APPROXIMATION TO THE SQUARE ROOT OF A POSITIVE OPERATOR

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Abstract. A generalization of successive approximations to the square root of a positive operator on a Hilbert space due to Riesz-Nagy and Halmos is discussed from the viewpoint of operator means and operator inequalities: For the arithmetic mean ∇ and a positive operator A, a sequence $\{A_n\}$ satisfying

$$A \geq A_n^2 \geq 0 \quad \text{and} \quad A_{n+1} \geq 2A_n \ \nabla (A - A_n^2) \qquad \text{for } n = 0, 1, 2, \cdots$$

converges monotone increasingly to the square root $\sqrt{A}$ of A in the strong operator topology, in which the operator sequence is selected seemingly at random. Moreover, we discuss a harmonic mean version for Newton's method.

1 Introduction. Throughout this note, a capital letter means a bounded linear operator on a Hilbert space H. An operator A is said to be positive, in symbol, $A \geq 0$ if $(Ax, x) \geq 0$ for all $x \in H$. In particular, we denote by $A > 0$ if $A \geq 0$ is invertible. The order $A \geq B$ for selfadjoint operators A and B is defined by $A - B \geq 0$.

The arithmetic mean ∇ and the harmonic mean ! are defined as

$$A \ \nabla \ B = \frac{A + B}{2} \quad \text{and} \quad A \ ! \ B = \left(\frac{A^{-1} + B^{-1}}{2} \right)^{-1}$$

for positive operators A and B, respectively.

For the existence of the square root of a positive operator on a Hilbert space, Riesz and Nagy [7] showed that for a positive operator A, the successive approximation defined recursively by $B_0 = 0$ and the equations

$$B_{n+1} = (1 - A) \ \nabla \ B_n^2 \quad \text{for } n = 0, 1, 2, \cdots \tag{1}$$

converges monotone increasingly in the strong operator topology. Its limit B necessarily satisfies $(1 - B)^2 = A$, also see Halmos [5, Problem 95].

If we replace B_n in (1) by $1 - A_n$, then the equations (1) is rephrased by

$$A_{n+1} = 2A_n \ \nabla \ (A - A_n^2) \quad \text{for } n = 0, 1, 2, \cdots \tag{2}$$

and the sequence $\{A_n\}$ converges monotone increasingly to the square root $\sqrt{A}$ of A in the strong operator topology, see Furuta's book [4, §2.1.5 Theorem 3].

On the other hand, in the preceding paper [2], we considered the following result by means of the inequality instead of the equality in the successive approximation: A sequence $\{A_n\}$ satisfying

$$0 \leq A_n \leq 1 \quad \text{and} \quad (1 - A_n) \ \sharp \ A_{n+1} \geq \frac{1}{2} \qquad \text{for } n = 0, 1, 2, \cdots \tag{\#}$$

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converges uniformly to $\frac{1}{2}$, where the geometric mean $\sharp$ is defined by

$$A \sharp B = A^{\frac{1}{2}}(A^{-\frac{1}{2}}BA^{-\frac{1}{2}})^{\frac{1}{2}}A^{\frac{1}{2}}$$

for positive invertible operators A and B.

From the viewpoint of operator means and operator inequalities, a generalization of successive approximations to the square root of a positive operator on a Hilbert space is discussed in this note. For a positive operator A, a sequence $\{A_n\}$ satisfying

$$A \geq A_n^2 \geq 0 \quad \text{and} \quad A_{n+1} \geq 2A_n \ \nabla (A - A_n^2) \qquad \text{for } n = 0, 1, 2, \cdots$$

converges monotone increasingly to $\sqrt{A}$ in the strong operator topology, in which an operator sequence is selected seemingly at random. Moreover, we discuss a harmonic mean version for Newton's method: A sequence $\{A_n\}$ satisfying

$$A \leq A_n^2 \quad \text{and} \quad A_{n+1}^2 \leq A \ ! \ A_n^2 \qquad \text{for } n = 0, 1, 2, \cdots$$

converges monotone decreasingly to $\sqrt{A}$ in the strong operator topology. They may be observed as a method to generalize successive approximations.

