, 3.4 and 3.5. Then $\{A^j\}$ converges to normality.

PROOF. $\delta_j = \|A^{j-1}\|_E^2 - \|A^j\|_E^2 \rightarrow 0$ ($j \rightarrow \infty$) for now W^j is even optimal. As in the preceding theorem $C(A^j) \rightarrow 0$ ($j \rightarrow \infty$).

REMARK. When A^j is almost normal an orthogonal transform $\tilde{A} := U A^j U$ of A^j such that $U (A^j + (A^j)^*) U$ is diagonal approximately exhibits the eigenvalues of A provided the spectrum has the following property: if $\mu \pm i\nu$, $\nu \neq 0$, is a pair of conjugate eigenvalues of A , then no other eigenvalues with real part μ is in the spectrum of A [7,8].

In each step of the norm-reducing process one may choose the specimen in the set of row equivalent shears that optimally contributes to the diagonalisation of the symmetric part of the current matrix.

5. IMPLEMENTATIONAL ASPECTS OF THE ALGORITHM

The parallel norm-reducing process described in the preceding section is summarized as follows:

ALGORITHM 5.1. Given $A \in \mathbb{R}^{n \times n}$ with $n = 2k$ the following algorithm overwrites A with $U^{-1}AU$.

Do until $\|C(A)\|_E \leq \delta \|A\|_E \wedge |(a_{\ell\ell} - a_{mm})a_{\ell m}| < \delta \|A\|_E$, $\ell \neq m$, where $\delta = \text{macheps}$,

(i) determine k disjoint index pairs (ℓ_j, m_j) , $j = 1, \dots, k$, such that

$$\sum_{j=1}^k ((c_{\ell_j, \ell_j} - c_{m_j, m_j})^2 + 4c_{\ell_j, m_j}^2) \geq \frac{4}{n-1} \|C(A)\|_E^2 \quad (5.1)$$

(ii) If $P = (e_{\ell_1}, e_{m_1}, \dots, e_{\ell_k}, e_{m_k})$, e_j being the j -th unit vector, then

$$A := P^T A P \quad (5.2)$$

(iii) for $\ell = 1, \dots, k$.

Determine $\cos \phi_\ell$ and $\sin \phi_\ell$, $-\pi/2 < \phi_\ell \leq \pi/2$ from

$$\begin{cases} \cos 2\phi_\ell = (c_{2\ell-1, 2\ell-1} - c_{2\ell, 2\ell})/N \\ \sin 2\phi_\ell = -2c_{2\ell-1, 2\ell}/N \end{cases} \quad (5.3)$$

where

$$N = ((c_{2\ell-1, 2\ell-1} - c_{2\ell, 2\ell})^2 + 4c_{2\ell-1, 2\ell}^2)^{\frac{1}{2}}. \quad (5.4)$$

If $c_{2\ell-1, 2\ell} = 0$ then just set $\cos \phi_\ell = 1$.

Compute

$$A := Q^T A Q \quad (5.5)$$

where $Q = \text{diag}(Q_1, \dots, Q_k)$, with

$$Q_\ell = \begin{pmatrix} \cos \phi_\ell & \sin \phi_\ell \\ -\sin \phi_\ell & \cos \phi_\ell \end{pmatrix} = \begin{pmatrix} c_\ell & s_\ell \\ -s_\ell & c_\ell \end{pmatrix} \quad (5.6)$$

