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Backward Stability of Iterations for Computing the Polar Decomposition

Nick Higham
School of Mathematics
The University of Manchester

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

Joint work with Yuji Nakatsukasa

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Polar Decomposition

Any $A \in \mathbb{C}^{s \times n}$ with $s \geq n$ has a **polar decomposition** $A = UH$, where $U \in \mathbb{C}^{s \times n}$ has orthonormal columns and H is Hermitian positive semidefinite.

Applications

- Orthogonalization.
- Orthogonal Procrustes problem.
- Graphics and imaging.
- Algorithms for symmetric eigenproblem and SVD.
  See MS1 (Monday), Nakatsukasa.

Computation

SVD

If $A = P\Sigma Q^*$ is an SVD then $U = PQ^*$, $H = Q\Sigma Q^*$.

Newton Iteration

For square, nonsingular A:

$$X_{k+1} = \frac{1}{2}\left(\mu_k X_k + \mu_k^{-1} X_k^{-*}\right), \quad X_0 = A.$$

H (1986):

- Gave optimal μ_k.
- Cgce in 9 iterations with cheap μ_k approximations.
- **Is the algorithm backward stable?**

QR-based Dynamically Weighted Halley

Nakatsukasa, Bai & Gygi (2010).

$$X_{k+1} = X_k(a_k I + b_k X_k^* X_k)(I + c_k X_k^* X_k)^{-1}, \quad X_0 = A/\alpha.$$

- $a_k = 3$, $b_k = 1$, $c_k = 3 \Rightarrow$ Halley.
- $\alpha \gtrsim \|A\|_2$.
- a_k, b_k, c_k satisfy scalar recurrences. Need lower bound for the smallest singular value of A.
- Cubically cgt, ≤ 6 iterations for cgce to double prec.

QR-based implementation (QDWH)

$$\begin{bmatrix} \sqrt{c_k} X_k \\ I \end{bmatrix} = \begin{bmatrix} Q_1 \\ Q_2 \end{bmatrix} R,$$

$$X_{k+1} = \frac{b_k}{c_k} X_k + \frac{1}{\sqrt{c_k}} \left(a_k - \frac{b_k}{c_k} \right) Q_1 Q_2^*.$$

Notation

ϵ denotes a matrix or scalar such that

$$\|\epsilon\| \le f(n)u,$$

where

- $f =$ modest function depending only on n,
- any norm,
- $u > 0$ is a small, fixed parameter.

We are not interested in tracking the constant $f(n)$,

Backward Stability

Assume $\widehat{H}$ is Hermitian. Alg is backward stable if

$$
\begin{aligned}
\widehat{U}\widehat{H} &= A + \Delta A, & \|\Delta A\| &= \epsilon\|A\|,\\
\widehat{H} &= H + \Delta H, & \|\Delta H\| &= \epsilon\|H\|,\\
\widehat{U} &= U + \Delta U, & \|\Delta U\| &= \epsilon\|U\|,
\end{aligned}
$$

where H Hermitian psd and U unitary.

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We develop a global analysis of iterations for the polar decomposition that

- can show some are backward stable,
- correctly predicts that others are not stable.

Strategy

- Want to bound backward error of numerically converged iterate.
- Take account of rounding errors within each iteration and error propagation between iterations.

Assumptions

Iteration

$$X_{k+1} = f_k(X_k), \qquad X_0 = A, \qquad X_k \to U.$$

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Mixed stable evaluation of iteration

There is an $\widetilde{X}_k \in \mathbb{C}^{n\times n}$ such that

$$\widehat{X}_{k+1} = f_k(\widetilde{X}_k) + \epsilon\|\widehat{X}_{k+1}\|_2, \qquad \widetilde{X}_k = \widehat{X}_k + \epsilon\|\widehat{X}_k\|_2.$$

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f_k does not significantly decrease relative size of σ_i

$$\frac{f_k(\sigma_i)}{\|f_k(\widetilde{X}_k)\|_2} \ge \frac{1}{d}\left(\frac{\sigma_i}{\|\widetilde{X}_k\|_2}\right), \qquad d \ge 1.$$

