Recent Results on Accuracy and Stability of Numerical Algorithms

Nick Higham
Department of Mathematics
University of Manchester

higham@ma.man.ac.uk
http://www.ma.man.ac.uk/~higham/

THE UNIVERSITY of MANCHESTER

Contents

- Area of a Triangle by Heron's Formula
- Fused Multiply-Add Instruction
- Gaussian Elimination with Rook Pivoting
- Newton's Method
- The Exchange Operator

Floating Point Arithmetic: Standard Model

$$fl(x \text{ op } y) = (x \text{ op } y)(1+\delta),$$
$$|\delta| \le u, \quad \text{op} = +, -, *, /.$$

Here, u is the unit roundoff, or machine precision.
In IEEE double precision arithmetic $u = 2^{-53} \approx 1.1 \times 10^{-16}$.
In IEEE, all arithmetic ops performed *as if* first calculated to infinite precision, then rounded.
Default: round to nearest, round to even in case of tie.

Example

$$fl(abc) = ab(1+\delta_1) \cdot c(1+\delta_2) = abc(1+\delta_1)(1+\delta_2)$$
$$\approx abc(1+\delta_1+\delta_2).$$

Area of a Triangle

Heron's formula for area A of triangle with sides of length a, b, and c:

$$A = \sqrt{s(s-a)(s-b)(s-c)}, \qquad s = (a+b+c)/2.$$

Inaccurate for needle-shaped triangles, e.g., $a \approx b + c$.

Kahan (1983): let $a \geq b \geq c$, then evaluate $4A$ as

$$\sqrt{(a+(b+c))(c-(a-b))(c+(a-b))(a+(b-c))}.$$

Gives an accurate answer for all data.

Examples

In IEEE double:

a	10	1	1
b	11	1	$\sin(\texttt{eps})$
c	12	1e-13	$\cos(\texttt{eps})$
Exact	5.152123e+1	5.000000e-14	1.110223e-16
Kahan	5.152123e+1	5.000000e-14	1.110223e-16
Heron	5.152123e+1	*4.996004e-14*	*0.000000e+0*

Subtraction

Theorem 1 (Sterbenz) *Let x and y be floating point numbers with $y/2 \leq x \leq 2y$. Then $x - y$ is computed exactly (assuming $x - y$ does not underflow).*

Recall $a \geq b \geq c$,

$$\sqrt{(a + (b + c))(c - (a - b))(c + (a - b))(a + (b - c))}.$$

Examine $c - (a - b)$. We have

$$b \leq a \leq b + c \leq 2b$$

so by the theorem, $a - b$ is exact. Hence

$$fl(c - (a - b)) = (c - (a - b))(1 + \delta), \qquad |\delta| \leq u.$$

Fused Multiply-Add Instruction

Intel IA-64 architecture has a fused multiply-add instruction with just one rounding error:

$$fl(x + y * z) = (x + y * z)(1 + \delta), \qquad |\delta| \leq u.$$

With an FMA:

- ★ Inner product $x^T y$ can be computed with half the rounding errors.
- ★ The algorithm

$$w = b * c$$
$$e = w - b * c$$
$$x = (a * d - w) + e$$

computes $x = \det([\begin{smallmatrix} a & b \\ c & d \end{smallmatrix}])$ with high relative accuracy (Kahan).

Fused Multiply-Add Instruction (cont.)

But

- What does `a*d + c*b` mean?
- The product

$$(x + iy)^*(x + iy) = x^2 + y^2 + i(xy - yx)$$

  may evaluate to non-real with an FMA.

