Faddeev Leverrier Method

- ✓ Recall: eigenvalues are the roots of the *characteristic polynomial* given by, $\det(\boldsymbol{A} - \lambda\boldsymbol{I}) = 0$
- ✓ For an $n \times n$ matrix, the polynomial is of the order n
- ✓ This method is an algorithm to obtain the coefficients of the characteristic polynomial:

$$(-1)^n(\lambda^n - a_{n-1}\lambda^{n-1} - \cdots - a_2\lambda^2 - a_1\lambda - a_0) = 0$$

- ✓ Algorithm:
  - ✓ Initialize: $\boldsymbol{A}_{n-1} = \boldsymbol{A}$; $a_{n-1} = \text{trace}\ (\boldsymbol{A}_{n-1})$
  - ✓ $\boldsymbol{A}_i = \boldsymbol{A}(\boldsymbol{A}_{i+1} - a_{i+1}\boldsymbol{I})$; $a_i = \frac{\text{trace}(\boldsymbol{A}_i)}{n-i}$
  - ✓ $i = (n-2), (n-3), \ldots 2, 1, 0.$
- ✓ Compute the roots of the polynomial using *Mueller's* or *Bairstow's* algorithm for the eigenvalues

Faddeev Leverrier Method: Example

$$A = \begin{bmatrix} 2 & -1 & 0 & 0 \\ -1 & 4 & -1 & 0 \\ 0 & -1 & 4 & -1 \\ 0 & 0 & -1 & 2 \end{bmatrix}$$

Characteristic polynomial:

$$(-1)^4(\lambda^4 - a_3\lambda^3 - a_2\lambda^2 - a_1\lambda - a_0) = 0$$

Initialize: $A_3 = A;\ a_3 = \text{trace}\,(A_3) = 12$

$$A_2 = A(A_3 - a_3 I)$$

$$(A_3 - a_3 I) = \begin{bmatrix} -10 & -1 & 0 & 0 \\ -1 & -8 & -1 & 0 \\ 0 & -1 & -8 & -1 \\ 0 & 0 & -1 & -10 \end{bmatrix}; \qquad A_2 = \begin{bmatrix} -19 & 6 & 1 & 0 \\ 6 & -30 & 4 & 1 \\ 1 & 4 & -30 & 6 \\ 0 & 1 & 6 & -19 \end{bmatrix}$$

$$a_2 = \frac{\text{trace}(A_2)}{4-2} = \frac{-98}{2} = -49$$

Faddeev Leverrier Method: Example

$$A_1 = A(A_2 - a_2 I)$$

$$(A_2 - a_2 I) = \begin{bmatrix} 30 & 6 & 1 & 0 \\ 6 & 19 & 4 & 1 \\ 1 & 4 & 19 & 6 \\ 0 & 1 & 6 & 30 \end{bmatrix}; \qquad A_1 = \begin{bmatrix} 54 & -7 & -2 & -1 \\ -7 & 66 & -4 & -2 \\ -2 & -4 & 66 & -7 \\ -1 & -2 & -7 & 54 \end{bmatrix}$$

$$a_1 = \frac{\mathrm{trace}(A_1)}{4-1} = \frac{240}{3} = 80$$

$$A_0 = A(A_1 - a_1 I)$$

$$(A_1 - a_1 I) = \begin{bmatrix} -26 & -7 & -2 & -1 \\ -7 & -14 & -4 & -2 \\ -2 & -4 & -14 & -7 \\ -1 & -2 & -7 & -14 \end{bmatrix}; \quad A_0 = \begin{bmatrix} -45 & 0 & 0 & 0 \\ 0 & -45 & 0 & 0 \\ 0 & 0 & -45 & 0 \\ 0 & 0 & 0 & -45 \end{bmatrix}$$

