Polar Decomposition

Thomas Seleiro

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2. Prove that the singular values of A are the eigenvalues of H.

We know that any matrix $A \in \mathbb{C}^{m\times n}$, $m \geq n$ has a thin singular value decomposition $A = P\Sigma Q^*$ where $P \in \mathbb{C}^{m\times n}$ has orthogonal columns, $Q \in \mathbb{C}^{n\times n}$ is unitary, and $\Sigma \in \mathbb{C}^{n\times n}$ is diagonal with $\Sigma = \text{diag}(\sigma_1, \ldots, \sigma_r)$ where $\text{rank}(A) = r$ and $\sigma_1 \geq \ldots \geq \sigma_r \geq 0$, the singular values of A. Thus we can write

$$A = (PQ^*)(Q\Sigma Q^*) =: UH \tag{1}$$

where U and H satisfy the properties of a polar decomposition.

In particular we have $H = Q\Sigma Q^*$ where Σ is diagonal and Q is orthogonal. Thus the diagonal values of Σ are the eigenvalues of H, which are the singular values of A.

3. Prove that A is normal ($A^*A = AA^*$) iff U and H commute.

We first suppose that U and H commute. Note that for the product HU to be well defined, we must have $m = n$ which implies $U \in \mathbb{C}$ is unitary. Since $A = UH = HU$ we get

$$A^*A = (UH)^*(UH) = H^*(U^*U)H = H^2 \tag{2}$$

$$AA^* = (HU)(HU)^* = H(UU^*)H^* = H^2 \tag{3}$$

so A is normal.

Now suppose A is normal. Since $A^*A \in \mathbb{C}^{n\times n}$ and $AA^* \in \mathbb{C}^{m\times m}$, A normal requires $m = n$. Using the singular value decomposition of A, we have

$$AA^* = (P\Sigma Q^*)(Q\Sigma P^*) = P\Sigma^2 P^* \tag{4}$$

where $\Sigma^2 = \text{diag}(\sigma_1^2, \ldots, \sigma_r^2)$. Equating (2) and (4), we get $H^2 = P\Sigma^2 P^*$. From [1, p.405], we know that there is a unique Hermitian positive semi-definite matrix $(AA^*)^{1/2}$ such that $(AA^*)^{1/2}(AA^*)^{1/2} = AA^* = H^2$. It is obvious by its construction that H is said matrix, but we also note that $(P\Sigma P^*)(P\Sigma P^*) = P\Sigma^2 P^* = AA^*$. Therefore $H = P\Sigma P^*$ and

$$HU = (P\Sigma P^*)(PQ^*) = P\Sigma Q^* = A = UH \tag{5}$$

by the properties of the SVD of A. Therefore U and H commute.

4. Verify the formula

$$U = \frac{2}{\pi} A \int_0^\infty (t^2 I - A^* A)^{-1} dt \qquad (*)$$

for full rank A by using the singular value decomposition (SVD) of A to diagonalize the formula.

Since $A^*A = (Q\Sigma P^*)(P\Sigma Q^*) = Q\Sigma^2 Q^*$, we have

$$t^2 I + A^* A = Q(t^2 I)Q^* + Q\Sigma^2 Q^* = QDQ^* \qquad (6)$$

where $D := \mathrm{diag}(t^2 + \sigma_i)$. Inverting (6) gives

$$(t^2 I + A^* A)^{-1} = QD^{-1}Q^*, \qquad D^{-1} = \mathrm{diag}\left(\frac{1}{\sigma_i^2 + t^2}\right) \qquad (7)$$

Since Q and Q^* do not depend on t, they can be taken outside the integral, leaving the right hand side of (*) in the form

$$\frac{2}{\pi} A\, Q \int_0^\infty D^{-1} dt\, Q^*. \qquad (8)$$

The integral is a diagonal matrix where the ith diagonal component is

$$\int_0^\infty \frac{1}{\sigma_i^2 + t^2}\, dt = \left[\frac{1}{\sigma_i} \arctan\left(\frac{t}{\sigma_i}\right)\right]_0^\infty = \frac{\pi}{2\sigma_i} \qquad (9)$$

using [2, 4.2.4.4]. So the right-hand side of (*) is

$$A\, Q\, \mathrm{diag}\left(\sigma_i^{-1}\right) Q^* = P\Sigma Q^*\, Q\Sigma^{-1} Q^* = PQ^* = U \qquad (10)$$

