Computing Matrix Eigenvalues

Recall the master-plan we have for computing all the eigenpairs of a given symmetric matrix A

$$\underbrace{A \xrightarrow[\text{Direct Method}]{\text{Similarity Transform}} \text{Tridiagonal}}_{\text{Phase I}} \Big| \underbrace{\xrightarrow[\text{Iterative}]{\text{Similarity Transform}} \text{Diagonal}}_{\text{Phase II}}$$

- To do both Phases, we need a technique for similarity transforming a matrix to a reduced form with many zeros.

- The technique we will use is called <u>Householder reflections</u>

- We will also see how this technique can be used to decompose a matrix into a form known as QR where Q is an orthogonal matrix and R is upper-triangular. Called the <u>QR decomposition</u> of A and is different than the QR algorithm.

- <u>Householder Reflections</u>:

- <u>Central Purpose</u>: Given vectors $x, y \in \mathbb{R}^n$, find a matrix $H \in \mathbb{R}^{n\times n}$ s.t. $Hx = y$.
If we require $x^T x = y^T y$ then by letting $w = \dfrac{y-x}{\|y-x\|_2}$ and

$H = I - 2ww^T$ we find (which you need to show) that

$$Hx = y.$$

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- Why is this important to our goal of introducing zeros into the matrix A?

Consider $A = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{bmatrix}$

Now let $x = \begin{bmatrix} a_{11} \\ a_{21} \\ \vdots \\ a_{n1} \end{bmatrix}$ & $y = \begin{bmatrix} \pm\|x\|_2 \\ 0 \\ \vdots \\ 0 \end{bmatrix}$

Then $x^T x = y^T y$.

So, we can form H from $w = \dfrac{y-x}{\|y-x\|_2}$, and thus obtain

$$\begin{bmatrix} & & \\ & H & \\ & & \end{bmatrix} \begin{bmatrix} x & & A & \end{bmatrix} = \left[\begin{array}{c|ccc} \pm\|x\| & a_{12}^{(2)} & \cdots & a_{1n}^{(2)} \\ 0 & a_{22}^{(2)} & \cdots & a_{2n}^{(2)} \\ \vdots & \vdots & & \vdots \\ 0 & a_{n2}^{(2)} & \cdots & a_{nn}^{(2)} \end{array}\right] = A^{(2)}$$

We choose the sign so that $y-x$ cannot cancel digits in the first component. This leads to a more stable method

i.e. if $x_1 < 0$ choose pl
if $x_1 > 0$ " min

Call $H = H^{(1)} = \tilde{H}^{(1)}$ & $x = x^{(1)}$ & $y = y^{(1)}$ &

Now, let $x^{(2)} = \begin{bmatrix} a_{22}^{(2)} \\ a_{32}^{(2)} \\ \vdots \\ a_{n2}^{(2)} \end{bmatrix}$ & $y^{(2)} = \begin{bmatrix} \pm\|x^{(2)}\| \\ 0 \\ \vdots \\ 0 \end{bmatrix}$ (Note these $x^{(2)}, y^{(2)} \in \mathbb{R}^{n-1}$)

Again, choose appropriately.

Then again form $\tilde{H}^{(2)}$ from $w^{(2)} = \dfrac{y^{(2)} - x^{(2)}}{\|y^{(2)} - x^{(2)}\|_2}$ and thus obtain

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$$\underbrace{\begin{bmatrix} 1 & 0 & \cdots & 0 \\ 0 & & & \\ \vdots & & \tilde{H}^{(2)} & \\ 0 & & & \end{bmatrix}}_{H^{(2)}} \begin{bmatrix} & & \\ & A^{(2)} & \\ & & \end{bmatrix} = \begin{bmatrix} \pm\|x^{(1)}\| & a_{12}^{(2)} & a_{13}^{(2)} & \cdots & a_{1n}^{(2)} \\ 0 & \pm\|x^{(2)}\| & a_{23}^{(3)} & \cdots & a_{2n}^{(3)} \\ 0 & 0 & \vdots & & \\ \vdots & \vdots & \vdots & & \\ & & a_{n3}^{(3)} & & a_{nn}^{(3)} \end{bmatrix} = A^{(3)}$$

Repeat this process for the 3^{rd} column of $A^{(3)}$, 4^{th} column of $A^{(4)}$, etc.

