A visualisation for conveying the dynamics of iterative eigenvalue algorithms over PSD matrices

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Abstract

We propose a new way of visualising the dynamics of iterative eigenvalue algorithms such as the QR algorithm, over the important special case of PSD (positive semi-definite) matrices. Many subtle and important properties of such algorithms are easily found this way. We believe that this may have pedagogical value to both students and researchers of numerical linear algebra. The fixed points of iterative algorithms are obtained visually, and their stability is analysed intuitively. It becomes clear that what it means for an iterative eigenvalue algorithm to “converge quickly” is an ambiguous question, depending on whether eigenvalues or eigenvectors are being sought. The presentation is likely a novel one, and using it, a theorem about the dynamics of general iterative eigenvalue algorithms is proved. There is an accompanying video series, currently hosted on Youtube, that has certain advantages in terms of fully exploiting the interactivity of the visualisation.

1 Simple iterative eigenvalue algorithms

The (naive) QR algorithm [2, 8, 3] evaluated on matrix $M$ begins with setting $M_0 = M$ and then repeating the following two steps until convergence:

1. Find the QR decomposition $M_n = Q_n R_n$.
2. Set $M_{n+1} = R_n Q_n$.

The thing to note is that $M_{n+1} = Q_n^T M_n Q_n$. We only concern ourselves with PSD matrices\textsuperscript{1} so the fixed points of the iteration above are all diagonal matrices with non-negative real entries.

We’ve also investigated a variant of the LR algorithm evaluated on a PSD matrix $M$ that begins with setting $M_0 = M$ and then repeating:

\textsuperscript{1}A PSD (positive semi-definite) matrix is a symmetric real matrix whose eigenvalues are all non-negative. Equivalently, it is a matrix $M$ for which $v^T M v \geq 0$ for all vectors $v$. 



1. Find the Cholesky decomposition $M_n = L_n L_n^T$.

2. Set $M_{n+1} = L_n^T L_n$.

Observe that all $M_n$ are similar to each other because $M_{n+1} = L_n^{-1} M_n L_n$. Each $M_n$ is also PSD. Therefore by the spectral theorem, the stronger fact follows that all $M_n$ are orthogonally similar to each other.

Note that while there are more modern and sophisticated versions of the QR algorithm [3], the original one is still widely taught, and remains simpler than its more recent improvements. We think there are conceptual advantages to better understanding the original one.

2 Account of visualisation

In this paper, we present a visualisation of the QR algorithm. Our visualisation makes many properties of the naive QR algorithm, and its various improvements, intuitive. Our visualisation may be beneficial to students and researchers. Our visualisation is also qualitative, and using it we can show that many features of the QR algorithm are in fact universal to iterative eigenvalue algorithms, and not just specific to the QR algorithm.

The QR algorithm is an iterative eigenvalue algorithm. By iterative, we mean that it employs a function $f$ from a set to itself, and evaluates it repeatedly on some starting value $x$ to produce the sequence: $x, f(x), f(f(x)), f(f(f(x))) \ldots$ until it converges close enough to a fixed point of $f$. It’s easy to verify that for the QR algorithm the fixed points are matrices whose eigenvalues are easily found. The issue is that in general, function iterations have very complicated dynamics. For some functions $f$ and starting values $x$, the iteration can diverge, or even be chaotic. When working over $\mathbb{R}$, the usual visualisation that’s employed is sometimes called the cobweb plot, and using it one can develop a good intuition for the dynamics of some instances of function iteration. We cannot use cobweb plots to understand the dynamics of iterative eigenvalue algorithms however, because even in the smallest non-trivial case, the $2 \times 2$ case, the function $f$ maps $\mathbb{R}^4 \to \mathbb{R}^4$.

We focus only on PSD matrices (positive semi-definite). It can be argued that this special case is sufficient for computing SVDs (Singular Value Decompositions), eigendecompositions of symmetric matrices, and eigendecompositions of orthogonal matrices[2]. The PSD case is especially amenable to visualisation. We won’t try to justify further our focus on the PSD case.