5. Derive Newton's method for computing U by considering equations $(X + E) * (X + E) = I$, where E is a "small perturbation". (Newton's method is $X_{k+1} = (X_k + X_k^{-*})/2, X_0 = A$)

We know that U is the closest unitary matrix to A, and since $U^*U = I$, we try to find a solution to the equation

$$F(X) = 0, \qquad F(X) := X^* X - I \qquad (11)$$

using a Newton method starting at A. The general form of the Newton method [(3), p.] is

$$F(X_{k+1}) + DF_{X_k}[X_{k+1} - X_k] = 0 \qquad (12)$$

where DF_{X_k} is the Fréchet derivative and, is the first order E term in

$$F(X + E) - F(X) = X^* E + E^* X + E^* E. \qquad (13)$$

So $DF_{X_k}[E] = X^*E + E^*X$. Substituting in (12),

$$X_k^* X_k - I + X_k^* \left(X_{k+1} - X_k\right) + \left(X_{k+1}^* - X_k^*\right) X_k = 0 \tag{14}$$
$$X_k^* X_k - I + X_k^* X_{k+1} - X_k^* X_k + X_{k+1}^* X_k - X_k^* X_k = 0 \tag{15}$$
$$X_k^* X_{k+1} + X_{k+1}^* X_k = X_k^* X_k + I \tag{16}$$

We know that for any matrix we can write $B = 1/2(B + B^*) + 1/2(B - B^*)$, where the terms on the right-hand side are the Hermitian and skew Hermitian components respectively [1, p.170]. Setting the skew Hermitian part to zero, and taking $B = X_k^* X_{k+1}$ gives

$$X_k^* X_{k+1} = \frac{1}{2}\left(X_k^* X_k + I\right) \tag{17}$$
$$X_{k+1} = \frac{1}{2}\left(X_k + X_k^{-*}\right) \tag{18}$$

6. Prove that Newton's method converges, and at a quadratic rate, by using the SVD of A.

For the Newton iteration to be well defined, we require that A and the iterates X_k be invertible.

We have the SVD of $A = P\Sigma Q^*$ and $U = PQ^*$. The iterates X_k also have a singular value decomposition, which we write $X_k = P_k \Sigma_k Q_k^*$. Using this in eq. (18) gives

$$X_{k+1} = (X_k + X_k^{-*})/2 = \frac{1}{2}(P_k \Sigma_k Q_k^* + P_k \Sigma_k^{-1} Q_k^*) \tag{19}$$
$$= P_k \frac{1}{2}(\Sigma_k + \Sigma_k^{-1}) Q_k^* \tag{20}$$

So we can identify the factors in the SVD of X_{k+1} (up to reordering of rows) and get

$$P_k = P, \qquad Q_k = Q, \qquad \Sigma_{k+1} = \frac{1}{2}\left(\Sigma_k + \Sigma_k^{-1}\right) \tag{21}$$

We now have

$$U - X_{k+1} = PQ^* - P\left[\frac{1}{2}\left(\Sigma_k + \Sigma_k^{-1}\right)\right] Q^* \tag{22}$$
$$= \frac{1}{2} P \left[(I - \Sigma_k) + \left(I - \Sigma_k^{-1}\right)\right] Q^* \tag{23}$$
$$\tag{24}$$

