The matrix square root

Next (and last, for us) matrix function: $A^{1/2}$, principal square root.

$A^{1/2}$ is well defined unless A has:

- Real eigenvalues $\lambda_i < 0$, or
- Non-trivial Jordan blocks at $\lambda_i = 0$ (because $g(x) = x^{1/2}$ is not differentiable).

Condition number / sensitivity

The Fréchet derivative of $f(X) = X^2$ is

$$L_{f,X}(E) = XE + EX, \quad \widehat{L} = I \otimes X + X^T \otimes I.$$

The Fréchet derivative of $g(Y) = Y^{1/2}$ is its inverse,

$$\widehat{L}_{g,Y} = (I \otimes Y^{1/2} + (Y^{1/2})^T \otimes I)^{-1}$$

with eigenvalues $\frac{1}{\lambda_i^{1/2} + \lambda_j^{1/2}}$, $i, j = 1, \ldots, n$.

In particular, g is ill-conditioned for matrices that either:

- have a small eigenvalue (taking $i = j$), or
- have two complex conjugate eigenvalues close to the negative real axis (because then $\lambda_i^{1/2} \approx ai$, $\lambda_j^{1/2} \approx -ai$).

Modified Schur method

Recall: Schur method:

1. Reduce to a triangular T using a Schur form;
2. Compute diagonal of $S = f(T)$;
3. Compute off-diagonal entries from $ST = TS$
   Involves a denominator $t_{ii} - t_{jj}$: if it is 0, we must work on blocks.

In the case of $A^{1/2}$, we can use $S^2 = T$ to get the off-diagonal entries instead:

$$s_{ii}s_{ij} + s_{i,i+1}s_{i+1,j} + \cdots + s_{ij}s_{jj} = t_{ij}.$$

This involves a denominator $s_{ii} + s_{jj}$: always invertible because $s_{ii} + s_{jj} \in RHP$.

This is (more or less) what Matlab uses, by the way (it does it in a divide-and-conquer way).

Stability of Schur method for `sqrtm`

Rounding error analysis for

$$s_{ij} = \frac{t_{ij} - s_{i,i+1}s_{i+1,j} - \cdots - s_{i,j-1}s_{j-1,j}}{s_{ii} + s_{jj}}.$$

(replacing each s_{ij} with the computed $\tilde{s}_{ij}$, and considering errors in all operations) leads to

$$\tilde{S}^2 = T + \delta T, \quad |\delta T| \leq |S|^2 \mathcal{O}(n\mathrm{u}).$$

Combining it with a (backward-stable) Schur factorization and switching to norm, we get that $X = A^{1/2}$ is computed with backward error

$$\|\hat{X}^2 - A\|_F \leq \mathcal{O}(n^3\mathrm{u}) \|X\|_F^2,$$

This is weaker than backward stability: there could be cancellation in the product X^2, so $\|X\|_F^2$ is not really the same thing as $\|A\|_F$.

Newton method

Newton method on $X^2 - A$:

$$X_{k+1} = X_k - E, \quad \text{where } E \text{ solves } EX_k + X_k E = X_k^2 - A.$$

Much more expensive than the Schur method: we solve a Sylvster equation at each step (and this requires a Schur form).

Trick: If X_0 commutes with A (for instance, taking $X_0 = \alpha I$), then $E = (2X_0)^{-1}(X_0^2 - A)$ solves that equation; then E, X_1 commute with A, too, and so on.

Resulting iteration:

(Modified) Newton iteration (MN)

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

At each step, $X_k A = AX_k$.

Square root and sign

Theorem

Assume A has no eigenvalues in $\mathbb{R}^-$. Then, the MN iteration converges to the principal square root $A^{1/2}$ for each starting point $X_0 = \alpha I$ or $X_0 = \alpha A$, with $\alpha > 0$.

Proof Pre-multiply by $A^{-1/2}$, and use commutativity:

$$A^{-1/2}X_{k+1} = \frac{1}{2}\left(A^{-1/2}X_k + (A^{-1/2}X_k)^{-1}\right).$$

This is the sign iteration! Hence $A^{-1/2}X_k \to \text{sign}(A^{-1/2}X_0) = I$.