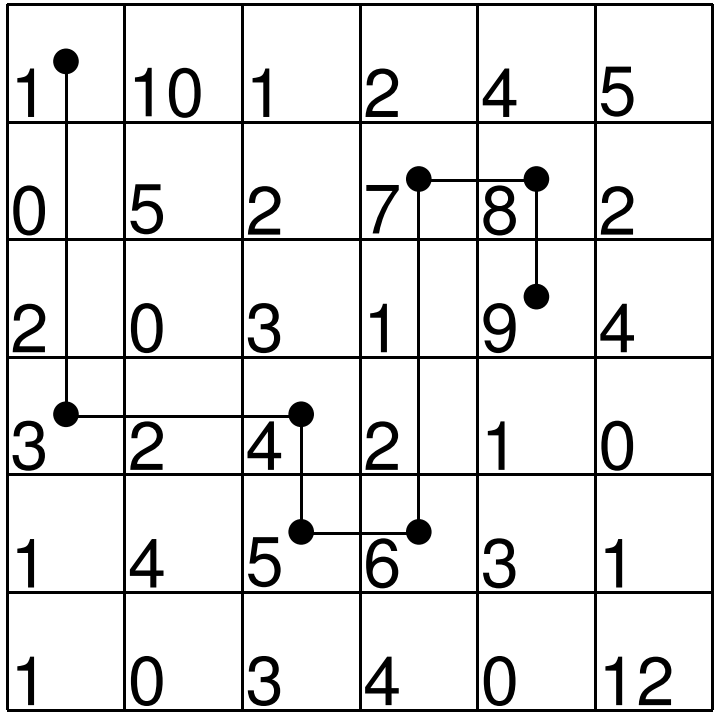
- $b^2 - 4ac$ can evaluate negative even when $b^2 \geq 4ac$.

Gaussian Elimination with Rook Pivoting

On kth stage of GE, swap rows k, r and columns k, s, where

$$|a_{rs}^{(k)}| = \max_{k \le i \le n} |a_{is}^{(k)}| = \max_{k \le j \le n} |a_{rj}^{(k)}|.$$

Intermediate between partial and complete pivoting.



Properties of Rook Pivoting

- **Cost of pivot search**: worst-case $O(n^3)$, but in practice $O(n^2)$. Foster (1997): if all $a_{ij}^{(k)}$ are iid random variables then $O(n^2)$.
- **Growth factor bounds**:

$$\rho_n \leq \begin{cases} 2^{n-1}, & \text{partial (Wilkinson),} \\ 1.5n^{\frac{3}{4}\log n}, & \text{rook (Foster),} \\ c\,n^{1/2}n^{\frac{1}{4}\log n}, & \text{complete (Wilkinson).} \end{cases}$$

