

On the condition number and perturbation of matrix functions with respect to unitarily invariant norms

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Abstract

Consider a given matrix function f and an arbitrary unitarily invariant matrix norm $\|\cdot\|$. We present here new results for the *absolute condition number* of the matrix function, i.e., $\kappa = \max_{S \neq 0} \frac{\|L_f(A, S)\|}{\|S\|}$, where L_f is the Frechét derivative of f , and new results for the perturbation $\|f(A + E) - f(A)\|$. More precisely, we show that under certain conditions, the absolute condition number is given by the maximum norm of the Loewner matrix $\{f[\lambda_i, \lambda_j]\}_{i,j}$, where $f[x, y]$ is the divided difference and $\lambda_1, \dots, \lambda_n$ are the eigenvalues of A . The derived expression does not depend on which unitarily invariant norm is chosen, showing that the absolute condition number is independent of norm (for the given generality setting). With the formula for the condition number we show that, under similar conditions, the perturbation is bounded by an expression involving the divided difference for the union of eigenvalues of A and $A + E$. More precisely,

$$\|f(A + E) - f(A)\| \leq \|E\| \max_{\lambda, \mu \in \sigma(A) \cup \sigma(A+E), \lambda \neq \mu} |f[\lambda, \mu]|.$$

This result is compared with perturbation results for particular choices of the matrix function f . Finally, the result is illustrated by an application to the error analysis of an iterative method in *electronic structure calculations*. The explicit bound can be used to achieve a user-given total error, by controlling the error of the inner iteration.

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