Finding Eigenvalues using Automatic Differentiation

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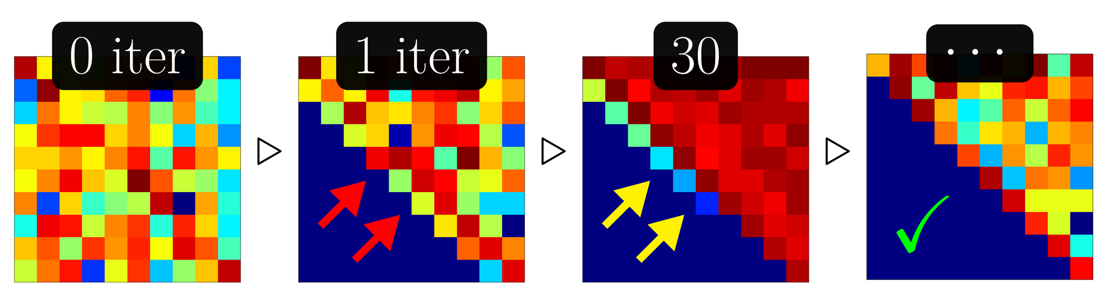
Abstract

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

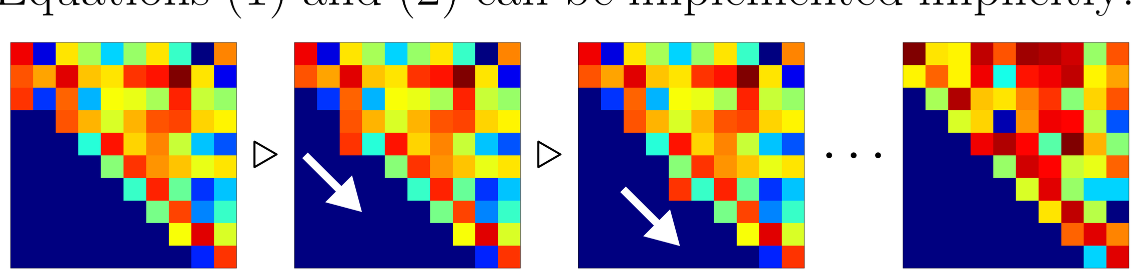
A general matrix is first reduced to Hessenberg form, then the **QR algorithm** is used to reduce the subdiagonal entries to zero iteratively:



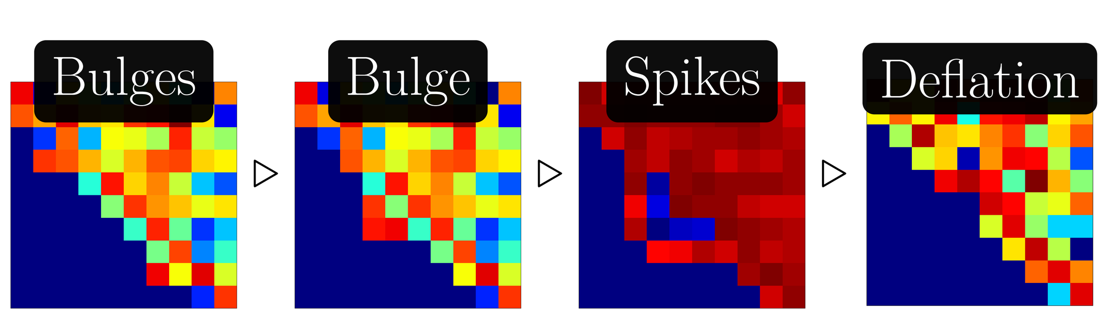
Since the resulting matrix is strictly upper triangular, **the eigenvalues are the diagonal entries**. The QR algorithm consists of repeated iterations of:

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

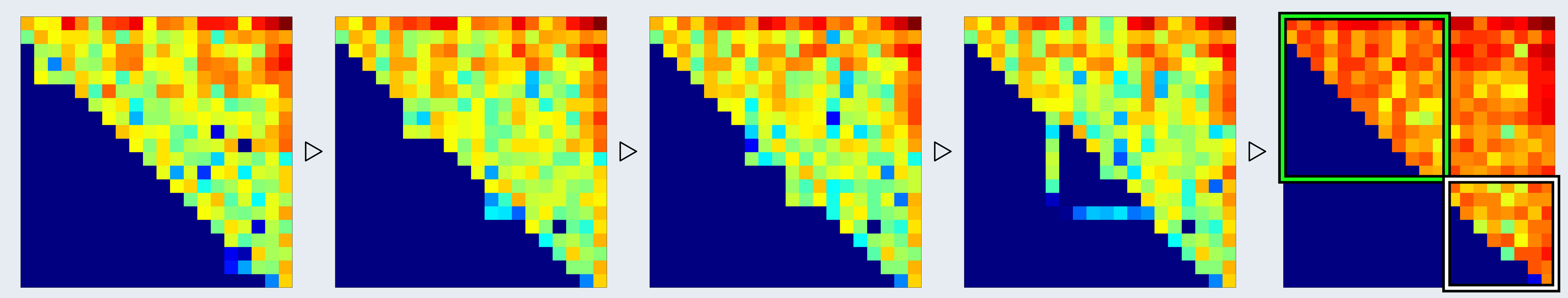
Equations (1) and (2) can be implemented implicitly:



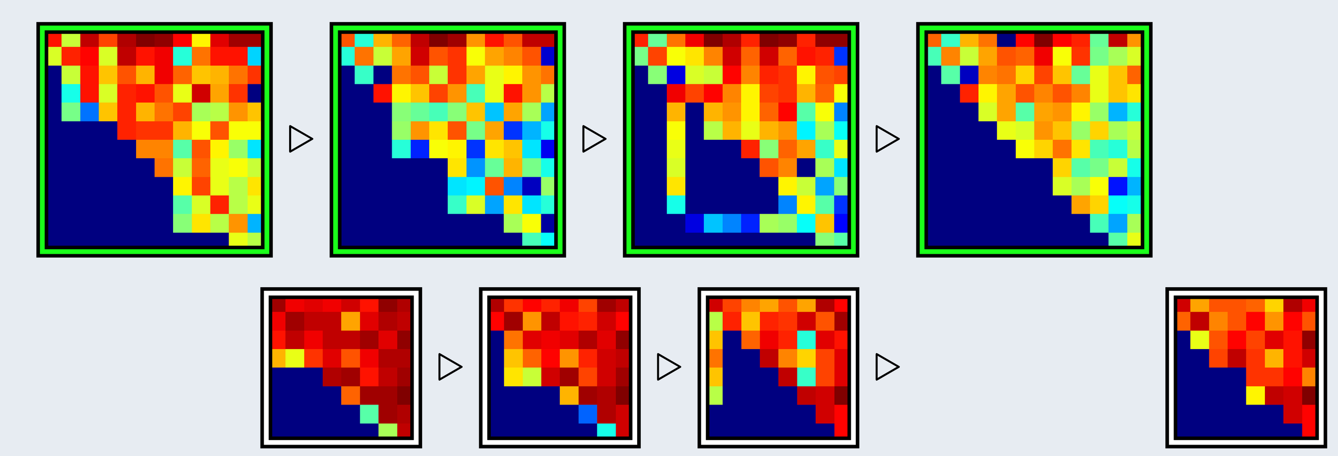
A *bulge* is chased down the diagonal. To speed convergence [4], the bulge is seeded with one or more *shifts*, which are **parameter choices**. A second bulge can be chased from the bottom. A **Schur decomposition is used to form *spikes*** around this bulge. Under the right conditions, the problem can be subdivided recursively into the top-left and bottom-right quarters. This is shown below.



Proposed Technique: Inducing Recursive Middle Deflation



Subdivision is a HUGE performance win.

