AN OPEN PROBLEM FOR SPECTRAL-NORM ESTIMATION IN MATRIX FUNCTION PERTURBATION THEORY AND ITS IMPLICATION IN QUANTUM CHEMISTRY

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Let $X, E \in \mathbb{C}^{n\times n}$ be Hermitian matrices. We are here concerned with the problem to find a bound of the type

$$\|f(X+E) - f(X)\|_\beta \leq \gamma \|E\|_\beta. \tag{1}$$

For the Frobenius norm ($\beta = \mathrm{F}$) it is known from [1] that γ can be chosen as $\gamma = \gamma_F = \max_{a\neq b\in\{\lambda_i\}\cup\{\tilde{\lambda}_j\}} |f[a,b]|$, where $\lambda_1,\ldots,\lambda_n$ are the eigenvalues of X and $\tilde{\lambda}_1,\ldots,\tilde{\lambda}_n$ are the eigenvalues of $X+E$. On the other hand, in certain situations, the Frobenius norm has properties making it unnatural. In particular, in the field of quantum chemistry, a bound of the type (1) for the spectral norm ($\beta = 2$) would be more physically meaningful and provide a rigorous support for efficient strategies to carry out approximations.

We study an approach involving a characterization of the condition number which holds for any unitary norm (e.g. Frobenius norm and the spectral norm). Let $\kappa_f(\cdot)$ denote the condition number and let $g(\alpha)$ be any function such that $g(\alpha) \leq \kappa_f(X + \alpha E)$. Then, from the definition of the condition number and reasoning with Fréchet derivatives (see [3, Equation (20)]) we know that

$$\|f(X+E) - f(X)\| \leq \|E\| \max_{\alpha\in[0,\,1]} g_{\max}(\alpha). \tag{2}$$

We also have the following consequence of the Daleckiĭ and Kreĭn [2, Theorem 3.11]

$$\kappa_f(A) = \max_{Z\in\Omega} \frac{\|G\circ Z\|_\beta}{\|Z\|_\beta}. \tag{3}$$

where $\Omega = \{Z \in \mathbb{R}^{n\times n} : Z \neq 0\}$ and $\circ$ denotes the Hadamard product and the elements of $G \in \mathbb{R}^{n\times n}$ consist of the divided differences $f[\lambda_i, \lambda_j]$ where $\lambda_i \in \sigma(A)$. (See also [3, Lemma 1].)

Consequently, a bound of the type (1) can be found if the right-hand side of (3) can be estimated in a relevant way. This approach is presented in a preliminary report [3], where the main result unfortunately does not hold under the given conditions. We present this here as a conjecture with counterexample. (The proof of [3, Lemma 2] is invalid due to lack of uniform convergence in the [3, Equation 11].)

Conjecture. *Suppose $A \in \mathbb{R}^{n\times n}$ is a symmetric matrix with positive elements. Under further relevant assumptions on A or Ω, we conjecture that*

$$\max_{Z\neq 0} \frac{\|A\circ Z\|_2}{\|Z\|_2} = \max_{i,j} |a_{i,j}|.$$

Under the conditions that the conjecture is true, it follows from (2) and (3) that a

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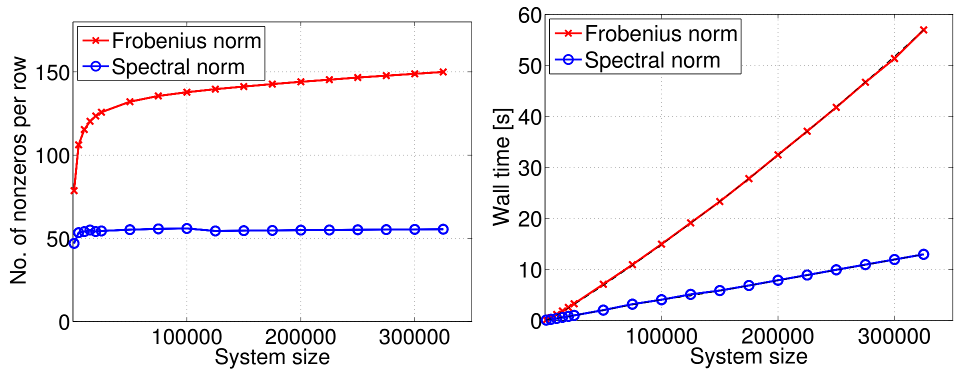

FIG. 1. *Test calculations for model Hamiltonians described in [3, Section 4]. Left panel: Average number of nonzero entries per row in $\widetilde{H}$. Right panel: Wall time for calculation of the square $\widetilde{H}^2$.*

bound of the type (1) for $\alpha = 2$ holds with

$$\gamma = \gamma_2 = \max_{a \neq b \in \{\lambda_i\} \cup \{\tilde{\lambda}_j\}} |f[a, b]|. \tag{4}$$

Counter example. Unfortunately, the conclusion of the conjecture above does not hold if the *further relevant assumptions* are removed. This can be seen from the following example. Let

$$Z = \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}, \quad A = \begin{pmatrix} 1 & 1 \\ 1 & 0.1 \end{pmatrix}.$$

Then

$$\kappa_f(A) > \frac{\|A \circ Z\|_2}{\|Z\|_2} \approx 1.1252 > 1.$$

Quantum chemistry application. Although the setting of this result is for matrix functions in general, this work is mainly motivated by an application occurring in the field of *electronic structure theory*. In this field, an imporant iteration involves approximation intermediate matrices such that they can be efficiently represented. A bound for the error introduced by this approximation can be expressed as (1). See [3, Section 4] for a more elaborate explanation and references. In Figure 1, we demonstrate the use of the spectral norm and the advantage in comparison to the Frobenius norm. The figure is based on the assumption the matrices and matrix function involved satisfy the conditions for the conjecture. If the conjecture does not hold, there could be situations where the error is larger than predicted and consequently not provide a reliable procedure for the estimation.

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