Theorem

Theorem

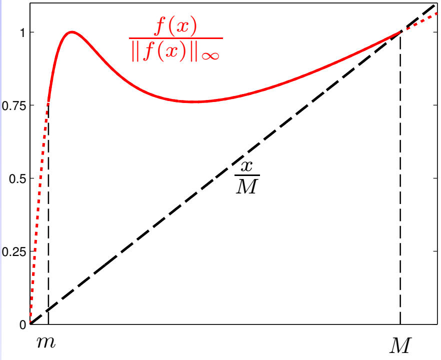
Suppose that, for some integer ℓ, $\widehat{X}_\ell^* \widehat{X}_\ell = I + \epsilon$, *and let* $\widehat{U} = \widehat{X}_\ell$ *and* $\widehat{H} = \frac{1}{2}(\widehat{U}^* A + (\widehat{U}^* A)^*)$. *Then*

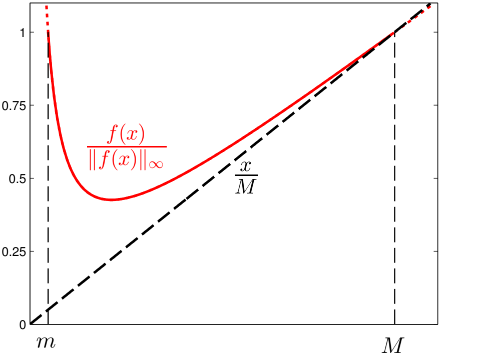
$$\begin{aligned} \widehat{U}\widehat{H} &= A + d\epsilon \|A\|_2, \\ \widehat{H} &= H + d\epsilon \|H\|_2, \end{aligned}$$

where H is the Hermitian polar factor of A. Furthermore,

$$\widehat{U} = U + d\epsilon\kappa_2(A).$$

Condition on f_k





QDWH iteration

$$f(x) = x\frac{a + bx^2}{1 + cx^2},$$

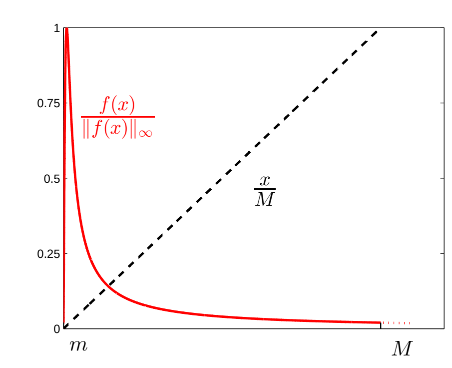
a stable mapping, $d = 1$.

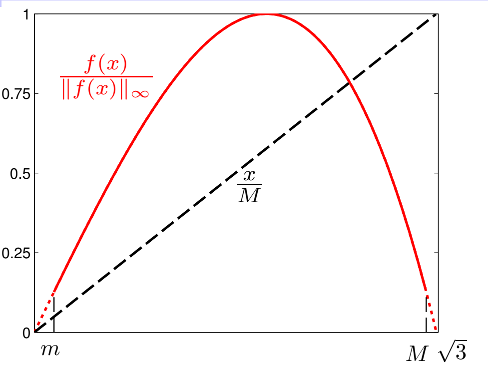
Scaled Newton iteration

$$f(x) = \tfrac{1}{2}(\mu x + (\mu x)^{-1}),$$

a stable mapping, $d = 1$.

Condition on f_k... cont.





Inverse Newton iteration

$f(x) = 2\mu x(1 + \mu^2 x^2)^{-1}$,

an unstable mapping.

Newton–Schulz iteration

$f(x) = \frac{1}{2}x(3 - x^2)$,

an unstable mapping if $M \approx \sqrt{3}$.

QDWH: Stability of Iteration

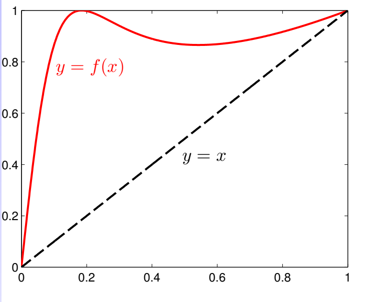
QR-based implementation (QDWH)

$$\begin{bmatrix} \sqrt{c_k} X_k \\ I \end{bmatrix} = \begin{bmatrix} Q_1 \\ Q_2 \end{bmatrix} R,$$

$$X_{k+1} = \frac{b_k}{c_k} X_k + \frac{1}{\sqrt{c_k}} \left(a_k - \frac{b_k}{c_k} \right) Q_1 Q_2^*.$$

- Assume Householder QR factorization with column pivoting and either row pivoting or row sorting.
- The QR factorization has row-wise b'errs of order $\rho_i u$, where growth factors $\rho_i \le \sqrt{s}(1+\sqrt{2})^{n-1}$ (Cox & H, 1998). ρ_i usually small in practice.
- Can prove that "mixed stable evaluation of iteration" condition holds.