Note that at each step the vector size shrinks by 1 and thus so does the # rows & columns in $\tilde{H}^{(k)}$.

To summarize, after n steps we will have

$$H^{(n)}H^{(n-1)}\cdots H^{(1)}A = \begin{bmatrix} \pm\|x^{(1)}\|_2 & a_{12}^{(2)} & a_{13}^{(2)} & \cdots & a_{1n}^{(2)} \\ & \pm\|x^{(2)}\|_2 & a_{23}^{(3)} & \cdots & a_{2n}^{(3)} \\ & & \pm\|x^{(3)}\|_2 & a_{34}^{(4)} \cdots & a_{3n}^{(4)} \\ & 0 & & \ddots & \vdots \\ & & & & a_{n-1,n}^{(n)} \\ & & & & \pm\|x^{(n)}\|_2 \end{bmatrix}$$

- As you will show on your homework Householder matrices are both orthogonal and symmetric. Thus letting

$$Q^T = H^{(n)}H^{(n-1)}\cdots H^{(1)}$$ (Product of orthogonal matrices as orthogonal)

- We have a <u>QR decomposition</u> of A as

$$A = QR$$

- Note that we never actually form H, since $H = I - 2ww^T$ and HA would cost $O(n^3)$ operations whereas $(I-2ww^T)H = A - \underbrace{2w\underbrace{w^TA}_{O(n^2)}}_{O(n^2)} \sim O(n^2)$

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- While we have constructed a method for computing the QR decomposition of a square matrix A, it turns out this idea can also be extended to when A is not square.
- The QR decomposition plays a major role in solving underdetermined or overdetermined linear systems as we will soon find out.

- Now back to the task at hand: Reducing a symmetric A to tridiagonal form using similarity transforms.

- Recall that a similarity transform is given by

$$B^{-1}AB \quad \text{(Perserves eigenvalues of } A)$$

where B is some non-singular matrix.

- It is obviously beneficial to chose B to be orthogonal so that $B^{-1} = B^T$. Since we have just seen that Householder matrices can introduce zeros in a matrix and they are orthogonal (and symmetric!) let's see how to use these to do the tri-diagonal reduction.

Tridiagonal Reduction of a Symmetric Matrix.

Let $A \in \mathbb{R}^{n \times n}$ be symmetric, and define $A^{(1)} = A$.

$$A^{(1)} = \begin{bmatrix} a_{11}^{(1)} & a_{21}^{(1)} & a_{31}^{(1)} & \cdots & a_{n1}^{(1)} \\ a_{21}^{(1)} & a_{22}^{(1)} & a_{32}^{(1)} & & a_{n2}^{(1)} \\ a_{31}^{(1)} & a_{32}^{(1)} & & & \vdots \\ \vdots & & & \ddots & \\ a_{n1}^{(1)} & a_{n2}^{(1)} & \cdots & & a_{nn}^{(1)} \end{bmatrix}$$

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Consider the the vector formed by the first column of A without the entry in the first row.

$$\Rightarrow \quad z^{(1)} = \begin{bmatrix} a_{21}^{(1)} \\ a_{31}^{(1)} \\ \vdots \\ a_{n1}^{(1)} \end{bmatrix}$$

Let $\tilde{H}^{(1)}$ be the Householder reflection matrix designed for $z^{(1)}$ i.e.

$$\tilde{H}^{(1)} z^{(1)} = \begin{bmatrix} \pm\|z^{(1)}\|_2 \\ 0 \\ \vdots \\ 0 \end{bmatrix}$$

Now, consider the product

$$\underbrace{\begin{bmatrix} 1 & 0 & \cdots & 0 \\ 0 & & & \\ \vdots & & \tilde{H}^{(1)} & \\ 0 & & & \end{bmatrix}}_{H^{(1)}} \underbrace{\begin{bmatrix} & & \\ & A & \\ & & \end{bmatrix}}_{A} = \begin{bmatrix} a_{11}^{(1)} & a_{21}^{(1)} & \cdots & a_{n1}^{(1)} \\ \|z\|_2 & \times & & \times \\ 0 & \vdots & & \\ \vdots & \vdots & & \\ 0 & \times & & \times \end{bmatrix}$$