And since

$$-\Sigma_k^{-1}(I - \Sigma_k)^2 = -\Sigma_k^{-1}\left(I - 2\Sigma_k + \Sigma_k^2\right) \tag{25}$$
$$= 2I - \Sigma_k - \Sigma_k^{-1} \tag{26}$$

we are left with $U - X_{k+1} = -P\Sigma_k^{-1}(I - \Sigma_k)^2 Q^*/2$. Taking the 2-norm on both sides and exploiting the fact that P and Q are orthogonal,

$$\begin{aligned}
\|U - X_{k+1}\|_2 &\leq \frac{1}{2}\left\|P\Sigma_k^{-1}\right\|_2 \left\|(I-\Sigma_k)^2 Q^*\right\|_2 && (27)\\
&= \frac{1}{2}\left\|\Sigma_k^{-1}\right\|_2 \left\|(I-\Sigma_k)^2\right\|_2 && (28)\\
&\leq \frac{1}{2}\|X_k\|_2 \|I - \Sigma_k\|_2^2 && (29)\\
&= \frac{1}{2}\|X_k\|_2 \|U - X_k\|_2^2 && (30)
\end{aligned}$$

To achieve quadratic convergence, we need to bound $\|X_k\|$ by a constant. We do so by observing that

$$\|X_{k+1}\|_2 = \max_{i=1:n} \frac{\sigma_i + \sigma_i^{-1}}{2} \leq \max\left\{\|X_k\|_2, \left\|X_k^{-1}\right\|_2\right\} \tag{31}$$

and so for all k, $\|X_k\|_2 \leq M := \max\{\|A\|_2, \|A^{-1}\|_2\}$. Thus we conclude that the Newton method converges quadratically.

7. Use the SVD to analyse the convergence of the Newton-Schulz iteration for computing U:

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

We assume $A \in \mathbb{C}^{m\times n}$ and $m \geq n$. We replace A in the expression of X_1 with the thin SVD $A = P\Sigma Q^*$ and get

$$\begin{aligned}
X_1 = \frac{1}{2}P\Sigma Q^*(3I - Q\Sigma P^* P\Sigma Q^*) &= \frac{1}{2}P\Sigma(Q^*Q)(3I - \Sigma^2)Q^* && (32)\\
&= P\left[\frac{1}{2}(3\Sigma - \Sigma^3)\right]Q^*. && (33)
\end{aligned}$$

Thus we can write $X_1 = P\Sigma_1 Q^*$ where $\Sigma_1 = (3\Sigma - \Sigma^3)/2$. Applying the same method recursively we can write $X_k = P\Sigma_k Q^*$ with

$$\Sigma_k = \operatorname{diag}(\sigma_i^{(k)}), \qquad \Sigma_{k+1} = \operatorname{diag}(3\sigma_i^{(k)} - (\sigma_i^{(k)})^3). \tag{34}$$

In order for the method to converge, we require every diagonal element of $(\Sigma_k)_{k\in\mathbb{N}}$ to converge. Since we want X_k to converge to $U = PQ^*$, we want each diagonal element to converge to 1.

We consider the real sequence $(x_k)_{k\in\mathbb{N}}$ defined by the recurrence relation

$$x_{k+1} = p(x_k), \qquad x_0 \geq 0, \qquad p(x) := \frac{1}{2}(3x - x^3), \tag{35}$$

where the condition $x_0 \geq 0$ is motivated by the singular values of A.

We first note that p is an odd function with roots at 0, $\pm\sqrt{3}$ and local maxima at ± 1 ($p(\pm 1) = \pm 1$). Since the leading coefficient of p is negative, p is positive on $[0, \sqrt{3}]$ and negative on $[\sqrt{3}, \infty)$. We now study the convergence of (x_k) for different values of x_0.

- For $x_0 = 0$ or $\sqrt{3}$, x_0 is a root of p so $x_k \to 0$ as $k \to \infty$.
- For $0 < x_0 \leq 1$, $p(0,1) = (0,1)$ and $p(x) > x$ on $(0,1)$ so $x_k \to 1$ as $k \to \infty$.
- For $1 < x_0 < \sqrt{3}$, $p(x_0) \in (0,1)$ so $x_n = p^n(x_0) = p^{n-1}(p(x_0)) \to 1$ as $k \to \infty$.
- For $x_0 > \sqrt{3}$, $p(x_0)$ is negative so we cannot guarantee convergence to 1. It is easy to show that for $x_0 \geq \sqrt{5}$ the iteration diverges, since $|p(x)| \geq x$ and p is unbounded for $|x| \geq \sqrt{5}$.

