Simultaneous *Inverse* Iteration $\iff$ QR Algorithm

- Last lecture we showed that “pure” QR $\iff$ simultaneous iteration applied to $I$, and the first column evolves as in power iteration.

- But it is also equivalent to simultaneous *inverse* iteration applied to a “flipped” $I$, and the last column evolves as in inverse iteration.

- To see this, recall that $A^k = Q^{(k)}R^{(k)}$ with

$$Q^{(k)} = \prod_{j=1}^{k} Q^{(j)} = \begin{bmatrix} q_1^{(k)} & q_2^{(k)} & \cdots & q_m^{(k)} \end{bmatrix}$$

- Invert and use that $A^{-1}$ is symmetric:

$$A^{-k} = (R^{(k)})^{-1}Q^{(k)T} = Q^{(k)}(R^{(k)})^{-T}$$
Simultaneous *Inverse* Iteration ⇐⇒ QR Algorithm

- Introduce the “flipping” permutation matrix

\[
P = \begin{bmatrix} 1 & \cdots & 1 \\ \vdots & & \vdots \\ 1 & & 1 \end{bmatrix}
\]

and rewrite that last expression as

\[
A^{-k} P = [Q^{(k)} P][P(R^{(k)})^{-T} P]
\]

- This is a QR factorization of $A^{-k} P$, and the algorithm is equivalent to simultaneous iteration on $A^{-1}$

- In particular, the last column of $Q^{(k)}$ evolves as in inverse iteration
The Shifted QR Algorithm

- Since the QR algorithm behaves like inverse iteration, introduce shifts $\mu^{(k)}$ to accelerate the convergence:

\[
A^{(k-1)} - \mu^{(k)} I = Q^{(k)} R^{(k)}
\]

\[
A^{(k)} = R^{(k)} Q^{(k)} + \mu^{(k)} I
\]

- We then get (same as before):

\[
A^{(k)} = (Q^{(k)})^T A^{(k-1)} Q^{(k)} = (\underline{Q}^{(k)})^T A \underline{Q}^{(k)}
\]

and (different from before):

\[
(A - \mu^{(k)} I)(A - \mu^{(k-1)} I) \cdots (A - \mu^{(1)} I) = \underline{Q}^{(k)} \underline{R}^{(k)}
\]

- Shifted simultaneous iteration – last column of $\underline{Q}^{(k)}$ converges quickly
Choosing $\mu^{(k)}$: The Rayleigh Quotient Shift

- Natural choice of $\mu^{(k)}$: Rayleigh quotient for last column of $Q^{(k)}$

\[
\mu^{(k)} = \frac{(q_m^{(k)})^T A q_m^{(k)}}{(q_m^{(k)})^T q_m^{(k)}} = (q_m^{(k)})^T A q_m^{(k)}
\]

- Rayleigh quotient iteration, last column $q_m^{(k)}$ converges cubically

- Convenient fact: This Rayleigh quotient appears as $m, m$ entry of $A^{(k)}$
  since $A^{(k)} = (Q^{(k)})^T A Q^{(k)}$

- The Rayleigh quotient shift corresponds to setting $\mu^{(k)} = A_{mm}^{(k)}$
Choosing $\mu^{(k)}$: The Wilkinson Shift

- The QR algorithm with Rayleigh quotient shift might fail, e.g. with two symmetric eigenvalues

- Break symmetry by the *Wilkinson shift*

\[ \mu = a_m - \text{sign}(\delta) b_{m-1}^2 \left/ \left( |\delta| + \sqrt{\delta^2 + b_{m-1}^2} \right) \right. \]

where $\delta = (a_{m-1} - a_m) / 2$ and $B = \begin{bmatrix} a_{m-1} & b_{m-1} \\ b_{m-1} & a_m \end{bmatrix}$ is the lower-right submatrix of $A^{(k)}$

- Always convergence with this shift, in worst case quadratically
A Practical Shifted QR Algorithm

Algorithm: “Practical” QR Algorithm

\[
(Q^{(0)})^T A^{(0)} Q^{(0)} = A
\]

for \(k = 1, 2, \ldots\)

Pick a shift \(\mu^{(k)}\) e.g., choose \(\mu^{(k)} = A^{(k-1)}_{mm}\)

\[
Q^{(k)} R^{(k)} = A^{(k-1)} - \mu^{(k)} I
\]

QR factorization of \(A^{(k-1)} - \mu^{(k)} I\)

\[
A^{(k)} = R^{(k)} Q^{(k)} + \mu^{(k)} I
\]

Recombine factors in reverse order

If any off-diagonal element \(A^{(k)}_{j,j+1}\) is sufficiently close to zero,

set \(A_{j,j+1} = A_{j+1,j} = 0\) to obtain

\[
\begin{bmatrix}
A_1 & 0 \\
0 & A_2
\end{bmatrix}
= A^{(k)}
\]

and now apply the QR algorithm to \(A_1\) and \(A_2\)
Stability and Accuracy

• The QR algorithm is backward stable:

\[
\tilde{Q}\tilde{\Lambda}\tilde{Q}^T = A + \delta A, \quad \frac{\|\delta A\|}{\|A\|} = O(\epsilon_{\text{machine}})
\]

where \(\tilde{\Lambda}\) is the computed \(\Lambda\) and \(\tilde{Q}\) is an exactly orthogonal matrix.

• The combination with Hessenberg reduction is also backward stable.

• Can be shown (for normal matrices) that \(|\tilde{\lambda}_j - \lambda_j| \leq \|\delta A\|_2\), which gives

\[
\frac{|\tilde{\lambda}_j - \lambda_j|}{\|A\|} = O(\epsilon_{\text{machine}})
\]

where \(\tilde{\lambda}_j\) are the computed eigenvalues.
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