The visualisation is based on the one-to-one correspondence between $n \times n$ PSD matrices, and ellipsoids centred at the origin of $\mathbb{R}^n$. The correspondence is

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[2] Briefly: For symmetric matrices, one can perform a shift $M' = M + \mu I$ for some easily chosen $\mu \in \mathbb{R}$ which makes $M'$ PSD. For an orthogonal matrix $M$, we can use the matrix logarithm (or Cayley Transform) as a first step towards making a matrix $M'$ which is PSD. SVD is reducible to eigendecomposition of symmetric matrices in various ways.
given by $M \mapsto \{ Mv \mid v \in S^n \}$ where $S^n$ is the origin-centred hypersphere in $\mathbb{R}^n$. Every PSD matrix corresponds to a unique ellipsoid, and every ellipsoid (that is origin-centred) corresponds to a unique PSD matrices. We therefore sometimes talk about ellipsoids and their semi-axes, instead of about matrices and their eigen-values/vectors. We go as far as to say “the ellipsoid” instead of “the PSD matrix” sometimes.\footnote{This all follows from the spectral theorem.}

Table 1:

Our input ellipse is in blue. Our output ellipse for 1 iteration is in red. We also visualise the LR algorithm in green for comparison. We visualise the naive QR algorithm.

We make some immediate observations:

1. The algorithm always converges for PSD matrices.
2. In every iteration, the angle between the large semi-axes and the $x$-axis diminishes.
3. The large semi-axis is in the same pair of quadrants for the output ellipse as for the input ellipse.
4. The fixed points only occur when the semi-axes are aligned with the coordinate axes. For a given ellipse, this can happen two ways.
5. If the large semi-axis is aligned with the $x$-axis, then this fixed point is stable.
6. If the large semi-axis is aligned with the $y$-axis, then this fixed point is unstable. Being close to this fixed point is undesirable, because 1 iteration moves you away from it, into the direction of the other fixed point. The
closer you are to the unstable fixed point, the more slowly you move away from it.

7. The rotation of the ellipse gets slower the closer it is to being a circle. This presents unsolvable difficulties for finding eigenvectors in general as opposed to eigenvalues.

8. Opposite to point 7, the rotation of the ellipse gets faster the closer it is to being a degenerate line segment. This can be harnessed to speed up the algorithm.

9. If the ellipse $M$ gets scaled to $M' = \lambda M$, then the angle of rotation remains the same.

10. The input ellipse is congruent (in the sense of Euclidean geometry and not of linear algebra) to the output ellipse.

Observation 7 has profound origins. It is a consequence of eigenvector instability. When the geometric multiplicity of some eigenvalue $\lambda$ of a matrix $M$ is 2 or more, then an infinitesimal perturbation of $M$ can violently change the eigenspaces. Therefore, the slowness of rotation in the near-circular case is a manifestation of an unsolvable difficulty which is intrinsic to the eigendecomposition problem. Changing to a different algorithm won’t make it go away.

Further discussion of observation 7 requires us to know what a nearly diagonal matrix looks like in the ellipse model:

i. A near-circle.

ii. An ellipse whose semi-axes are nearly coordinate-axis aligned.

These two scenarios (i and ii) have little overlap. We can find eigenvalues in both scenarios (because of the Gershgorin circle theorem), but not eigenvectors, for which we require scenario ii. The eigenvector problem is uncomputable in general.

This uncomputability is perhaps not a “big deal”. It often suffices to find the eigendecomposition of a matrix close by to the input matrix, even though this may violently change the eigenspaces. A discussion of why this can ever be acceptable is left to a footnote.\footnote{To understand why, we recall the distinction between forwards numerical stability and backwards numerical stability, and the difference in applications of each. An algorithm $\hat{f}$ for computing a function $f$ is forwards-stable if $\hat{f}(x) \approx f(x)$ for all $x$. An algorithm $\tilde{f}$ for computing a function $f$ is backwards stable if given $x$ there is an $\tilde{x} \approx x$ such that $\tilde{f}(x) \approx f(\tilde{x})$. Clearly, forwards stability is desirable, but we’ve shown that for the eigendecomposition problem it is unattainable. Backwards stability remains attainable, but what’s the point of it? We explain. Let $f: \mathbb{R} \rightarrow \mathbb{R}$ be some continuous function. Eigendecomposition enables us to extend $f$ to the set of PSD matrices by assuming that $f(PP^{-1}) = Pf(D)P^{-1}$ is true. We can only compute eigendecompositions in a backwards stable way, which means that we can make $M \approx PDP^{-1}$ true but not $M = PDP^{-1}$. This is fine though, because by the continuity of $f$ we have that $f(M) \approx Pf(D)P^{-1}$, so the approximation error from computing $f$ via the eigendecomposition of $M$ can be made negligible. Be careful though, because while...}
The fix for observation 6 is to make the function being iterated discontinuous. This is obvious in 2 dimensions thanks to the visualisation, but it is also true in all dimensions. A more general version of this is the statement of theorem 1. A continuous choice of function \( f \) might be nicer, but continuity can’t hold everywhere.