2 Approximations.

2 Approximations. First of all, based on ideas in the preceding paper [2], by replacing the equality in (2) by the inequality, we show the following theorem in which an operator sequence is selected seemingly at random. Here we denote by $A_n \downarrow A$ a series of selfadjoint operators $\{A_n\}$ such that $A_1 \geq A_2 \geq \ldots$ and $A_n \to A$ in the strong operator topology for a selfadjoint operator A.

Theorem 1. *Let A be a positive operator. If a sequence $\{A_n\}$ of positive operators satisfies*

$$A \geq A_n^2 \geq 0 \quad \textit{and} \quad A_{n+1} \geq 2A_n \ \nabla (A - A_n^2) \qquad \textit{for } n = 0, 1, 2, \cdots,$$

then the sequence $\{A_n\}$ converges monotone increasingly to $\sqrt{A}$ in the strong operator topology.

Proof. Since $A \geq A_n^2 \geq 0$, we have

$$A_{n+1} \geq A_n + \frac{1}{2}(A - A_n^2) \geq A_n \qquad \text{for } n = 0, 1, 2, \cdots.$$

Since $\{A_n\}$ is non-decreasing and bounded above by $0 \leq A_n \leq \|A\|^{\frac{1}{2}}$, there exists a positive operator B such that $A_n \uparrow B$. Since $A_n \to B$ (strongly), it follows that $A_n^2 \to B^2$ (strongly) and hence that

$$A \geq B^2 \quad \text{and} \quad B \geq 2B \ \nabla \ (A - B^2).$$

The latter inequality implies $B^2 \geq A$ and so we have $B^2 = A$ as desired. □

We can easily generalize Theorem 1 under a general setting. If we put $f(t) = \sqrt[n]{t}$ in Corollary 2, then it follows that $f(t)$ is operator monotone and $f^{-1}(t) = t^n$ and thus we obtain the approximation to the n-th root of a given positive operator.

Corollary 2. *Let A be a positive operator and f an operator monotone function on the interval $[0, \infty)$. If a sequence $\{A_n\}$ of positive operators satisfies*

$$A \geq f^{-1}(A_n) \geq 0 \quad \textit{and} \quad A_{n+1} \geq 2A_n \ \nabla (A - f^{-1}(A_n)) \qquad \textit{for } n = 0, 1, 2, \cdots,$$

then the sequence $\{A_n\}$ converges monotone increasingly to $f(A)$ in the strong operator topology.

Next, we consider a generalized Newton's method which is introduced by [3] for operators as follows: Let A be a positive operator. If a sequence $\{A_n\}$ of positive invertible operators satisfies

$$A \geq A_n^2 \geq 0, \quad A_n A = A A_n \quad \text{and} \quad A_{n+1} \geq A_n \ \nabla \ (A A_n^{-1}) \quad \text{for } n = 0, 1, 2, \cdots$$

then the sequence $\{A_n\}$ converges monotone increasingly to $\sqrt{A}$ in the strong operator topology by a similar way to Theorem 1.

We show a harmonic mean version for Newton's method which is seemingly simple by presentation.

Theorem 3. *Let A be a positive operator. If a sequence $\{A_n\}$ of positive operators satisfies*

$$A \leq A_n^2 \quad \textit{and} \quad A_{n+1}^2 \leq A \ ! \ A_n^2 \qquad \textit{for } n = 0, 1, 2, \cdots,$$

then the sequence $\{A_n\}$ converges monotone decreasingly to the square root $\sqrt{A}$ in the strong operator topology.

To prove Theorem 3, we need the following lemma on the harmonic mean.

Lemma 4. (1) *If A and B are positive invertible operators, then $A \ ! \ B = B$ implies $A = B$.*

(2) *If A and B are positive operators and $A \geq B$, then $A \ ! \ B = A$ implies $A = B$.*

Proof. (1). Since A and B are invertible, we have

$$B^{-1} = (A \ ! \ B)^{-1} = A^{-1} \ \nabla \ B^{-1}$$

and hence $A^{-1} = B^{-1}$. Therefore it follows that $A = B$.

