Error control technique of quadrature-based algorithms for the von Neumann Entropy

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Abstract

This study considers a quadrature-based method for computing the von Neumann entropy. For a positive semidefinite Hermitian matrix $A \in \mathbb{C}^{n\times n}$, the von Neumann entropy is defined as $\mathrm{tr}(-A\log(A))$, where $\mathrm{tr}(\cdot)$ denotes the trace (the sum of diagonal entries of a square matrix) and $\log(A)$ denotes the matrix logarithm. In numerical computation, we require evaluating the quadratic form $\boldsymbol{b}^\top(-A\log(A))\boldsymbol{b}$ for a vector $\boldsymbol{b} \in \mathbb{R}^n$. The computation of an integral representation of $\boldsymbol{b}^\top(-A\log(A))\boldsymbol{b}$ is reduced to solving dozens or hundreds of shifted linear systems. Current approaches usually analyze the quadrature discretization error [1], but rarely take into account the additional error introduced by solving these shifted linear systems with iterative solvers.

In this study, we bound this error using the residuals of the approximate solutions of these linear systems. This yields a stopping criterion for iterative solvers that keeps the error in $\boldsymbol{b}^\top(-A\log(A))\boldsymbol{b}$ below a prescribed tolerance. Numerical results demonstrate that the proposed criterion enables the computation of $\boldsymbol{b}^\top(-A\log(A))\boldsymbol{b}$ within the prescribed tolerance.

***K*eywords** matrix function · von Neumann entropy · numerical quadrature

References

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