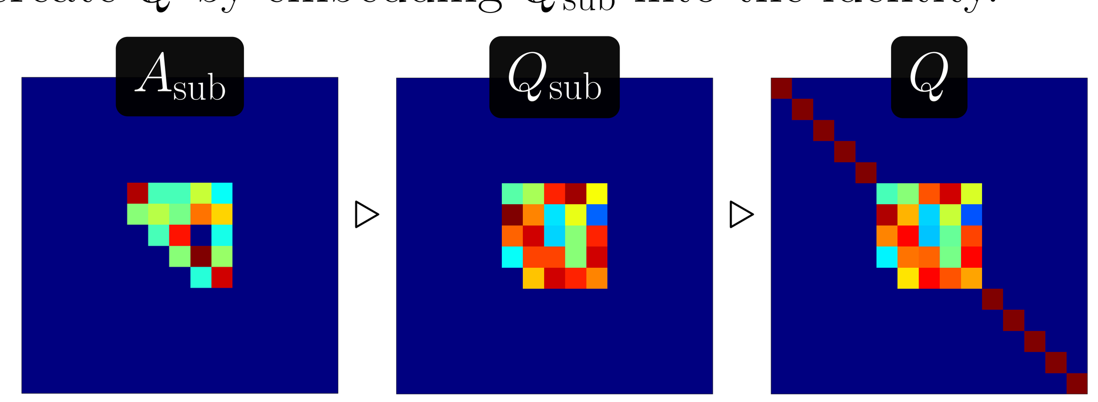


Schur Decomposition

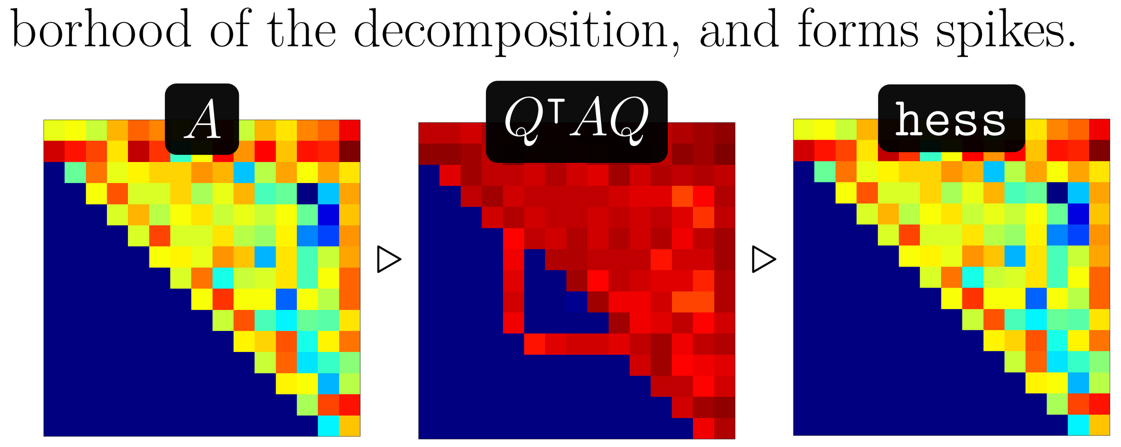
Schur decompositions allow spikes to be created [1]. For an input matrix A, they form symmetric Q and diagonal T such that **Q diagonalizes A into T**:

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

Consider a submatrix A_{sub} and compute Q_{sub}, then create Q by embedding Q_{sub} into the identity.



Applying Q to A zeros the subdiagonal in the neighborhood of the decomposition, and forms spikes.



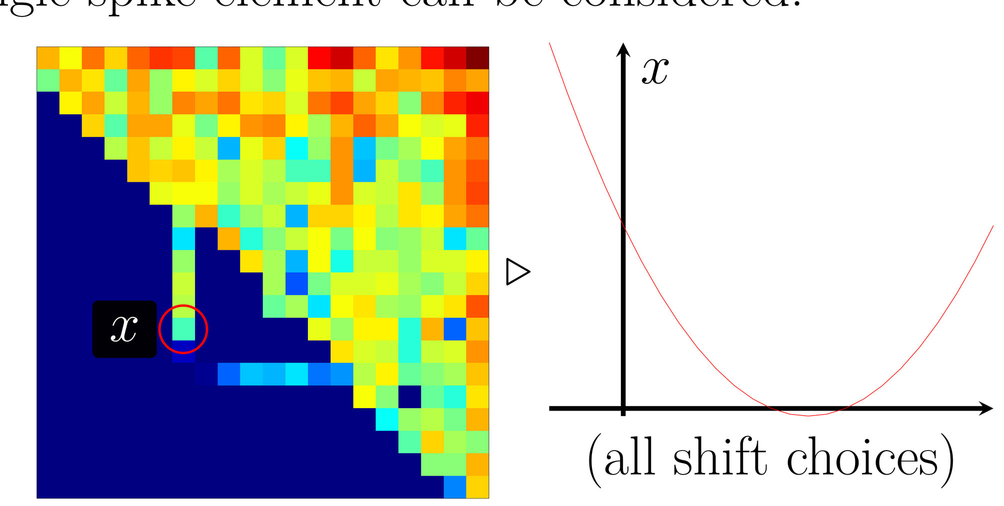
This matrix is then reduced to Hessenberg form again. If roughly half of the values on the spike are near zero, then the Hessenberg form has a zero on the subdiagonal. This allows for matrix deflation (shown in large center box above).

Achieving Deflation

Middle deflations are improbable because they rely on the spikes having many zeros, and the spike values depend on shift choices. Deflations can be induced with proper shift choices. Specifically, the proper shifts can be found by solving:

$$\min_{\text{shifts}} \sum |\text{spike values}| \tag{4}$$

Satisfaction of (4) implies that spikes will be close to zero, allowing for middle deflation. Graphically, a single spike element can be considered:



This element x can be driven to zero with proper shift choices. Many effective methods for minimizing functions rely upon derivative information (e.g. Newton's Method). **Automatic Differentiation** (AD) methods allow for differentiation of matrix operations [2] and the Schur decomposition itself [3]. In this way, AD tools can be used to deflate matrices through optimal shift choices.

Conclusions

We have presented an algorithm which can aggressively target middle deflation as opposed to existing algorithms which do not. The algorithm utilizes AD methods which are highly parallelizable. We are currently prototyping this algorithm in GNU Octave. Very efficient implementations are possible.

Future Work

- Characterize performance
- Optimization (time and space)
- Publication

References

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

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[3] A. Struthers, *Automatic differentiation in linear algebra and statistics*.

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

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