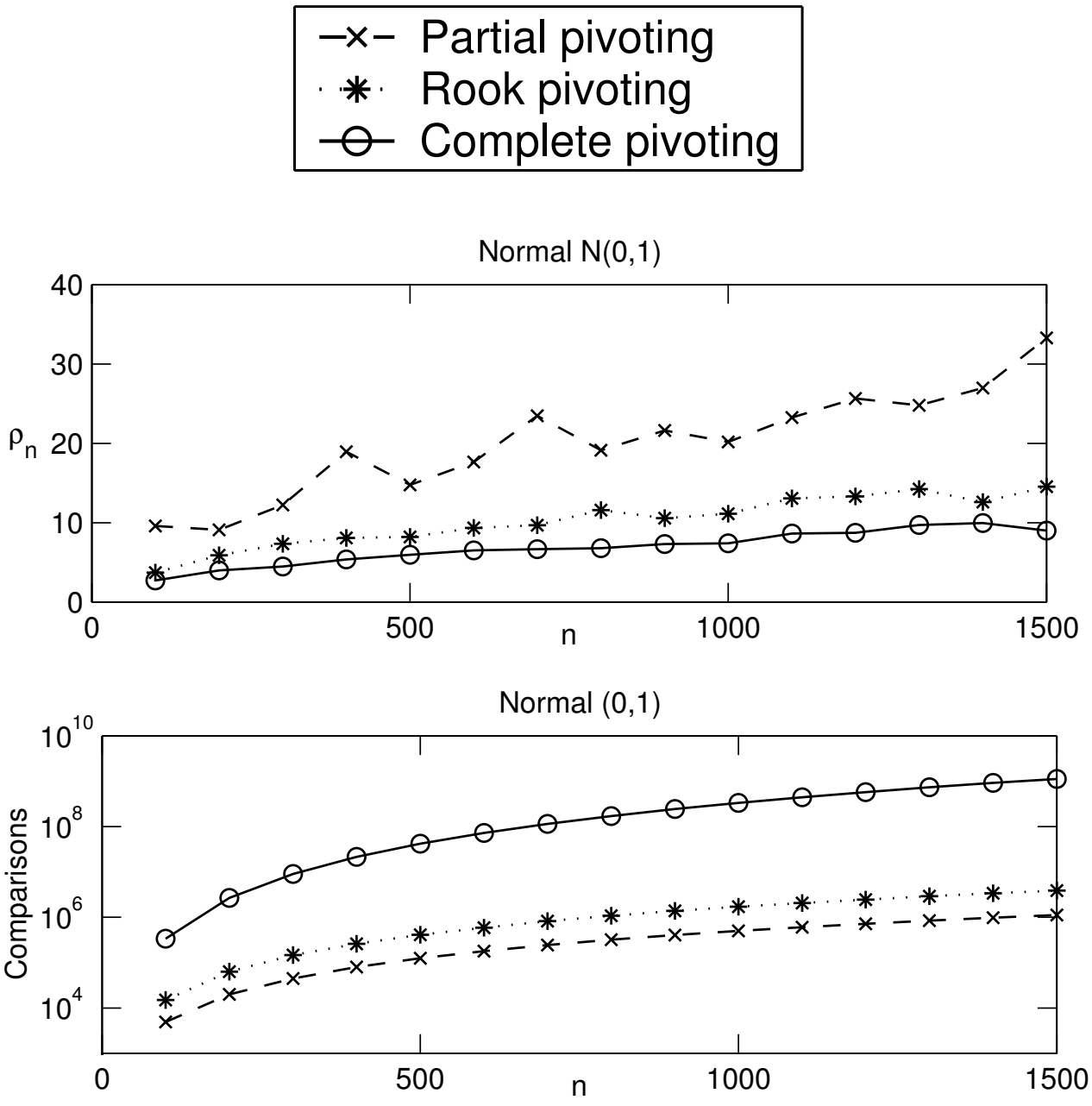
- **LU factors**: in $PAQ = LU$,

$$\operatorname{cond}(U) = \| \, |U^{-1}||U| \, \|_\infty \leq 2^n - 1,$$

because $|u_{ij}| \geq |u_{ii}|$. For GE with any pivoting scheme,

$$\frac{\|x - \widehat{x}\|_\infty}{\|x\|_\infty} \leq 3nu \operatorname{cond}(A) \operatorname{cond}(U) + O(u^2).$$

Numerical Experiment



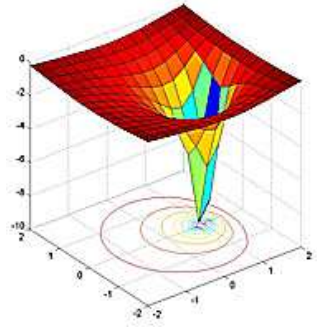
History of Rook Pivoting

- Introduced for nonsymmetric matrices by Neal & Poole (1992): “A Geometric Analysis of Gaussian Elimination”.
- Related strategy for symmetric indefinite matrices introduced by Fletcher (1976).
- Ashcraft, Grimes & Lewis (1998) noted that Bunch–Kaufman pivoting strategy does not bound L factor in $PAP^T = LDL^T$. Motivated their definition of *symmetric rook pivoting*.

Rook Pivoting Summary

- ★ For nonsymmetric A, mainly of pedagogical interest. May give insight into growth factor for partial pivoting.
- ★ *Symmetric* rook pivoting of real practical interest. E.g., when bounded L required: modified Cholesky factorization of Cheng & H (1998).

Matrix Computation Toolbox (H, 2002)



`http://www.ma.man.ac.uk/ higham/mctoolbox`

Functions `gep`, `ldlt_symm`.

Newton's Method

$F : \mathbb{R}^m \mapsto \mathbb{R}^m$ continuously differentiable.
$J(v)$: Jacobian matrix of F.

Assume that J is Lipschitz:

$$\|J(\bar{v}) - J(v)\| \leq \beta \|\bar{v} - v\| \quad \text{for all} \quad v, \bar{v} \in \mathbb{R}^m.$$

Attempt to solve $F(v) = 0$ by Newton's method.