$$a_0 = \frac{\mathrm{trace}(A_0)}{4-0} = \frac{-180}{4} = -45$$

$$\lambda^4 - 12\lambda^3 + 49\lambda^2 - 80\lambda + 45 = 0$$

Similarity Transformation

- ✓ Two $n \times n$ matrices $\boldsymbol{A}$ and $\boldsymbol{B}$ are similar if there exists another $n \times n$ invertible matrix $\boldsymbol{S}$ such that $\boldsymbol{A} = \boldsymbol{SBS}^{-1}$ or $\boldsymbol{B} = \boldsymbol{S}^{-1}\boldsymbol{AS}$
- ✓ The process of obtaining the similar matrix $\boldsymbol{B}$ from matrix $\boldsymbol{A}$ using the relation $\boldsymbol{B} = \boldsymbol{S}^{-1}\boldsymbol{AS}$ is called *similarity transformation*!
- ✓ Similar matrices have the same eigenvalues!
- ✓ Some matrices can be diagonalized using similarity transformation
  - ✓ $\boldsymbol{A} = \boldsymbol{X\Lambda X}^{-1}$; where $\boldsymbol{\Lambda}$ is a diagonal matrix containing eigenvalues and $\boldsymbol{X}$ is a square matrix containing eigenvectors in the columns $\boldsymbol{AX} = \boldsymbol{X\Lambda}$

$$[\boldsymbol{Ax_1} \quad \boldsymbol{Ax_2} \quad \dots \quad \boldsymbol{Ax_n}] = [\lambda_1\boldsymbol{x_1} \quad \lambda_2\boldsymbol{x_2} \quad \dots \quad \lambda_n\boldsymbol{x_n}]$$

Computation of Eigenvalues

- ✓ Recall: What is an orthogonal matrix?
  - ✓ Each column vector is *orthonormal* to each other
  - ✓ $\boldsymbol{Q}^{\mathrm{T}}\boldsymbol{Q} = \boldsymbol{I}$ or $\boldsymbol{Q}^{\mathrm{T}} = \boldsymbol{Q}^{-1}$
- ✓ A $n \times n$ matrix is *non-defective* if it has n independent eigenvectors (rank n, non-zero determinant, inverse exists, etc.)
- ✓ For every *non-defective* real matrix $\boldsymbol{A}$ with real eigenvalues, there is an orthogonal matrix $\boldsymbol{Q}$ and an upper-triangular matrix $\boldsymbol{U}$ such that $\boldsymbol{A} = \boldsymbol{QUQ}^{\mathrm{T}}$
- ✓ If $\boldsymbol{A}$ is complex, $\boldsymbol{Q}$ is unitary such that $\boldsymbol{A} = \boldsymbol{QUQ}^{\mathrm{H}}$
- ✓ Therefore, $\boldsymbol{A}$ and $\boldsymbol{U}$ are similar matrices, $\boldsymbol{A} = \boldsymbol{QUQ}^{\mathrm{T}}$
- ✓ The upper triangular matrix $\boldsymbol{U}$ contains the eigenvalues of $\boldsymbol{A}$ on its diagonal.

Computation of Eigenvalues

- ✓ All *non-defective* matrices are similar to upper triangular matrices
- ✓ $\boldsymbol{A} = \boldsymbol{QUQ}^{\mathrm{T}}$ or $\boldsymbol{U} = \boldsymbol{Q}^{\mathrm{T}}\boldsymbol{AQ}$, $\boldsymbol{U}$ contains the eigenvalues of $\boldsymbol{A}$ on its diagonal.
- ✓ Therefore, a non-defective matrix $\boldsymbol{A}$ can be transformed to an upper-triangular matrix $\boldsymbol{U}$ through *similarity transformation* and the diagonal elements of $\boldsymbol{U}$ will be the eigenvalues.
- ✓ This transformation cannot be achieved in one step. It is achieved through a sequence of *similarity transformation* using *QR-decomposition*!