QDWH: Condition on Iteration Function



Plot of
$f_k(x) = x(a_k + b_k x^2)/(1 + c_k x^2)$
for $\ell = 0.1$.

Prove condition using results below.

$$b = (a-1)^2/4, \quad c = a + b - 1, \quad 3 \le a \le \frac{2+\ell}{\ell},$$

$$x \le f(x) \le 1 = f(1) \quad \text{for } 0 < x < 1,$$

$$f'(x) \ge 0 \quad \text{for } x \ge 1,$$

$g(x) = \dfrac{f(x)}{x}$ satisfies $g(0) = a$, $g(1) = 1$, $g'(x) < 0$ for $x > 0$,

$$0 \le f'(1) = (a-3)^2/(a+1)^2 < 1 \text{ for } a \ge 3.$$

QDWH Experiment

105 $n \times n$ matrices with $\kappa_2(A) \le u^{-1}/2$.
Report pairs

$$\frac{\|A - \widehat{U}\widehat{H}\|_F}{\|A\|_F}, \frac{\|\widehat{U}^*\widehat{U} - I\|_F}{\sqrt{n}}.$$

Pivoting	$n = 100$	$n = 250$
None	2.7e-15, 1.1e-15	8.3e-15, 1.7e-15
Col	1.9e-15, 1.7e-15	4.0e-15, 3.9e-15
Row & col	1.8e-15, 1.6e-15	3.5e-15, 3.5e-15

Can construct examples of instability for no pivoting, but they are rare.

Scaled Newton Iteration

$$X_{k+1} = \frac{1}{2}\left(\mu_k X_k + \mu_k^{-1} X_k^{-*}\right), \quad X_0 = A.$$

H (1985) : $\mu_k = \left(\dfrac{\|X_k^{-1}\|_1 \|X_k^{-1}\|_\infty}{\|X_k\|_1 \|X_k\|_\infty}\right)^{1/4}, \quad \mu_k = \left(\dfrac{\|X_k^{-1}\|_F}{\|X_k\|_F}\right)^{1/2}.$

Byers & Xu (2008) : $\mu_{k+1} = \left[\dfrac{2}{\mu_k + \mu_k^{-1}}\right]^{1/2}, \ \mu_0 = \left[\dfrac{\|A^{-1}\|_2}{\|A\|_2}\right]^{1/2}.$

- Mixed stable condition holds if matrix inverse computed using mixed backward–forward stable method.
- Condition on f_k holds.

Conclusion

Scaled Newton is backward stable.

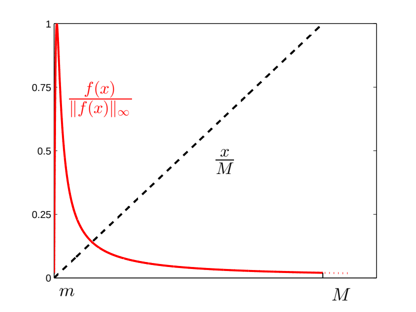
History for Scaled Newton

- **H** (1985) raised the question of backward stability.
- **Kiełbasiński & Ziętak** (2003): long and complicated analysis proving backward stability, assuming matrix inverses are computed in a mixed backward–forward stable way.
- **Byers & Xu** (2008): alternative proof using much simpler arguments, but analysis incomplete (Kiełbasiński & Ziętak, 2010).

Inverse Newton Iteration

$$X_{k+1} = 2\mu_k X_k (I + \mu_k^2 X_k^* X_k)^{-1}, \quad X_0 = A.$$

- Byers & Xu (2001) and Nakatsukasa, Bai & Gygi (2010) observe that a QR-based implementation is not backward stable.
- $d \neq O(1)$ in condition on f_k: $d \gtrsim \kappa_2(A)^{1/2}/2$.



Newton–Schulz Iteration

$$X_{k+1} = \frac{1}{2} X_k (3I - X_k^* X_k), \qquad X_0 = A,$$

Converges when $\|A\|_2 < \sqrt{3}$.

Condition for stability

$\|A\|_2$ safely less than $\sqrt{3}$.

Conclusions

- New, general analysis that separates
  - **stability of the iteration evaluation**,
  - **inherent properties of the iteration function**.
- **Scaled Newton**: backward stable if inverses computed in mixed backward–forward stable way.
- **QR-based dynamically weighted Halley** (QDWH): backward stable when Householder QR with column pivoting and row pivoting/sorting used—and stable in practice without pivoting!
- **Scaled inverse Newton**: not backward stable.
- **Newton–Schulz**: conditionally backward stable.

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