Assume there is v_* such that $F(v_*) = 0$ and $J_* = J(v_*)$ is nonsingular.

Newton's Method in Floating Point

Implement Newton as

Solve $J(v_i)d_i = -F(v_i)$, let $v_{i+1} = v_i + d_i$.

In floating point arithmetic,

$$\widehat{v}_{i+1} = \widehat{v}_i - \left(J(\widehat{v}_i) + E_i\right)^{-1} \left(F(\widehat{v}_i) + e_i\right) + \varepsilon_i.$$

- e_i is error in computing residual $F(\widehat{v}_i)$ at precision $\bar{u}$,

$$\|e_i\| \leq u\|F(\widehat{v}_i)\| + \psi(F, \widehat{v}_i, \bar{u}).$$

- E_i is error in forming $J(\widehat{v}_i)$ and solving linear system for d_i,

$$\|E_i\| \leq u\,\phi(F, \widehat{v}_i, n, u).$$

- ε_i is error made when adding correction $\widehat{d}_i$ to $\widehat{v}_i$,

$$\|\varepsilon_i\| \leq u\,(\|\widehat{v}_i\| + \|\widehat{d}_i\|).$$

Limiting Forward Error & Residual

Theorem 2 (Tisseur, 2001) *If*

- $J(v_*)$ *not too ill conditioned,*
- J*-evaluation and solver not too inaccurate/unstable,*
- $\|v_0 - v_*\|$ *not too large,*
- *Lipschitz constant* β *not too large,*

then Newton in floating point arithmetic yields a sequence $\{\widehat{v}_{i+1}\}$ *whose normwise relative error & residual decrease until*

$$\frac{\|\widehat{v}_{i+1} - v_*\|}{\|v_*\|} \approx \frac{\|J(v_*)^{-1}\|}{\|v_*\|}\psi(F, v_*, \bar{u}) + u,$$

$$\|F(\widehat{v}_{i+1})\| \approx \psi(F, \widehat{v}_i, \bar{u}) + u\|J(\widehat{v}_i)\|\|\widehat{v}_i\|.$$

Applications

Can apply to iterative refinement: solving $F(v) = 0$ with a "good" starting value, e.g.

- linear system $Ax = b$,
- eigenvalue problem $Ax = \lambda x$,
- generalized eigenproblem $Ax = \lambda Bx$, and higher degree ...

- in fixed precision: $\bar{u} = u$, or
- in mixed precision, e.g., $\bar{u} = u^2$.

Refinement can

★ ameliorate instability of algorithm (fixed precision),

★ overcome ill conditioning of problem (mixed precision).