Remark: if A has a negative eigenvalue $\lambda < 0$, there is another obstruction: neither version of Newton can converge, because $A^{1/2}$ is non-real. To restore convergence, we need to add a small imaginary part to X_0.

Theory and practice

Problem All of this holds in exact arithmetic, but the method won't work in practice in machine arithmetic! Try `rng(4); A = randn(5);`. These two iterations behave quite differently:

True Newton

$$X_{k+1} = X_k - E, \quad \text{where } E \text{ solves } EX_k + X_k E = X_k^2 - A.$$

Modified Newton

$$X_{k+1} = \frac{1}{2}(X_k + X_k^{-1} A).$$

TN converges, but MN diverges after an initial "pseudo-convergence".

Numerically, the two sequences behave quite differently, and the commutativity property $X_k A = AX_k$ is lost in MN in a few iterations.

Local stability

The geometric picture The two iterations coincide on the manifold of matrices that commute with A, $\{X \in \mathbb{C}^{n\times n} \colon AX = XA\}$, but not on the rest of $\mathbb{C}^n$.

Numerical perturbations take us outside of the manifold, and then they do not coincide anymore.

While TN is quadratically convergent, MN does not even have an stable fixed point in $A^{1/2}$: even when started very close to $A^{1/2}$, the iteration diverges.

We can prove this formally.

Local stability

Local stability of a fixed point of $X_{k+1} = h(X_k)$ depends on the eigenvalues of its Jacobian.

The Jacobian / Fréchet derivative of $h(X) = \frac{1}{2}(X + X^{-1}A)$ is

$$L_{h,X}(E) = \frac{1}{2}(E + X^{-1}EX^{-1}A)$$

(use $(X+E)^{-1} - X^{-1} = (X+E)^{-1}EX^{-1} = X^{-1}EX^{-1} + o(\|E\|)$).

Hence $L_{h,A^{1/2}} = \frac{1}{2}(E + A^{-1/2}EA^{1/2})$, or
$\hat{L}_{h,A^{1/2}} = \frac{1}{2}\left(I + (A^{1/2})^T \otimes A^{-1/2}\right)$.

It has eigenvalues $\frac{1}{2} + \frac{1}{2}\lambda_i^{1/2}\lambda_j^{-1/2}$, where λ_i are the eigenvalues of A.

It is easy to construct examples in which $L_{h,A^{1/2}}$ has eigenvalues with modulus > 1, hence $A^{1/2}$ is an unstable fixed point of $h(X)$.

Denman–Beavers iteration

However, the stability properties are significantly different for slight variations of the modified Newton's method.

Setting $Y_k = A^{-1}X_k$, we can get

Denman–Beavers iteration [Denman–Beavers, '76]

$$X_{k+1} = \frac{1}{2}(X_k + Y_k^{-1}),$$
$$Y_{k+1} = \frac{1}{2}(Y_k + X_k^{-1}),$$

(It corresponds to using the relation with the matrix sign and using Newton for the matrix sign to compute $\operatorname{sign}\left(\begin{bmatrix} 0 & A \\ I & 0 \end{bmatrix}\right)$.)

Local stability of the DB iteration

Theorem

The DB iteration satisfies $\lim(X_k, Y_k) = (A^{1/2}, A^{-1/2})$, *and it is locally stable.*

We have

$$L_{DB,(X,Y)}(\begin{bmatrix} E \\ F \end{bmatrix}) = \frac{1}{2}\begin{bmatrix} E - Y^{-1}FY^{-1} \\ F - X^{-1}EX^{-1} \end{bmatrix}$$

All $(X, Y) = (M, M^{-1})$ are fixed points, and in these the Jacobian is idempotent, i.e., $(K_{DB,(B,B^{-1})})^2 = K_{DB,(B,B^{-1})}$.

Hence its eigenvalues are $0, 1$, and all the Jordan blocks are simple $\implies$ bounded powers $\implies$ local stability.

Other variants are available [Higham book, Ch. 6].