(iv) Compute

$$\beta := \left(\sum_{\ell, m=1}^k a_{2\ell, 2m-1}^2 \right)^{\frac{1}{2}}, \quad \gamma := \left(\sum_{\ell, m=1}^k a_{2\ell-1, 2m}^2 \right)^{\frac{1}{2}} \quad (5.7)$$

and

$$x := \begin{cases} (\beta/\gamma)^{\frac{1}{2}} & , \beta\gamma \neq 0 \end{cases} \quad (5.8)$$

$$x := \begin{cases} \frac{1}{2} \left(1 - \frac{1}{8} \|A\|_E^{-2} \beta^2 \right)^{\frac{1}{2}} & , \beta \neq 0, \gamma = 0 \end{cases} \quad (5.9)$$

$$x := \begin{cases} 2 \left(1 - \frac{1}{8} \|A\|_E^{-2} \gamma^2 \right)^{-\frac{1}{2}} & , \gamma \neq 0, \beta = 0 \end{cases} \quad (5.10)$$

$$x := \begin{cases} 1 & , \beta = \gamma = 0 \end{cases} \quad (5.11)$$

(v) Find

$$\cos \theta_\ell \text{ and } \sin \theta_\ell, \quad -\frac{\pi}{4} < \theta_\ell \leq \frac{\pi}{4}, \quad \ell = 1, \dots, k$$

such that

$$\cotan 2\theta_\ell = \frac{a_{2\ell, 2\ell} - a_{2\ell-1, 2\ell-1}}{a_{2\ell, 2\ell-1} x^2 + a_{2\ell-1, 2\ell} / x^2} \quad (5.12)$$

(vi) Compute

$$A := W^{-1} A W \quad (5.13)$$

where $W = \text{diag}(W_1, \dots, W_k)$ with

$$W_\ell = \begin{pmatrix} x \cos \theta_\ell & x \sin \theta_\ell \\ -\sin \theta_\ell/x & \cos \theta_\ell/x \end{pmatrix}, \quad \ell = 1, \dots, k. \quad (5.14)$$

The computation of $C(A)$ already requires $O(n^3)$ flops, so (i) is not a practical course of action.

Inspired by the caterpillar permutations introduced by Brent and Luk for systolic arrays we avoid the expensive search for an optimal set of k distinct index pairs and perform a serial process. The caterpillar permutation P_c will be illustrated for $n = 8$.

$$\begin{array}{cccc} 1 & 3 & + & 5 & + & 7 \\ & \nearrow & & & & \downarrow \\ 2 & + & 4 & + & 6 & + & 8 \end{array}$$

So

$$P_c(1, 2, 3, 4, 5, 6, 7, 8) = (1, 4, 2, 6, 3, 8, 5, 7).$$

Generally

$$P_c(i) = \begin{cases} 1 & , i = 1 \\ i+2 & , i = 2, 4, \dots, 2k-2 \\ i-2 & , i = 5, 7, \dots, 2k-1 \\ i-1 & , i = 3. \end{cases} \quad (5.15)$$

It is easy to see that $P_c^{n-1} = I$.

ALGORITHM 5.2. Given $A \in \mathbb{R}^{n \times n}$ with $n = 2k$ the following algorithm overwrites A with $U^{-1}AU$.

Do until

$$|a_{\ell\ell} - a_{mm}| |a_{\ell m} + a_{m\ell}| \leq \delta \|A\|_E \quad (5.16)$$

(i) Perform the stages (iii), (iv), (v), and (vi) of algorithm 5.1.

(ii) Compute $A := PAP^T$, where P is the caterpillar per mutation given in (5.14).

At the moment there is no proof of the convergence of the last algorithm.

Let algorithm 5.2 be performed with parallel processors G_ℓ , $\ell = 1, \dots, k$ for the concurrent computation with pairs of rows or columns. The following steps can be successively executed with the k parallel processors.

$$\left. \begin{array}{l} \text{a.1)} \quad c_{2\ell-1, 2\ell-1} + (A A)_{2\ell-1, 2\ell-1} \\ \text{a.2)} \quad c_{2\ell, 2\ell} + (A A)_{2\ell, 2\ell} \\ \text{a.3)} \quad c_{2\ell-1, 2\ell} + (A A)_{2\ell-1, 2\ell} \end{array} \right\} 2n \text{ steps}$$