(2). Since the harmonic mean is represented as

$$A \ ! \ B = \max \left\{ X \geq 0 \ : \ \begin{pmatrix} 2A & 0 \\ 0 & 2B \end{pmatrix} \geq \begin{pmatrix} X & X \\ X & X \end{pmatrix} \right\},$$

the hypothesis $A \ ! \ B = A$ implies

$$\begin{pmatrix} 2A & 0 \\ 0 & 2B \end{pmatrix} \geq \begin{pmatrix} A & A \\ A & A \end{pmatrix}.$$

For every vector $x \in H$, it follows that

$$0 \leq \left(\begin{pmatrix} A & -A \\ -A & 2B - A \end{pmatrix} \begin{pmatrix} x \\ x \end{pmatrix}, \begin{pmatrix} x \\ x \end{pmatrix} \right) = 2((B - A)x, x) \leq 0$$

by the hypothesis $A \geq B$. Therefore we have $A = B$. □

Proof of Theorem 3. By the hypothesis, we have

$$A_{n+1}^2 \leq A \; ! \; A_n^2 \leq A_n^2 \; ! \; A_n^2 = A_n^2.$$

Since $\{A_n\}$ is non-increasing by the Löwner-Heinz theorem and bounded below by $A_n \geq 0$, there exists a positive operator B such that $A_n \downarrow B$. Since $A_n^2 \to B^2$ (strongly), it follows that

$$B^2 \geq A \quad \text{and} \quad B^2 \leq A \; ! \; B^2.$$

Therefore, we have $B^2 \leq A \; ! \; B^2 \leq B^2 \; ! \; B^2 = B^2$ and hence $A \; ! \; B^2 = B^2$. It follows from (2) of Lemma 4 that $B^2 = A$ as desired. □

As a dual case of Theorem 3, We have the following corollary by (1) of Lemma 4.

Corollary 5. *Let A be a positive operator. If a sequence $\{A_n\}$ of positive invertible operators satisfies*

$$A \geq A_n^2 > 0 \quad \textit{and} \quad A_{n+1}^2 \geq A \; ! \; A_n^2 \qquad \textit{for } n = 0, 1, 2, \cdots,$$

then the sequence $\{A_n\}$ converges monotone increasingly to $\sqrt{A}$ in the strong operator topology.

Remark. (1) In the results of this section, as we have observed in [2], it follows from Dini's theorem that monotone increasing strongly convergence implies uniformly convergence.

(2) Lemma 4 (1) is indebted to J.I.Fujii and Lemma 4 (2) is due to M.Fujii. It is pointed out by him that the assumption of the invertibility can not omited by the following simple example: If P is a projection, then $1 \; ! \; P = P$ does not deduce to $1 = P$.

(3) M.Fujii also pointed out that the formulation of Theorem 3 is deducible by Newton's method. Let $A_{n+1} = A_n \; \nabla \; AA_n^{-1}$ under the assumption of the invertibility and the commutativity of operators. Then we have

$$A_{n+1}^{-1} = A_n^{-1} \; \nabla \; \frac{A^{-1}}{A_n^{-1}} = A_n^{-1} \; \nabla \; \left(\frac{A}{A_n}\right)^{-1}$$

and so

$$A_{n+1} = \left(A_n^{-1} \; \nabla \; \left(\frac{A}{A_n}\right)^{-1}\right)^{-1} = A_n \; ! \; \frac{A}{A_n}.$$

Now assuming $A_{n+1} = A_n$ for sufficiently large n, we have consequently $A_{n+1}^2 = A_n^2 \; ! \; A$ as desired.