Computation of Eigenvalues

- ✓ QR-decomposition: A *non-defective* matrix $\boldsymbol{A}$ can be decomposed into an orthogonal matrix $\boldsymbol{Q}$ and an upper-triangular matrix $\boldsymbol{R}$ such that $\boldsymbol{A} = \boldsymbol{QR}$
- ✓ A sequence of matrix is generated through *similarity transformation* as follows:
  - ✓ Initialize: $\boldsymbol{A_0} = \boldsymbol{A}$
  - ✓ QR-Decomposition: $\boldsymbol{A_k} = \boldsymbol{Q_k R_k}$
  - ✓ Similarity Transformation:

$$\boldsymbol{A_{k+1}} = \boldsymbol{Q_k}^{\mathrm{T}} \boldsymbol{A Q_k} = \boldsymbol{Q_k}^{\mathrm{T}} \boldsymbol{Q_k R_k Q_k} = \boldsymbol{R_k Q_k}$$

- ✓ Stopping criteria: $\max_j \left| \frac{\lambda_j^{k+1} - \lambda_j^k}{\lambda_j^k} \right| \leq \varepsilon$
- ✓ How to perform QR-decomposition?
  - ✓ Detailed process: proof by induction, inefficient computation
  - ✓ Gram-Schmidt Orthogonalization: efficient computation

QR-Decomposition

- ✓ We seek a decomposition of the form: $\boldsymbol{A} = \boldsymbol{QR}$

$$
\begin{array}{cccccc}
\boldsymbol{a}^{(1)} & \boldsymbol{a}^{(2)} & & \boldsymbol{a}^{(j)} & & \boldsymbol{a}^{(n)} \\
\end{array}
$$

$$
\begin{bmatrix}
a_{11} & a_{12} & \dots & a_{1j} & \dots & a_{1n} \\
a_{21} & a_{22} & \dots & a_{2j} & \dots & a_{2n} \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
a_{i1} & a_{i2} & \dots & a_{ij} & \dots & a_{in} \\
\vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\
a_{n1} & a_{n2} & \dots & a_{nj} & \dots & a_{nn}
\end{bmatrix}
$$

$$
\begin{array}{cccccc}
\boldsymbol{q}^{(1)} & \boldsymbol{q}^{(2)} & & \boldsymbol{q}^{(j)} & & \boldsymbol{q}^{(n)} \\
\end{array}
\quad
\begin{array}{cccccc}
\boldsymbol{r}^{(1)} & \boldsymbol{r}^{(2)} & & \boldsymbol{r}^{(j)} & & \boldsymbol{r}^{(n)} \\
\end{array}
$$

$$
= \begin{bmatrix}
q_{11} & q_{12} & \dots & q_{1j} & \dots & q_{1n} \\
q_{21} & q_{22} & \dots & q_{2j} & \dots & q_{2n} \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
q_{i1} & q_{i2} & \dots & q_{ij} & \dots & q_{in} \\
\vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\
q_{n1} & q_{n2} & \dots & q_{nj} & \dots & q_{nn}
\end{bmatrix}
\begin{bmatrix}
r_{11} & r_{12} & \dots & r_{1j} & \dots & r_{1n} \\
0 & r_{22} & \dots & r_{2j} & \dots & r_{2n} \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
0 & 0 & \dots & r_{jj} & \dots & r_{in} \\
\vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\
0 & 0 & \dots & 0 & \dots & r_{nn}
\end{bmatrix}
$$

- ✓ Denote: $\boldsymbol{a}^{(k)}$, $\boldsymbol{q}^{(k)}$ and $\boldsymbol{r}^{(k)}$ as the k^{th} column vectors of matrices $\boldsymbol{A}$, $\boldsymbol{Q}$ and $\boldsymbol{R}$

QR-Decomposition: proof by induction

- ✓ $k = 1$: $\boldsymbol{a}^{(1)} = \boldsymbol{Q}\boldsymbol{r}^{(1)} = r_{11}\boldsymbol{q}^{(1)}$
  - ✓ $\boldsymbol{Q}$ is orthogonal: $\|\boldsymbol{q}^{(1)}\|_2 = 1$
  - ✓ $\|\boldsymbol{a}^{(1)}\|_2 = |r_{11}|\|\boldsymbol{q}^{(1)}\|_2 = r_{11}$
  - ✓ $\boldsymbol{q}^{(1)} = (1/\, r_{11})\boldsymbol{a}^{(1)}$