$$\left. \begin{array}{l} \text{b.1)} \quad c_{2\ell-1, 2\ell-1} + c_{2\ell-1, 2\ell-1} - (AA)_{2\ell-1, 2\ell-1} \\ \text{b.2)} \quad c_{2\ell, 2\ell} + c_{2\ell, 2\ell} - (AA)_{2\ell, 2\ell} \\ \text{b.3)} \quad c_{2\ell-1, 2\ell} + c_{2\ell-1, 2\ell} - (AA)_{2\ell-1, 2\ell} \end{array} \right\} 2n \text{ steps}$$

$$\text{c.} \quad \cos 2\phi_\ell, \sin 2\phi_\ell \text{ according to (5.3)}$$

$$\text{d.1)} \quad \begin{pmatrix} a_{2\ell-1, i} \\ a_{2\ell, i} \end{pmatrix} + \begin{pmatrix} c_\ell & -s_\ell \\ s_\ell & c_\ell \end{pmatrix} \begin{pmatrix} a_{2\ell-1, i} \\ a_{2\ell, i} \end{pmatrix}, \quad i = 1, \dots, n \quad 6n \text{ steps}$$

$$\text{d.2)} \quad \begin{pmatrix} a_{i, 2\ell-1} \\ a_{i, 2\ell} \end{pmatrix} + \begin{pmatrix} c_\ell & -s_\ell \\ s_\ell & c_\ell \end{pmatrix} \begin{pmatrix} a_{i, 2\ell-1} \\ a_{i, 2\ell} \end{pmatrix}, \quad i = 1, \dots, n \quad 6n \text{ steps}$$

$$\text{e.1)} \quad \beta_\ell + \sum_{i=1}^k a_{2\ell, 2i-1}^2 \quad n \text{ steps}$$

$$\gamma_\ell + \sum_{i=1}^k a_{2\ell-1, 2i}^2 \quad n \text{ steps}$$

$$E.2) \quad \beta + \left(\sum_{\ell=1}^k \beta_{\ell} \right)^{\frac{1}{2}} \quad \boxed{k \text{ flops}}$$

$$\gamma + \left(\sum_{\ell=1}^k \gamma_{\ell} \right)^{\frac{1}{2}} \quad \boxed{k \text{ flops}}$$

$$E.3) \quad x + (\beta/\gamma)^{\frac{1}{2}}$$

f. Find $c_{\ell} = \cos \theta_{\ell}$, $s_{\ell} = \sin \theta_{\ell}$, $\theta_{\ell} \in (-\frac{\pi}{4}, \frac{\pi}{4})$ from (5.12)

$$g.1) \quad \begin{pmatrix} a_{2\ell-1,1} \\ a_{2\ell,1} \end{pmatrix} + \begin{pmatrix} c_{\ell}/x & -xs_{\ell} \\ s_{\ell}/x & xc_{\ell} \end{pmatrix} \begin{pmatrix} a_{2\ell-1,1} \\ a_{2\ell,1} \end{pmatrix}, \quad i = 1, \dots, n \quad 6n \text{ steps}$$

$$g.2) \quad \begin{pmatrix} a_{1,2\ell-1} \\ a_{1,2\ell} \end{pmatrix}^T + \begin{pmatrix} a_{1,2\ell-1} \\ a_{1,2\ell} \end{pmatrix}^T \begin{pmatrix} xc_{\ell} & xs_{\ell} \\ -s_{\ell}/x & c_{\ell}/x \end{pmatrix}, \quad i = 1, \dots, n \quad 6n \text{ steps}$$

The k processors are simultaneously active in each stage of the process except for state E.2. Without further refinements, this process needs in each iteration $31n$ steps, each sweep consists of $n-1$ iterations. Condition (5.16) holds after $\sim \log n$ sweeps. So $\mathcal{O}(n \log n)$ iterations of each $39n$ parallel flops diagonalize A .

Recursive doubling in a, b, e.1 and E.2 for the computation of innerproducts and the use of n CPU's in d and g gives a reduction to $\mathcal{O}(\log n)$ steps per iteration.

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