Therefore, every diagonal sequence converges to 1 if $0 < \sigma_i < \sqrt{3}$ for $i = 1 : \text{rank}(A)$, or equivalently $\|A\|_2 < \sqrt{3}$ and A is full rank.

It follows that for a starting matrix A with full rank and $\|A\|_2 < \sqrt{3}$,

$$\|U - X_{k+1}\|_2 = \left\| PQ^* - P\left[\frac{1}{2}(3\Sigma_k - \Sigma_k^3)\right] Q^* \right\|_2 = \left\| I - \frac{1}{2}(3\Sigma_k - \Sigma_k^3) \right\|_2 \tag{36}$$

$$= \max_{i=1:n} \left| 1 - \frac{1}{2}\left(3\sigma_i^{(k)} - (\sigma_i^{(k)})^3\right) \right|, \tag{37}$$

which tends to 0 as $k \to \infty$.

8. Evaluate the operation count for one step of Newton's method and one step of the Newton-Schulz iteration (taking account of symmetry). Ignoring operation counts, how much faster does matrix multiplication have to be than matrix inversion for Newton-Schulz to be faster than Newton (assuming both take the same number of iterations)?

We first consider the kth step $X_{k+1} = (X_k + X_k^{-*})/2$ for the Newton iteration of a matrix $A \in \mathbb{C}^{n \times n}$. We identify 3 main operations:

- One matrix inversion of $X_k \in \mathbb{C}^{n \times n}$: $2n^3 + O(n^2)$ flops
- One matrix addition in $\mathbb{C}^{n \times n}$: n^2 flops
- One element-wise division in $\mathbb{C}^{n \times n}$: n^2 flops

So the total number of operations for the Newton method is $2n^3 + O(n^2)$.

We now consider a step of the Newton-Schulz iteration $X_k(3I - X_k^* X_K)/2$ for $X_0 = A \in \mathbb{C}^{m \times n}$. We fist note that $X_k^* X_k$, and by extension $(3I - X_K^* X_k)/2$, is Hermitian in $\mathbb{C}^{n \times n}$. Therefore only the upper triangular elements of these matrices need to be calculated, ie we only have to compute $\sum_{k=1}^{n} k = (n^2 + n)/2$ components. Calculating $X_k * X_k$, we use the Algorithm 1, using a total

Algorithm 1: Algorithm to compute the top diagonal elements of $X_k^* X_k$

$b_{ij} = (X_k^* X_k)_{ij}$;
for $i = 1 : n$ **do**
  for $j = i : n$ **do**
    for $r = 1 : m$ **do**
      $b_{ij} = b_{ij} + \overline{x_{ri}} x_{rj}$;
    end
  end
end

of $mn^2 + mn$ flops. Forming $3I - X_k^* X_k$ and dividing the result by 2 adds $n^2 + n$ operations. Finally multiplying by X_k takes $2mn^2$ flops for a total of $3mn^2 + O(n^2) + O(mn)$ flops per step.

9. Write a MATLAB M-file `poldec` that computes the polar decomposition of a nonsingular $A \in \mathbb{C}^{n \times n}$.

We wrote the MATLAB function `poldec` (see `poldec.m` in the github repository *https://github.com/ThomasSeleiro/PolarDecompProj*) that computes the polar decomposition of a matrix A.

The Newton method from (18) is used until the condition $\|X_k\|_2 < \sqrt{3}$ is met, at which point we use the Newton-Schulz method, since it is guaranteed to converge.

References

[1] Roger A Horn and Charles R Johnson. *Matrix analysis.* Cambridge University Press, Cambridge, 1985.

[2] Alan. Jeffrey and Hui-Hui Dai. *Handbook of mathematical formulas and integrals.* Academic Press/Elsevier, Burlington, MA, 4th ed. / edition, 2008.

[3] C T Kelley. *Solving nonlinear equations with Newton's method.* Fundamentals of Algorithms. Society for Industrial and Applied Mathematics, Philadelphia, 2003.