Observation 8 appears to be a (kind of) converse to observation 7, but it’s difficult to verify under what conditions an iterative eigenvalue algorithm behaves this way. In the case of the QR and LR algorithms, this behaviour may be directly verified, but it would be interesting to demonstrate that it is true for a large class of other algorithms.

Table 2: 3 × 3 PSD matrices. Observe that when pancakes, the ellipsoid aligns 1 semi-axis in 1 iteration.

Observation 8 can be combined with observation 9 to motivate shifting, and to demonstrate the limits of shifting and how they may be bypassed through the use of deflation. Shifting is the map \( M' = M + \mu I \) for some arbitrary \( \mu \in \mathbb{R} \). The effect this has is to increase the lengths of all the semi-axes by \( \mu \). To better understand this effect, we exploit observation 9 to scale down the ellipse so that its largest semi-axis has length exactly equal to 1. We then observe that the effect of shifting is that it either fattens or thins the ellipse. The fattest case is a perfect circle, which by observation 7 is the worst-case scenario. The thinnest case is a line segment, for which convergence is instant. In higher dimensions, the extreme cases are flat pancakes or perfect hyperspheres. Therefore, shifting is pancaking! Pancakes are, of course, the best; and blobs are, of course, the worst. But once you’ve got a perfect pancake, shifting runs out of steam as a speeding-up technique, so we may employ deflation to destroy the dimension of the ellipsoid that has been reduced to 0, so that we may pancake the remaining dimensions, and rekindle the speed-up.

The above analysis of observation 8 shows that iterative eigenvalue algorithms \( D \) may be close to the eigenvalue matrix of \( M \) (because eigenspectra vary continuously) the same is not true for \( P \), which may be far from any true eigenvector matrix of \( M \).

\(^5\) For the sake of conceptual understanding, the function \( f \) may be engineered to be continuous over a subspace of its domain over which it has a globally attractive fixed point, while the discontinuities outside of this subspace may serve to “kick” the input into the well-behaved subspace. The Wilkinson shift happens to be discontinuous, so it provides the needed discontinuities.
in which observation 8 holds can be used as improvers of cruder but faster eigenvalue estimation technique. If an eigenvalue estimation technique can crudely estimate the smallest eigenvalue, then this can be used as the value of the shift $\mu$, which can be used then to pancake the ellipsoid effectively, and which in turn will accelerate the iterative eigenvalue algorithm, and which may in turn make the crude estimation technique more accurate in subsequent iterations, and so on.

3 Account of generalisation to $n$ dimensions

It may not be obvious that the conclusions generalise straightforwardly to PSD matrices in $n$ dimensions, but they do:

- The algorithm converges for all PSD matrices.
- The stable fixed points are precisely the diagonal matrices of the form $\text{diag}(\lambda_n, \lambda_{n-1}, \ldots, \lambda_1)$ where all the $\lambda_i$'s are non-negative reals, and $\lambda_n \geq \lambda_{n-1} \geq \ldots \geq \lambda_1$. The other diagonal matrices are unstable fixed points, with convergence slowing down the smaller the angle an ellipsoid makes with them.
- The output of each iteration is orthogonally similar (as a matrix) to its input. In terms of Euclidean geometry, it is a congruent ellipsoid. (Be aware that “congruence” in Euclidean geometry means something different from in linear algebra).
- At eigenvalue clashes, the eigenvectors are unstable, but the algorithm may still converge quickly to a nearly diagonal matrix. In which case, only the eigenvalues and not the eigenvectors may be obtained under such circumstances.
- Shifting can be understood as “pancaking” the ellipsoid (once the semi-axes are scaled so that the largest semi-axis has length 1). Like in the 2D case, this speeds up convergence.
- Deflation can be thought of as continuing the “pancaking” (shifting) once one of the semi-axes has been fully pancaked.

These conclusions can be checked by doing the ellipsoid visualisation in 3 dimensions. But this isn’t necessary, as the 2D case is suggestive enough.