- ✓ $k = 2$: $\boldsymbol{a}^{(2)} = \boldsymbol{Q}\boldsymbol{r}^{(2)} = r_{12}\boldsymbol{q}^{(1)} + r_{22}\boldsymbol{q}^{(2)}$
  - ✓ $\boldsymbol{Q}$ is orthogonal: $\boldsymbol{q}^{(1)T}\boldsymbol{a}^{(2)} = r_{12}\boldsymbol{q}^{(1)T}\boldsymbol{q}^{(1)} + r_{22}\boldsymbol{q}^{(1)T}\boldsymbol{q}^{(2)} = r_{12}$
  - ✓ Also: $\|\boldsymbol{a}^{(2)} - r_{12}\boldsymbol{q}^{(1)}\|_2 = |r_{22}|\|\boldsymbol{q}^{(2)}\|_2 = r_{22}$
  - ✓ $\boldsymbol{q}^{(2)} = (1/\, r_{22})(\boldsymbol{a}^{(2)} - r_{12}\boldsymbol{q}^{(1)})$

QR-Decomposition: proof by induction

- ✓ $k = 1$: $\boldsymbol{a}^{(1)} = \boldsymbol{Q}\boldsymbol{r}^{(1)} = r_{11}\boldsymbol{q}^{(1)}$
  - ✓ $\boldsymbol{Q}$ is orthogonal: $\left\|\boldsymbol{q}^{(1)}\right\|_2 = 1$
  - ✓ $\left\|\boldsymbol{a}^{(1)}\right\|_2 = |r_{11}|\left\|\boldsymbol{q}^{(1)}\right\|_2 = r_{11}$
  - ✓ $\boldsymbol{q}^{(1)} = (1/\, r_{11})\boldsymbol{a}^{(1)}$

- ✓ $k = 2$: $\boldsymbol{a}^{(2)} = \boldsymbol{Q}\boldsymbol{r}^{(2)} = r_{12}\boldsymbol{q}^{(1)} + r_{22}\boldsymbol{q}^{(2)}$
  - ✓ $\boldsymbol{Q}$ is orthogonal: $\boldsymbol{q}^{(1)T}\boldsymbol{a}^{(2)} = r_{12}\boldsymbol{q}^{(1)T}\boldsymbol{q}^{(1)} + r_{22}\boldsymbol{q}^{(1)T}\boldsymbol{q}^{(2)} = r_{12}$
  - ✓ Also: $\left\|\boldsymbol{a}^{(2)} - r_{12}\boldsymbol{q}^{(1)}\right\|_2 = |r_{22}|\left\|\boldsymbol{q}^{(2)}\right\|_2 = r_{22}$
  - ✓ $\boldsymbol{q}^{(2)} = (1/\, r_{22})(\boldsymbol{a}^{(2)} - r_{12}\boldsymbol{q}^{(1)})$

- ✓ k^{th} step: $\boldsymbol{a}^{(k)} = \boldsymbol{Q}\boldsymbol{r}^{(k)} = r_{1k}\boldsymbol{q}^{(1)} + r_{2k}\boldsymbol{q}^{(2)} \ldots + r_{kk}\boldsymbol{q}^{(k)}$
  - ✓ $\boldsymbol{Q}$ is orthogonal: $\boldsymbol{q}^{(i)T}\boldsymbol{a}^{(k)} = r_{1k}\boldsymbol{q}^{(i)T}\boldsymbol{q}^{(1)} + r_{2k}\boldsymbol{q}^{(i)T}\boldsymbol{q}^{(2)} \ldots + r_{kk}\boldsymbol{q}^{(i)T}\boldsymbol{q}^{(k)} = r_{ik}$

    for $i = 1, 2, \ldots (k\text{-}1)$
  - ✓ Also: $\left\|\boldsymbol{a}^{(2)} - r_{1k}\boldsymbol{q}^{(1)} - r_{2k}\boldsymbol{q}^{(2)} \ldots - r_{k-1,k}\boldsymbol{q}^{(k-1)}\right\|_2 =$

