Finding Eigenvalues using Automatic Differentiation

Alex Hirzel, Peter Solfest, and Ryan Bruner

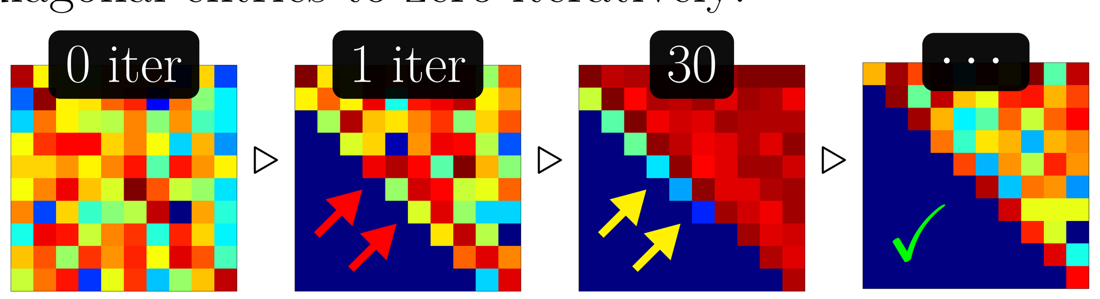
Michigan Technological University

Abstract

Eigenvalues are ubiquitous in all branches of science and engineering. The dominant eigenvalue algorithm reduces input matrices to almost diagonal and then creates and chases bulges using parameters called shifts. Good parameter choices can allow shrinking of the original problem allowing for a more aggressive deflation on the subproblem. Such deflations greatly improve performance. We apply automatic differentiation tools to achieve frequent deflations.

Existing Techniques

A general matrix is first reduced to Hessenberg form, then the **QR algorithm** is used to reduce the subdiagonal entries to zero iteratively:

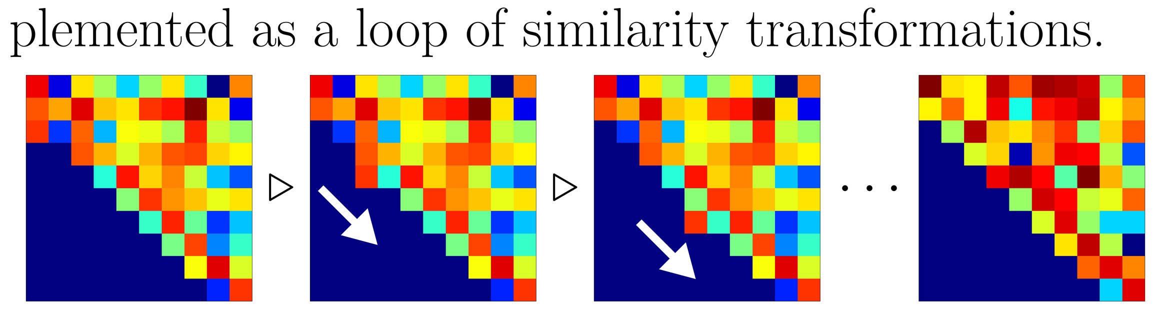


Since the resulting matrix is strictly upper triangular, **the eigenvalues are the diagonal entries**. The QR algorithm consists of repeated iterations of:

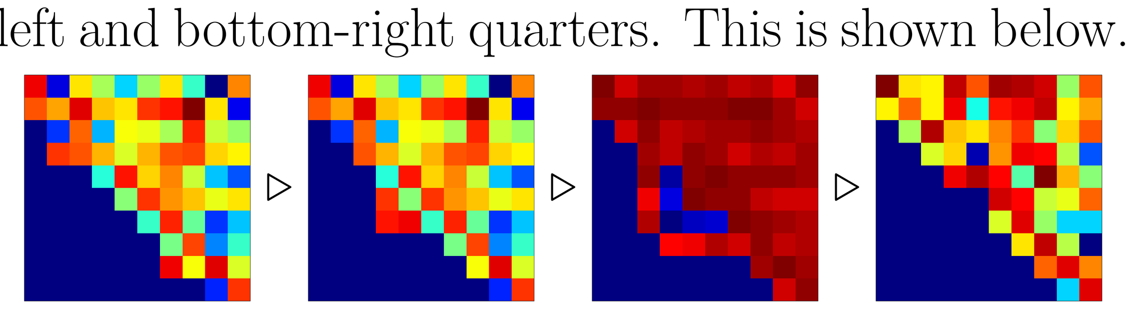
$$A_n \to Q_n R_n \tag{1}$$

$$A_{n+1} \leftarrow R_n Q_n = Q_n^{-1} A_n Q_n \tag{2}$$

As written, (1) and (2) require multiplication of large matrices. For this reason, the QR algorithm is implemented as a loop of similarity transformations.