Example

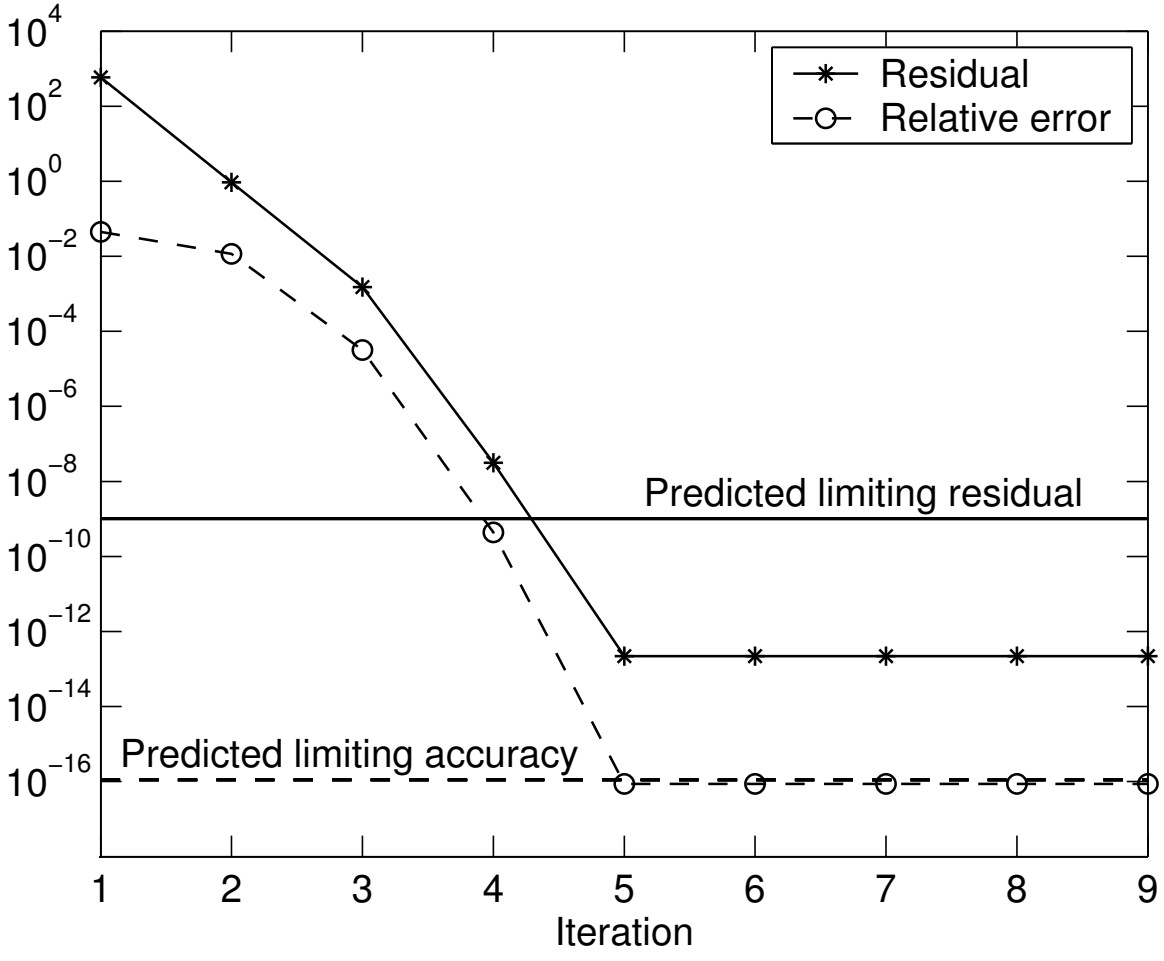
$$F(v) = \begin{bmatrix} (A - \lambda I)x \\ e_s^T x - 1 \end{bmatrix} = 0, \qquad v = \begin{bmatrix} x \\ \lambda \end{bmatrix}.$$

Smallest eigenpair of 10×10 Frank matrix, $\bar{u} = u^2$:

`eig`:

res $\approx 10^{-10}$

err $\approx 10^{-8}$



Newton's Method for ??

With $J = \mathrm{diag}(\pm 1)$,

$$X_{k+1} = \frac{1}{2}(X_k + J X_k^{-T} J), \qquad X_0 = A \in \mathbb{R}^{n \times n}.$$

Newton's Method for ??

With $J = \mathrm{diag}(\pm 1)$,

$$X_{k+1} = \frac{1}{2}(X_k + J X_k^{-T} J), \qquad X_0 = A \in \mathbb{R}^{n \times n}.$$

If $X_k \to X$ then $X = J X^{-T} J$, i.e.,

$$X^T J X = J.$$

Newton's Method for ??

With $J = \mathrm{diag}(\pm 1)$,

$$X_{k+1} = \frac{1}{2}(X_k + J X_k^{-T} J), \qquad X_0 = A \in \mathbb{R}^{n \times n}.$$

If $X_k \to X$ then $X = J X^{-T} J$, i.e.,

$$X^T J X = J.$$

Such X are $\boxed{J\text{-orthogonal}}$.

Newton's Method for ??

With $J = \mathrm{diag}(\pm 1)$,

$$X_{k+1} = \frac{1}{2}(X_k + J X_k^{-T} J), \qquad X_0 = A \in \mathbb{R}^{n \times n}.$$

If $X_k \to X$ then $X = J X^{-T} J$, i.e.,

$$X^T J X = J.$$

Such X are $\boxed{J\text{-orthogonal}}$.

Can prove: if $\lambda(J A^T J A)$ off negative real axis,

$$X_k \to A(J A^T J A)^{-1/2}.$$

Downdating Problem

Compute Cholesky factorization of a positive definite $C = A^T A - B^T B$, where $A \in \mathbb{R}^{p \times n}$ $(p \geq n)$ and $B \in \mathbb{R}^{q \times n}$.