    $|r_{kk}|\left\|\boldsymbol{q}^{(k)}\right\|_2 = r_{kk}$
  - ✓ $\boldsymbol{q}^{(k)} = (1/\, r_{kk})(\boldsymbol{a}^{(k)} - r_{1k}\boldsymbol{q}^{(1)} - r_{2k}\boldsymbol{q}^{(2)} \ldots + \mathrm{r}_{k\text{-}1,k}\mathbf{q}^{(k\text{-}1)})$

QR-Decomposition: proof by induction

- ✓ Proceeding this way up to step $\boldsymbol{n}$, all $\boldsymbol{n}$ columns of $\boldsymbol{Q}$ and all the elements of $\boldsymbol{R}$ can be computed. This concludes the proof that, $\boldsymbol{A} = \boldsymbol{QR}$ can be constructed!
- ✓ However, the algorithm in proof is tedious and inefficient!
- ✓ It is easier to construct the $\boldsymbol{Q}$ and $\boldsymbol{R}$ independently, directly from $\boldsymbol{A}$ using Gram-Schmidt orthogonalization!
- ✓ For eigenvalues:
  - ✓ Initialize: $\boldsymbol{A_0} = \boldsymbol{A}$
  - ✓ QR-Decomposition at each step: $\boldsymbol{A_k} = \boldsymbol{Q_k R_k}$
  - ✓ Similarity Transformation:

$$\boldsymbol{A_{k+1}} = \boldsymbol{Q_k}^{\mathrm{T}} \boldsymbol{A Q_k} = \boldsymbol{Q_k}^{\mathrm{T}} \boldsymbol{Q_k R_k Q_k} = \boldsymbol{R_k Q_k}$$

- ✓ Stopping criteria: $\max\limits_{j} \left| \dfrac{\lambda_j^{k+1} - \lambda_j^{k}}{\lambda_j^{k}} \right| \leq \varepsilon$

QR-Decomposition: Algorithm

- For a given matrix $\boldsymbol{A}$, formulate $\boldsymbol{Q}$ using Gram-Schmidt procedure (MTH 102) as follows:
  - Initialize: $\boldsymbol{q}^{(1)} = \frac{\boldsymbol{a}^{(1)}}{\left\|\boldsymbol{a}^{(1)}\right\|_2}$
  - $\boldsymbol{z}^{(k+1)} = \boldsymbol{a}^{(k+1)} - \sum_{i=1}^{k} \left(\boldsymbol{a}^{(k+1)^T} \boldsymbol{q}^{(i)}\right) \boldsymbol{q}^{(i)}$
  - $\boldsymbol{q}^{(k+1)} = \frac{\boldsymbol{z}^{(k+1)}}{\left\|\boldsymbol{a}^{(k+1)}\right\|_2}$

- Compute the elements of matrix $\boldsymbol{R}$ as follows:
  - $r_{ij} = \boldsymbol{q}^{(i)^T} \boldsymbol{a}^{(j)}$

Example: QR-Decomposition

$$\boldsymbol{A} = \begin{bmatrix} 3 & 4 & 1 \\ 3 & 5 & 1 \\ 2 & 2 & 1 \end{bmatrix} \qquad x_1 = \begin{bmatrix} 3 \\ 3 \\ 2 \end{bmatrix},\ x_2 = \begin{bmatrix} 4 \\ 5 \\ 2 \end{bmatrix} \text{ and } x_3 = \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}$$

$$\|x_1\| = \sqrt{3^2 + 3^2 + 2^2} = 4.6904 \qquad y_1 = \frac{x_1}{\|x_1\|} = \begin{bmatrix} 0.6396 \\ 0.6396 \\ 0.4264 \end{bmatrix}$$

$$z_2 = x_2 - \left(x_2^T y_1\right) y_1 = \begin{bmatrix} -0.2273 \\ 0.7727 \\ -0.8182 \end{bmatrix} \qquad \|z_2\| = 1.1481, \quad y_2 = \frac{z_2}{\|z_2\|} = \begin{bmatrix} -0.1980 \\ 0.6730 \\ -0.7126 \end{bmatrix}$$

