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Convergence of Eigenvector Continuation AVIK SARKAR, Michigan State University — Eigenvector continuation is a computational method that finds the extremal eigenvalues and eigenvectors of a Hamiltonian matrix with one or more control parameters. It does this by projection onto a subspace of eigenvectors corresponding to selected training values of the control parameters. The method has proven to be very efficient and accurate for interpolating and extrapolating eigenvectors. However, almost nothing is known about how the method converges, and its rapid convergence properties have remained mysterious. In this letter we present the first study of the convergence of eigenvector continuation. To perform the mathematical analysis, we introduce a new variant of eigenvector continuation that we call vector continuation. We first prove that eigenvector continuation and vector continuation have identical convergence properties and then analyze the convergence of vector continuation. Our analysis shows that, in general, eigenvector continuation converges more rapidly than perturbation theory. The faster convergence is achieved by eliminating a phenomenon that we call differential folding, the interference between non-orthogonal vectors appearing at different orders in perturbation theory.

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