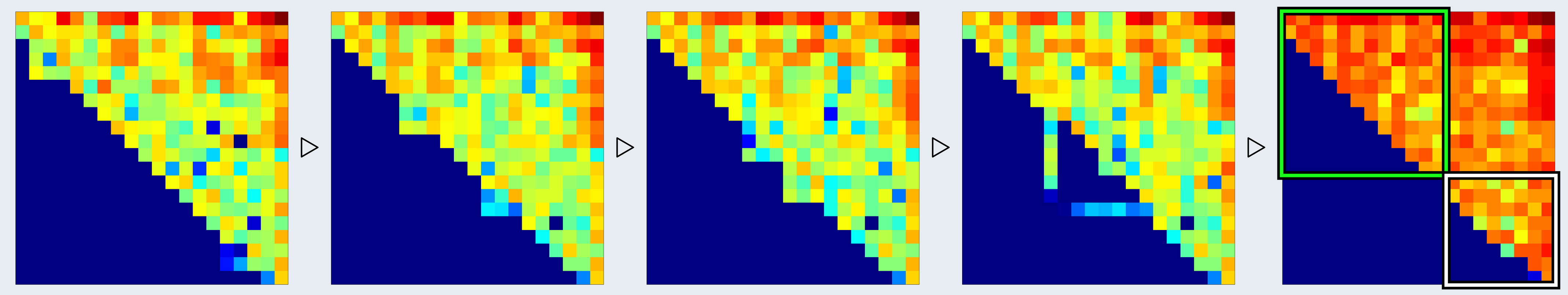


A *bulge* is repeatedly **chased down the diagonal**. To speed convergence [3], the bulge is seeded with one or more *shifts*, which represent **parameter choices**. A second bulge can be started from the bottom, and the two can meet in the middle. A **Schur decomposition is used to form *spikes*** around this bulge. Under the right conditions, the problem can be subdivided recursively into the top-left and bottom-right quarters. This is shown below.

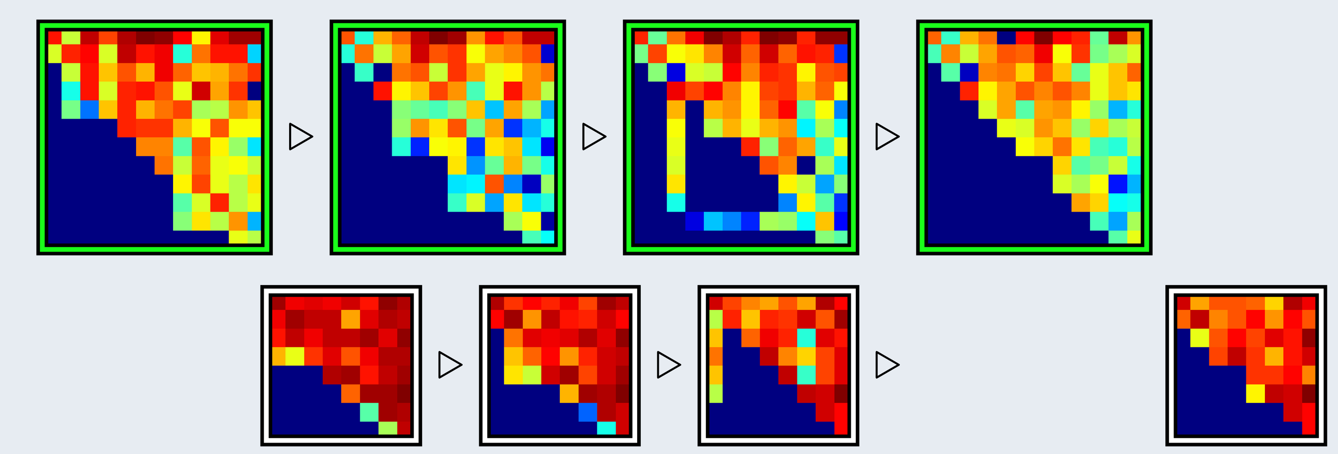


Proposed Technique: Inducing Recursive Middle Deflation

We expect middle deflation to be possible by chasing bulges from both corners simultaneously: [1] [2]



Subdivision is a HUGE performance win.