Example: QR-Decomposition

$$z_3 = x_3 - \left(x_3^T y_1\right) y_1 - \left(x_3^T y_2\right) y_2 = \begin{bmatrix} -0.1379 \\ 0.0690 \\ 0.1034 \end{bmatrix}$$

$$\|z_3\| = 0.1857, \quad y_3 = \frac{z_3}{\|z_3\|} = \begin{bmatrix} -0.7428 \\ 0.3714 \\ 0.5571 \end{bmatrix}$$

$$Q = \begin{bmatrix} 0.6396 & -0.1980 & -0.7428 \\ 0.6396 & 0.6730 & 0.3714 \\ 0.4264 & -0.7126 & 0.5571 \end{bmatrix}$$

Example: QR-Decomposition

$r_{11} = y_1^T x_1 = 4.6904$, $r_{12} = y_1^T x_2 = 6.6092$, $r_{13} = y_1^T x_3 = 1.7056$, $r_{22} = y_2^T x_2 = 1.1481$,
$r_{23} = y_2^T x_3 = -0.2375$ and $r_{33} = y_3^T x_3 = 0.1857$

$$R = \begin{bmatrix} 4.6904 & 6.6092 & 1.7056 \\ 0 & 1.1481 & -0.2375 \\ 0 & 0 & 0.1857 \end{bmatrix}$$

Example: Eigenvalues by Similarity Transformation

k	$A_k = R_kQ_k$			Q_k			R_k			e (%)
0	3.0000	4.0000	1.0000	0.6396	-0.1980	-0.7428	4.6904	6.6092	1.7056	
	3.0000	5.0000	1.0000	0.6396	0.6730	0.3714	0.0000	1.1481	-0.2375	
	2.0000	2.0000	1.0000	0.4264	-0.7126	0.5571	0.0000	0.0000	0.1857	
1	7.9545	2.3043	-0.0792	0.9968	-0.0757	-0.0257	7.9801	2.3703	-0.0546	866
	0.6331	0.9420	0.2941	0.0793	0.9765	0.2004	0.0000	0.7721	0.2723	
	0.0792	-0.1323	0.1034	0.0099	-0.2018	0.9794	0.0000	0.0000	0.1623	
2	8.1420	1.7215	0.2166	1.0000	-0.0078	-0.0006	8.1423	1.7269	0.2199	34.92
	0.0640	0.6990	0.4214	0.0079	0.9988	0.0482	0.0000	0.6863	0.4116	
	0.0016	-0.0328	0.1589	0.0002	-0.0482	0.9988	0.0000	0.0000	0.1790	
3	8.1556	1.6505	0.2983	1.0000	-0.0007	0.0000	8.1557	1.6509	0.2986	11.08
	0.0055	0.6656	0.4442	0.0007	0.9999	0.0130	0.0000	0.6645	0.4416	
	0.0000	-0.0086	0.1788	0.0000	-0.0130	0.9999	0.0000	0.0000	0.1845	
4	8.1568	1.6414	0.3199	1.0000	-0.0001	0.0000	8.1568	1.6415	0.3199	3.1
	0.0004	0.6587	0.4502	0.0001	1.0000	0.0036	0.0000	0.6587	0.4495	
	0.0000	-0.0024	0.1845	0.0000	-0.0036	1.0000	0.0000	0.0000	0.1861	
5	8.1568	1.6398	0.3259	1.0000	0.0000	0.0000	8.1568	1.6398	0.3259	0.88
	0.0000	0.6570	0.4519	0.0000	1.0000	0.0010	0.0000	0.6570	0.4517	
	0.0000	-0.0007	0.1861	0.0000	-0.0010	1.0000	0.0000	0.0000	0.1866	
6	8.1569	1.6395	0.3276	1.0000	0.0000	0.0000	8.1569	1.6395	0.3276	0.25
	0.0000	0.6565	0.4524	0.0000	1.0000	0.0003	0.0000	0.6565	0.4523	
	0.0000	-0.0002	0.1866	0.0000	-0.0003	1.0000	0.0000	0.0000	0.1867	
7	8.1569	1.6394	0.3281							0.07
	0.0000	0.6564	0.4525							
	0.0000	-0.0001	0.1867							