↑ nonzero number

Followed by the product $(H^{(1)}A)(H^{(1)})^T = (H^{(1)}A)H^{(1)}$

$$\begin{bmatrix} a_{11}^{(1)} & a_{21}^{(1)} & \cdots & & a_{n}^{(1)} \\ \|z^{(1)}\|_2 & \times & \times & \cdots & \times \\ 0 & \vdots & & & \\ \vdots & \vdots & & & \\ \vdots & \times & & & \times \end{bmatrix} \begin{bmatrix} 1 & 0 & \cdots & 0 \\ 0 & & & \\ \vdots & & \tilde{H}^{(1)} & \\ 0 & & & \end{bmatrix} = \underbrace{\begin{bmatrix} a_{11}^{(1)} & \|z^{(1)}\|_2 & 0 & \cdots & 0 \\ \|z^{(1)}\|_2 & \times & \times & & \times \\ 0 & \times & \cdots & & \vdots \\ \vdots & \vdots & & & \vdots \\ 0 & \times & \cdots & & \times \end{bmatrix}}_{A^{(2)}}$$

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- Note that ① $A^{(2)}$ is symmetric since

$$(A^{(2)})^T = (H^{(1)}A^{(1)}H^{(1)})^T = H^{(1)T}A^{(1)T}H^{(1)T} = H^{(1)}A^{(1)}H^{(1)} = A^{(2)}$$

and ② its eigenvalues are equivalent to $A^{(1)}$ since we have gotten $A^{(2)}$ from similarity transforming $A^{(1)}$.

$$\Rightarrow (H^{(1)})^{-1}A^{(1)}H^{(1)} = H^{(1)}A^{(1)}H^{(1)}.$$

and ③ It is one step closer to tridiagonal form.

Now, we can write $A^{(2)}$ as.

$$A^{(2)} = \begin{bmatrix} a_{11}^{(1)} & \|z^{(1)}\|_2 & 0 & \cdots & 0 \\ \|z^{(1)}\|_2 & a_{22}^{(2)} & a_{32}^{(2)} & \cdots & a_{n2}^{(2)} \\ 0 & a_{32}^{(2)} & x & & x \\ \vdots & \vdots & \vdots & & \vdots \\ 0 & a_{n2}^{(2)} & x & & x \end{bmatrix}.$$

Let $z^{(2)} = \begin{bmatrix} a_{22}^{(2)} \\ a_{32}^{(2)} \\ \vdots \\ a_{n2}^{(2)} \end{bmatrix}$ and form the Householder reflection matrix for $z^{(2)}$

$$\Rightarrow \check{H}^{(2)} z^{(2)} = \begin{bmatrix} \pm\|z^{(2)}\|_2 \\ 0 \\ \vdots \\ 0 \end{bmatrix}$$

Now consider the product

$$\underbrace{\begin{bmatrix} 1 & 0 & 0 & \cdots & 0 \\ 0 & 1 & 0 & \cdots & 0 \\ 0 & 0 & & & \\ \vdots & & & \check{H}^{(2)} & \\ 0 & 0 & & & \end{bmatrix}}_{H^{(2)}} \Bigg[\quad A^{(2)} \quad \Bigg] \underbrace{\begin{bmatrix} 1 & 0 & \cdots & & 0 \\ 0 & 1 & 0 & \cdots & 0 \\ 0 & 0 & & & \\ \vdots & \vdots & & \check{H}^{(2)} & \\ 0 & 0 & & & \end{bmatrix}}_{H^{(2)}}.$$

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- Because of the entries in the first and second column and row of $H^{(2)}$, the entries in the first and second column and row of $A^{(2)}$ are preserved and we obtain

$$H^{(2)} A^{(2)} H^{(2)} = \begin{bmatrix} a_{11}^{(1)} & \|z^{(1)}\|_2 & 0 & \cdots & & 0 \\ \|z^{(1)}\|_2 & a_{22}^{(2)} & \|z^{(2)}\|_2 & 0 & \cdots & 0 \\ 0 & \|z^{(2)}\|_2 & a_{33}^{(3)} & a_{43}^{(3)} & \cdots & a_{n3}^{(3)} \\ \vdots & 0 & a_{43}^{(3)} & x & \cdots & x \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & a_{n3}^{(3)} & x & \cdots & x \end{bmatrix} = A^{(3)}$$

Continuing this process of similarity transforming with a Householder matrix of one size smaller than the previous time.