If we can find a J-orthogonal Q such that

$$Q \begin{bmatrix} A \\ B \end{bmatrix} \begin{matrix} p \\ q \end{matrix} = \begin{bmatrix} R \\ 0 \end{bmatrix} \begin{matrix} n \\ p+q-n \end{matrix}, \qquad \begin{matrix} n \\ \end{matrix}$$

with $J = \mathrm{diag}(I_p, -I_q)$ and $R \in \mathbb{R}^{n \times n}$ upper triangular, then

$$C = \begin{bmatrix} A \\ B \end{bmatrix}^T J \begin{bmatrix} A \\ B \end{bmatrix} = \begin{bmatrix} A \\ B \end{bmatrix}^T Q^T J Q \begin{bmatrix} A \\ B \end{bmatrix} = R^T R.$$

Indefinite Least Squares Problem

$$\min_x (b - Ax)^T J (b - Ax),$$

where $A \in \mathbb{R}^{m \times n}$, $m \geq n$, and

$$J = \begin{bmatrix} I_p & 0 \\ 0 & -I_q \end{bmatrix}, \qquad p + q = m.$$

Normal equations:

$$A^T J A x = A^T J b.$$

Unique solution iff

$$A^T J A \text{ positive definite.}$$

Methods:

- Chandrasekaran, Gu & Sayed (1998): Cholesky–QR.
- Bojanczyk, H & Patel (2002): hyperbolic QR.

The Exchange Operator

Let $A \in \mathbb{R}^{n\times n}$. The system

$$\begin{array}{c} \\ p \\ q \end{array}\!\!\begin{array}{c} 1 \\ \left[\begin{array}{c} y_1 \\ y_2 \end{array}\right] \end{array} = \begin{array}{c} \\ p \\ q \end{array}\!\!\begin{array}{c} \begin{array}{cc} p & q \end{array} \\ \left[\begin{array}{cc} A_{11} & A_{12} \\ A_{21} & A_{22} \end{array}\right] \end{array} \begin{array}{c} 1 \\ \left[\begin{array}{c} x_1 \\ x_2 \end{array}\right] \\ \\ \end{array}\!\!\begin{array}{c} p \\ q \\ \\ \end{array}$$

where A_{11} is nonsingular, can be rewritten

$$\begin{bmatrix} x_1 \\ y_2 \end{bmatrix} = \mathrm{exc}(A) \begin{bmatrix} y_1 \\ x_2 \end{bmatrix},$$

where

$$\mathrm{exc}(A) = \begin{bmatrix} A_{11}^{-1} & -A_{11}^{-1}A_{12} \\ A_{21}A_{11}^{-1} & A_{22} - A_{21}A_{11}^{-1}A_{12} \end{bmatrix}.$$