4 Remark about the dual purpose of Wilkinson shifts, and the search for better shifting strategies

Wilkinson shifts are curiously enough not continuous. Wilkinson shifts appear to both “kick” the ellipsoid away from the unstable fixed point (if it’s too close to
it) and to “pancake” the ellipsoid. Both of these features speed up convergence. One might wonder though if these two properties: The kicking away from the unstable fixed point, and the pancaking of the ellipsoid, can be achieved separately. In particular, the shift $\mu$ can perhaps be made into a continuous function, with it serving only to “pancake” the ellipsoid. This might simplify the search for superior shifting strategies if we can narrow the search down to only continuous functions, with the discontinuity needed to do the “kicking” from the fixed point coming from elsewhere.

5 Axiomatic development of the theory of iterative eigenvalue algorithms

One advantage of the visualisation is that it is mostly qualitative. In particular, we see that the LR algorithm exhibits the same qualitative behaviour as the QR algorithm. We exploit this to show that much of the behaviour and theory of the QR algorithm is not caused by the QR decomposition as such, but is intrinsic to solving the eigenvalue estimation problem by the use of fixed-point iteration.

Consider the following axioms for a fixed-point iteration algorithm:

1. It consists of iterating some function $f$ over PSD matrices.
2. $f(M)$ is orthogonally similar to $M$.
3. The sequence $(f^n(M))_{n \in \mathbb{N}}$ converges for every $M$. It furthermore converges to a fixed point of $f$.
4. A fixed point can only be a diagonal matrix.
5. All fixed points are attractive. (This makes convergence fast).

We consider these 5 axioms to be highly desirable. Intriguingly, these rule out the possibility that $f$ can be continuous everywhere. This is the statement of theorem 1. Morally, the theorem holds because given a non-scalar matrix $M$, the topological space of matrices orthogonally similar to $M$ is connected, but has some “holes” in it. The influence these “holes” have is that they prevent axioms 1 to 5 being realised when $f$ is continuous, even though these 5 conditions are highly desirable. A work-around might be to make $f$ continuous over some neighbourhood of each fixed point, and use the discontinuity of $f$ outside these neighbours to make $f(x)$ only map into these neighbourhoods.

**Theorem 1** Assuming axioms 1 to 5, the function $f$ being iterated must have discontinuities in the set of PSD matrices.

**Proof** We restrict the domain and codomain of $f$ to the set of matrices orthogonally similar to some PSD matrix $M$, where $M$ is not a multiple of the identity matrix. The fact that we can do this follows from condition 2. We show that $f$ has at least two fixed points under continuity: Assume it
only has one fixed point $x$. It must be attractive by condition 5. By condition 3, all points attract to $x$. This results in the space of matrices orthogonally similar to $M$ being a contractible space, which it isn’t. We get a contradiction. Therefore $f$ has at least two fixed points orthogonally similar to $M$.

**Now we show that under continuity, one of these two fixed points is not attractive, which contradicts conditions 3 and 5.** The space of matrices orthogonally similar to some arbitrary matrix $M$ is connected. The set of points which attract to some attractive fixed point is always open. The basins of attraction of the attractive fixed points are disjoint, so by topological connectivity there are points not in their union, which are the points which don’t attract to an attractive fixed point. This contradicts conditions 3 and 5.

\[\square\]

6 Future work regarding visualisations

We ask the following questions. Forgive us if some happen to be easy:

- Can a visualisation technique for iterative eigenvalue algorithms be developed for non-symmetric matrices? The dynamics of the QR algorithm in the case of non-symmetric matrices (especially featuring shift policies) is not as well understood as in the symmetric case \[1\].

- Can a visualisation technique help to better understand Hessenberg matrices and their uses for finding eigenvalues and eigenvectors? We haven’t succeeded yet in producing anything useful for this. Even symmetric Hessenberg matrices would be interesting.

It’s important that visualisations be legible. Whether a visualisation is legible or not is perhaps subjective.

7 Novelty

We first put a visualisation of the QR algorithm onto the Wikipedia page on the QR algorithm on August 2021. We did so under a pseudonym. Afterwards, we left it for some time. We then later presented some of the material in this paper in a Youtube video series \[3\], also under a pseudonym. Based on a private correspondence with Professor David Watkins \[5\] (who has written numerous pedagogical papers on iterative eigenvalue algorithms like the QR algorithm \[6, 7\]) the presentation is likely a novel one. The emphasis is likely novel. Videos and lectures are an important accompaniment when trying to present material like the one here.
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