We will have

$$\underbrace{H^{(n-1)} H^{(n-2)} \cdots H^{(1)}}_{H^T} \underbrace{A}_{A} \underbrace{H^{(1)} \cdots H^{(n-2)} H^{(n-1)}}_{H} = \begin{bmatrix} a_{11}^{(1)} & \|z^{(1)}\|_2 & 0 & & \\ \|z^{(1)}\|_2 & a_{22}^{(2)} & \|z^{(2)}\|_2 & & \Large 0 \\ 0 & \|z^{(2)}\|_2 & a_{33}^{(3)} & \ddots & \\ & 0 & \ddots & \ddots & \|z^{(n-1)}\|_2 \\ \Large 0 & & & \|z^{(n-1)}\|_2 & a_{nn}^{(n)} \end{bmatrix}$$

i.e a symmetric tridiagonal matrix with the same eigenvalues as A.

Note that the entries in the tridiagonal matrix may be positive or negative depending on how we form $\tilde{H}^{(k)}$.

- The total FLOP count for this reduction is $\sim \frac{4}{3} n^3$

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- Now, since A is symmetric we know by the Principal Axis theorem that it has a Schur decomposition

$$Q^T A Q = \mathrm{diag}(\lambda_j).$$

- An obvious question is why can't we simply use Householder reflections to make A diagonal instead of tridiagonal? Consider how we would do this. First, we would multiply A by $H^{(1)}$ so as to zero out all the entries but the first in the first column of A.

$$\Rightarrow \begin{bmatrix} & & \\ & H^{(1)} & \\ & & \end{bmatrix} \begin{bmatrix} & & \\ & A^{(1)} & \\ & & \end{bmatrix} = \begin{bmatrix} \|a^{(1)}\| & \boxed{x \; \cdots \; x} \\ 0 & x \; \cdots \; x \\ \vdots & \vdots \quad\quad \vdots \\ 0 & x \; \cdots \; x \end{bmatrix}$$

Now, when we multiply on the left by $H^{(1)}$ we should not expect zeros to be introduced into the first row since this first row is not equal to $a^{(1)}$. Furthermore, the zero entries in the first column will become non-zero.

Thus $H^{(1)} A^{(1)} H^{(1)}$ is still a full matrix.

- Comments on the non-symmetric case.

We proceed with a non-symmetric matrix exactly as we did for the symmetric case however now the result is not a tridiagonal matrix but an upper Hessenberg matrix.

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Non-Symmetric Case (Cont).

$$H^{(n-1)}H^{(n-2)}\cdots H^{(1)}AH^{(1)}\cdots H^{(n-2)}H^{(n-1)} = \begin{bmatrix} x & x & \cdots & & x \\ x & x & & & \vdots \\ 0 & x & \ddots & & \vdots \\ & & \ddots & \ddots & \vdots \\ & & & x & x \end{bmatrix}$$ (Upper Hessenberg)

Methods For Finding the Eigenvalues/Eigenvectors of Tridiagonal matrix.

- First, we never try to solve the characteristic equation even though it is easier to compute for this matrix.

Methods.

1) Strum sequences (Atkinson. p.621-623)
   - Never used
2) Rayleigh Quotient iteration
3) QR iteration
   - Essentially RQI but we simultaneously find the eigenvalues and eigenvectors.
   - Most widely used
   - Deflation is built in.
4) Divide-and-Conquer
   - Currently the fastest method when $n > 25$.
   - Very complicated method that is hard to implement stably. Discovered in 1981, but a stable implementation was not discovered until 1992

- Recall that we have reduced A to tridiagonal form by $H^TAH = \breve{A}$. Thus as we compute the eigenvalues of $\breve{A}$ we have to get back to the eigenvalues of A by the transformation

$$\breve{A}\breve{v} = \lambda\breve{v} \Rightarrow H^TAH\breve{v} = \lambda\breve{v} \Rightarrow Av = \lambda v \quad \text{where } v = H\breve{v}$$