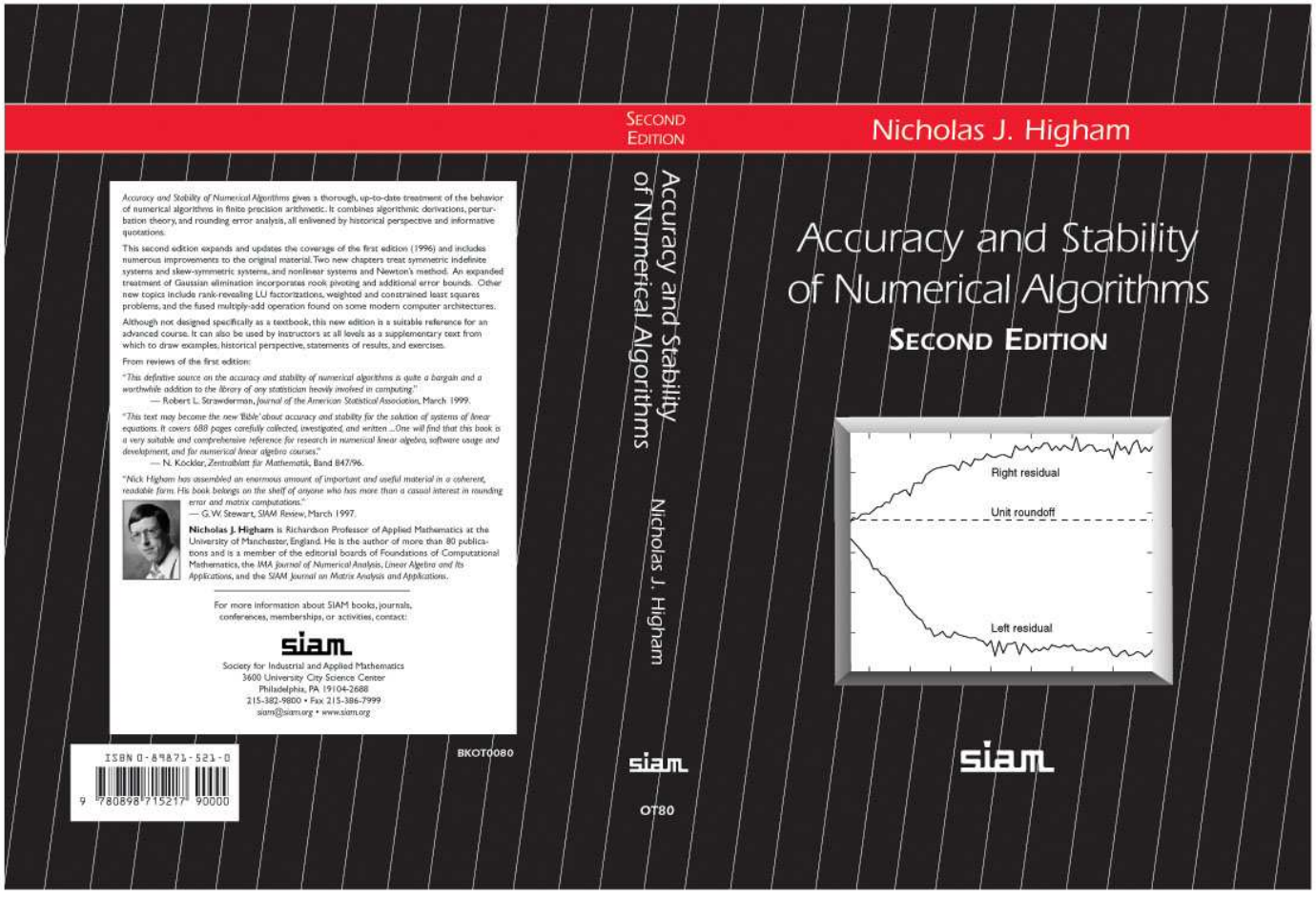
Theorem 2 *Let $A \in \mathbb{R}^{n\times n}$ be J orthogonal. Then $\mathrm{exc}(A)$ is orthogonal. Moreover, if A is orthogonal and A_{11} is nonsingular then $\mathrm{exc}(A)$ is J orthogonal.*

History of Exchange Operator

- Called *gyration operator* in network analysis (Duffin et al., 1966).
- Known as *sweep operator* in statistics. Used to express Gauss–Jordan elimination.
- Called *principal pivot transform* in linear algebra. A is a P-matrix implies $\mathrm{exc}(A)$ also a P-matrix.
- Numerical analysis: Pan & Plemmons (1989), Stewart & Stewart (1998), H (2002).

Uses of Exchange Operator

- Error analysis of products of J-orthogonal matrices (Stewart & Stewart, 1998; Bojanczyk, H & Patel, 2002):
  - map to orthogonal matrices using exc,
  - do error analysis on orthogonal,
  - map back to J-orthogonal using exc.
- Can derive a hyperbolic CS decomposition of a J-orthogonal matrix directly from usual CS decomposition of an orthogonal matrix (H, 2002).
- Can derive an algorithm for constructing random J-orthogonal matrices with prescribed norm and condition number (H, 2002).



Time to LaTeX ASNA

DX2-33	7.5 mins
Pentium 120Mhz	1.3 mins
Pentium 500Mhz	20 secs
Pentium 1Ghz	10 secs
Pentium 2.4Ghz	6 secs