3 operator means. In this section, we generalize the preceding results to operator means. The theory of operator means for positive (bounded linear) operators on a Hilbert space is established by Kubo and Ando [6] in connection with Löwner's theory for the operator monotone functions. A binary operation $(A, B) \in \mathcal{B}^+(H) \times \mathcal{B}^+(H) \to A \; m \; B \in \mathcal{B}^+(H)$ in the cone of positive operators on a Hilbert space H is called an *operator mean m* if the following conditions are satisfied:

(monotonicity) $A \le C$ and $B \le D$ imply $A\ m\ B \le C\ m\ D$.

(upper continuity) $A_n \downarrow A$ and $B_n \downarrow B$ imply $A_n\ m\ B_n \downarrow A\ m\ B$.

(transformer inequality) $T^*(A\ m\ B)T \le (T^*AT)\ m\ (T^*BT)$ for an operator T.

(normalized condition) $A\ m\ A = A$.

If T is invertible, then an operator mean m satisfies the transformer equality:

$$T^*(A\ m\ B)T = (T^*AT)\ m\ (T^*BT). \tag{3}$$

An operator mean m is called *symmetric* if $A\ m\ B = B\ m\ A$ for positive operators A and B.

Simple examples of symmetric operator means are the arithmetic mean ∇ and the harmonic mean !. Another one is the geometric mean $\sharp$ defined as

$$A \sharp B = A^{\frac{1}{2}}(A^{-\frac{1}{2}}BA^{-\frac{1}{2}})^{\frac{1}{2}}A^{\frac{1}{2}}.$$

If A commutes with B, then $A \sharp B = \sqrt{AB}$.

A partial order $\ge$ among two operartor means is introduced in a natural way: $m \le n$ means by definition that $A\ m\ B \le A\ n\ B$ for positive operators A and B. Like the numerical case, the arithmetic-geometric-harmonic mean inequality holds:

$$A\ !\ B \le A \sharp B \le A\ \nabla\ B \tag{4}$$

for positive operators A and B. Moreover, a symmetric operator mean have the following property due to Kubo-Ando [6].

Lemma 6 (Kubo-Ando). *Arithmetic mean is the maximum of all symmetric means while harmonic mean is the minimum: For a symmetric mean m*

$$A\ !\ B \le A\ m\ B \le A\ \nabla\ B$$

for positive operators A and B.

A *state* ϕ is a unital positive linear functional on a C*-algebra of operators acting on H such that $\|\phi\| = \phi(1) = 1$. Then we cite the following lemma due to Ando[1]:

Lemma 7 (Ando). *If ϕ is a state, then*

$$\phi(A \sharp B) \le \phi(A) \sharp \phi(B)$$

for positive operators A and B.

We show the following theorem related to (#) in §1 from the viewpoint of operator inequalities.

Theorem 8. *Let A be a positive operator. If a sequence $\{A_n\}$ of positive operators satisfies*

$$A \ge A_n^2 \ge 0 \quad \textit{and} \quad A \le \left(2A - A_n^2\right) \sharp A_{n+1}^2 \qquad \textit{for } n = 0, 1, 2, \cdots,$$

then the sequence $\{A_n\}$ converges monotone increasingly to $\sqrt{A}$ in the strong operator topology.

Proof. By the arithmetic-geometric mean inequality (4), we have

$$\begin{aligned} 0 \le A &\le \left(2A - A_n^2\right) \ \sharp\ A_{n+1}^2 \\ &\le \left(2A - A_n^2\right) \ \nabla\ A_{n+1}^2 = \frac{(2A - A_n^2) + A_{n+1}^2}{2} \end{aligned}$$

and hence $A_n^2 \le A_{n+1}^2$. It follows from the Löwner-Heinz theorem that $A_n \le A_{n+1}$. Since $\{A_n\}$ is non-decreasing and bounded above by $A_n \le \|A\|^{\frac{1}{2}}$, there exists a positive operator B such that $A_n \uparrow B$. Since $A_n^2 \to B^2$ (strongly), it follows that

$$B^2 \le A \quad \text{and} \quad A \le \left(2A - B^2\right) \ \sharp\ B^2.$$

Let ϕ be an arbitrary state on the C*-algebra generated by $\{A_n\}$ and A. Then it follows from Lemma 7 that