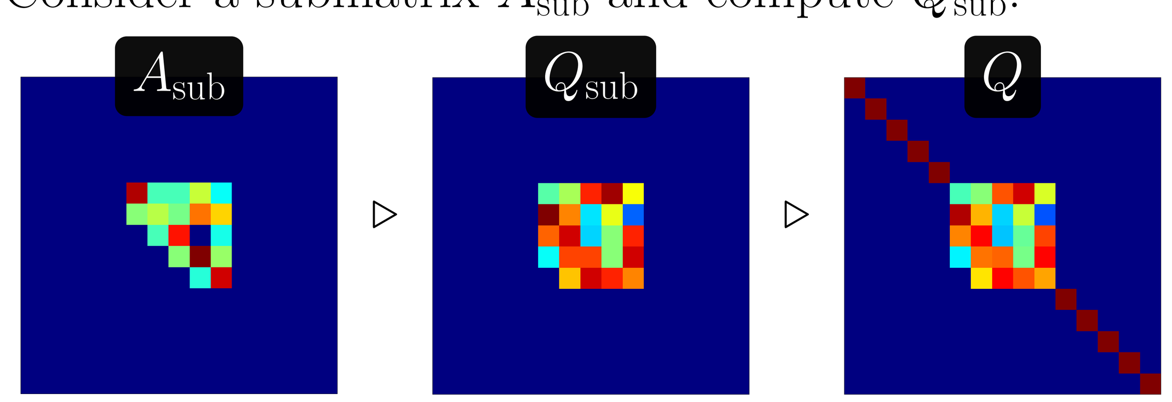


Schur Decomposition

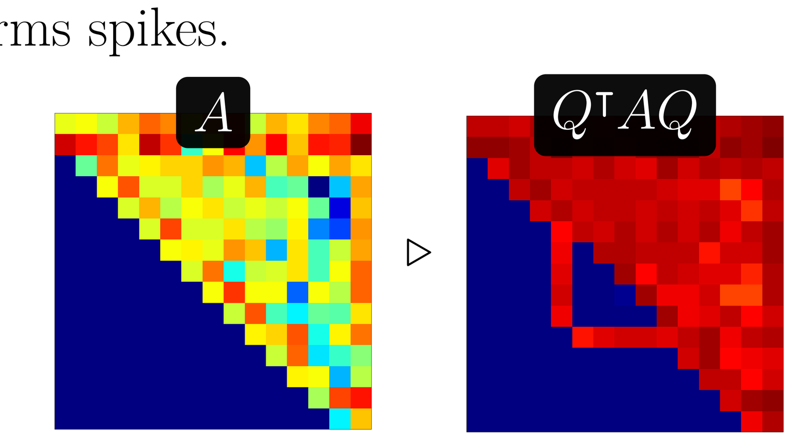
The Schur decomposition allows us to create spikes. For an input matrix A, it forms symmetric Q and diagonal T such that **Q diagonalizes A into T**, as

$$A = Q^{\intercal} T Q \tag{3}$$

Consider a submatrix A_{sub} and compute Q_{sub}:



We can then create Q by embedding Q_{sub} into the identity. Applying this to A creates zeros on the subdiagonal in the neighborhood of the decomposition, and forms spikes.



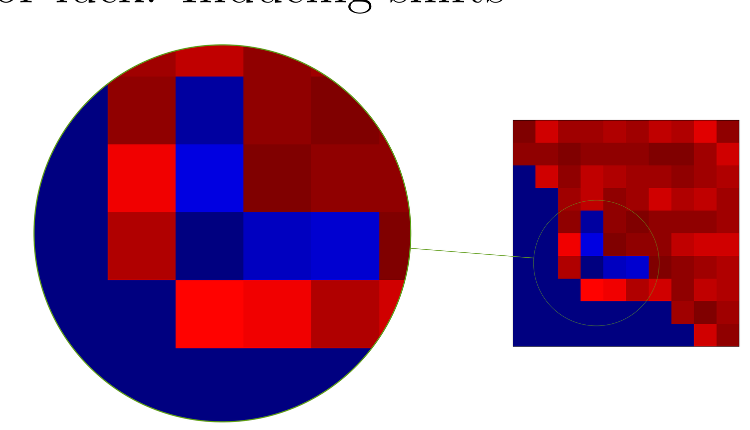
Automatic Differentiation (AD)

$$M_{n+1} = \texttt{MiddleDeflation}(M, \texttt{shifts})$$

AD tools can be applied to compute the sensitivities of the spike tips to the shifts.

$$\frac{dM_{n+1}}{d\texttt{shifts}} = \texttt{func}(M, \texttt{shifts})$$

In practice, middle deflations are improbable because they rely on the values of the spikes. The spike values depend on the shifts fed to the QR algorithm. are generated using a Schur decomposition. They occur when the spike tips become zero due to change or luck. Inducing shifts



We apply **automatic differentiation** (AD) tools to these spikes. AD tools allow *algorithms* to be differentiated in the same sense as algebraic functions. Classical calculus allows us to linearize a function $f(x)$ at $x = a$ as

$$f(x) \approx f(a) + f'(x) \cdot (x - a)$$

which solving for the root ($f(x) = 0$) gives us Newton's method

Conclusions and Future Work

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We successfully apply Automatic Differentiation techniques to induce deflations in the center of matrices. With the proper implementation, this will provide a large performance improvement over traditional algorithms in use today. Additionally, this is an enabling technique for extremely large eigenvalue

Future Work

The authors are pursuing publication.

References

[1] K. S. Braman, *Toward a Recursive QR Algorithm*, PhD thesis, Lawrence, KS, USA, 2003. AAI3103375.

[2] D. S. Watkins, *Bulge exchanges in algorithms of qr type*, SIAM Journal on Matrix Analysis and Applications, 19 (1998), pp. 1074–1096.

[3] D. S. Watkins, *The matrix eigenvalue problem: GR and Krylov subspace methods*, vol. 101, SIAM, 2007.

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Contact Information

- Email: `ahirzel@mtu.edu`
- Phone: +1 (906) 231 0866

Michigan Tech
Michigan Technological University