$$\begin{aligned} \phi(A) &\le \phi\left((2A - B^2) \ \sharp\ B^2\right) \\ &\le \phi(2A - B^2) \ \sharp\ \phi(B^2) \\ &= \left(2\phi(A) - \phi(B^2)\right) \ \sharp\ \phi(B^2) \\ &= \sqrt{(2\phi(A) - \phi(B^2))\,\phi(B^2)} \end{aligned}$$

and hence

$$0 \le \phi(A)^2 - (2\phi(A) - \phi(B^2))\phi(B^2) = -(\phi(A) - \phi(B^2))^2$$

Therefore we have $\phi(A - B^2) = 0$ for every state ϕ. □

Corollary 9. *Let m be an operator mean dominated by the geometric mean $\sharp$ and A a positive operator. If a sequence $\{A_n\}$ of positive operators satisfies*

$$A \ge A_n^2 \ge 0 \quad \textit{and} \quad A \le \left(2A - A_n^2\right) \ m\ A_{n+1}^2 \qquad \textit{for } n = 0, 1, 2, \cdots,$$

then the sequence $\{A_n\}$ converges monotone increasingly to $\sqrt{A}$ in the strong operator topology.

Proof. Since $A \le \left(2A - A_n^2\right) \ m\ A_{n+1}^2 \le \left(2A - A_n^2\ \right) \ \sharp\ A_{n+1}^2$, the result follows from Theorem 8. □

We can easily generalize Theorem 3 to operator means.

Corollary 10. *Let m be a symmetric operator mean and A a positive operator. If a sequence $\{A_n\}$ of positive invertible operators satisfies*

$$A \ge A_n^2 > 0 \quad \textit{and} \quad A_{n+1}^2 \ge A \ m\ A_n^2 \qquad \textit{for } n = 0, 1, 2, \cdots,$$

then the sequence $\{A_n\}$ converges monotone increasingly to $\sqrt{A}$ in the strong operator topology.

Proof. By a similar way to Theorem 3, there exist a positive operator B such that $A_n \uparrow B$ and hence

$$A \geq B^2 \quad \text{and} \quad B^2 \geq A\ m\ B^2.$$

Therefore we have $B^2 \geq A\ m\ B^2 \geq B^2\ m\ B^2 = B^2$ by the normalization of m and so $B^2 = A\ m\ B^2$. Then it follows from the transformer equality (3) and the symmetry of m that

$$1 = B^{-1}B^2B^{-1} = B^{-1}(A\ m\ B^2)B^{-1} = (B^{-1}AB^{-1})\ m\ 1 \geq (B^{-1}AB^{-1})\ !\ 1.$$

The last inequality is due to Lemma 6. Hence we have $1 \geq B^{-1}AB^{-1}$. This says that $B^2 = A$ as desired. □

Finally, we state the operator mean version of Newton's method, which is a generalized successive approximation to the n-th root of a given positive operator.

Corollary 11. *Let m be a symmetric operator mean and A a positive operator, and p a positive real number. If a sequence $\{A_n\}$ of positive invertible operators satisfies*

$$A_n^{p+1} \geq A,\ A_nA = AA_n \quad \textit{and} \quad A_{n+1} \leq A_n\ m\ (AA_n^{-p}) \qquad \textit{for } n = 0, 1, 2, \cdots,$$

then the sequence $\{A_n\}$ converges monotone decreasingly to the $(p+1)$-th root $\sqrt[p+1]{A}$ in the strong operator topology.

Proof. By Lemma 6, we have $0 \leq A_{n+1} \leq A_n\ m\ (AA_n^{-p}) \leq A_n\ \nabla\ (AA_n^{-p}) \leq A_n$ and so it follows that $\{A_n\}$ is non-increasing and bounded below. Hence there exists a positive operator B such that $A_n \downarrow B$ and $B^{p+1} \geq A$. Therefore we have

$$B \leq B\ \nabla\ AB^{-p}$$

and so $B^{p+1} = A$. □

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