Faddeev Leverrier Method

- ✓ Recall: eigenvalues are the roots of the *characteristic* polynomial given by, $det(A \lambda I) = 0$
- \checkmark 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:

$$(-1)^{n}(\lambda^{n} - a_{n-1}\lambda^{n-1} - \dots - a_{2}\lambda^{2} - a_{1}\lambda - a_{0}) = 0$$

- ✓ Algorithm:
 - ✓ Initialize: $A_{n-1} = A$; $a_{n-1} = \text{trace } (A_{n-1})$
 - $\checkmark A_i = A(A_{i+1} a_{i+1}I); a_i = \frac{\operatorname{trace}(A_i)}{n-i}$
 - \checkmark $i = (n-2), (n-3), \dots 2, 1, 0.$
- ✓ 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:
$$A_3 = A$$
; $a_3 = \text{trace}(A_3) = 12$

$$A_{2} = A(A_{3} - a_{3}I)$$

$$(A_{3} - a_{3}I) = \begin{bmatrix} -10 & -1 & 0 & 0 \\ -1 & -8 & -1 & 0 \\ 0 & -1 & -8 & -1 \\ 0 & 0 & -1 & -10 \end{bmatrix}; \quad A_{2} = \begin{bmatrix} -19 & 6 & 1 & 0 \\ 6 & -30 & 4 & 1 \\ 1 & 4 & -30 & 6 \\ 0 & 1 & 6 & -19 \end{bmatrix}$$

$$a_{2} = \frac{\operatorname{trace}(A_{2})}{4 - 2} = \frac{-98}{2} = -49$$

Faddeev Leverrier Method: Example

$$A_{1} = A(A_{2} - a_{2}I)$$

$$(A_{2} - a_{2}I) = \begin{bmatrix} 30 & 6 & 1 & 0 \\ 6 & 19 & 4 & 1 \\ 1 & 4 & 19 & 6 \\ 0 & 1 & 6 & 30 \end{bmatrix}; \quad A_{1} = \begin{bmatrix} 54 & -7 & -2 & -1 \\ -7 & 66 & -4 & -2 \\ -2 & -4 & 66 & -7 \\ -1 & -2 & -7 & 54 \end{bmatrix}$$

$$a_{1} = \frac{\text{trace}(A_{1})}{4 - 1} = \frac{240}{3} = 80$$

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

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

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

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

Similarity Transformation

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

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

Computation of Eigenvalues

- ✓ Recall: What is an orthogonal matrix?
 - ✓ Each column vector is *orthonormal* to each other
 - $\checkmark Q^{T}Q = I \text{ or } Q^{T} = Q^{-1}$
- ✓ 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 A with real eigenvalues, there is an orthogonal matrix Q and an upper-triangular matrix U such that $A = QUQ^T$
- ✓ If A is complex, Q is unitary such that $A = QUQ^H$
- ✓ Therefore, A and U are similar matrices, $A = QUQ^T$
- \checkmark The upper triangular matrix U contains the eigenvalues of A on its diagonal.

Computation of Eigenvalues

- ✓ All *non-defective* matrices are similar to upper triangular matrices
- ✓ $A = QUQ^{T}$ or $U = Q^{T}AQ$, U contains the eigenvalues of A on its diagonal.
- \checkmark Therefore, a non-defective matrix A can be transformed to an upper-triangular matrix U through *similarity* transformation and the diagonal elements of 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 A can be decomposed into an orthogonal matrix Q and an uppertriangular matrix R such that A = QR
- ✓ A sequence of matrix is generated through *similarity transformation* as follows:
 - ✓ Initialize: $A_0 = A$
 - ✓ QR-Decomposition: $A_k = Q_k R_k$
 - ✓ Similarity Transformation:

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

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

QR-Decomposition

 \checkmark We seek a decomposition of the form: A = QR

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

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

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

QR-Decomposition: proof by induction

$$\checkmark k = 1: a^{(1)} = Qr^{(1)} = r_{11}q^{(1)}$$

$$\checkmark$$
 Q is orthogonal: $||q^{(1)}||_2 = 1$

$$||a^{(1)}||_2 = |r_{11}|||q^{(1)}||_2 = r_{11}$$

$$\checkmark q^{(1)} = (1/r_{11})a^{(1)}$$

$$\checkmark k = 2: a^{(2)} = Qr^{(2)} = r_{12}q^{(1)} + r_{22}q^{(2)}$$

$$\checkmark$$
 Q is orthogonal: $q^{(1)T}a^{(2)} = r_{12}q^{(1)T}q^{(1)} + r_{22}q^{(1)T}q^{(2)} = r_{12}$

$$\checkmark$$
 Also: $\|\boldsymbol{a}^{(2)} - r_{12}\boldsymbol{q}^{(1)}\|_2 = |r_{22}| \|\boldsymbol{q}^{(2)}\|_2 = r_{22}$

$$\checkmark q^{(2)} = (1/r_{22})(a^{(2)} - r_{12}q^{(1)})$$

QR-Decomposition: proof by induction

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\checkmark  k = 1: \mathbf{a}^{(1)} = \mathbf{Q}\mathbf{r}^{(1)} = r_{11}\mathbf{q}^{(1)}
         \checkmark Q is orthogonal: \|q^{(1)}\|_2 = 1
         ||a^{(1)}||_2 = |r_{11}|||q^{(1)}||_2 = r_{11}

\checkmark q^{(1)} = (1/r_{11})a^{(1)}

\checkmark  k = 2: \mathbf{a}^{(2)} = \mathbf{Q}\mathbf{r}^{(2)} = r_{12}\mathbf{q}^{(1)} + r_{22}\mathbf{q}^{(2)}
         \checkmark Q is orthogonal: q^{(1)T}a^{(2)} = r_{12}q^{(1)T}q^{(1)} + r_{22}q^{(1)T}q^{(2)} = r_{12}
         \checkmark Also: \|\boldsymbol{a}^{(2)} - r_{12}\boldsymbol{q}^{(1)}\|_{2} = |r_{22}|\|\boldsymbol{q}^{(2)}\|_{2} = r_{22}
         \mathbf{q}^{(2)} = (1/r_{22})(\mathbf{q}^{(2)} - r_{12}\mathbf{q}^{(1)})
\checkmark kth step: a^{(k)} = Qr^{(k)} = r_{1k}q^{(1)} + r_{2k}q^{(2)} \dots + r_{kk}q^{(k)}
         \checkmark Q is orthogonal: q^{(i)T}a^{(k)} = r_{1k}q^{(i)T}q^{(1)} + r_{2k}q^{(i)T}q^{(2)} \dots + r_{kk}q^{(i)T}q^{(k)} = r_{ik}
                   for i = 1, 2, ... (k-1)
         \checkmark Also: \|\boldsymbol{a}^{(2)} - r_{1k}\boldsymbol{q}^{(1)} - r_{2k}\boldsymbol{q}^{(2)} \dots - r_{k-1,k}\boldsymbol{q}^{(k-1)}\|_{2} =
                   |r_{kk}| \|\boldsymbol{q}^{(k)}\|_{2} = r_{kk}
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 $\mathbf{q}^{(k)} = (1/r_{kk})(\mathbf{q}^{(k)} - r_{1k}\mathbf{q}^{(1)} - r_{2k}\mathbf{q}^{(2)} \dots + r_{k-1k}\mathbf{q}^{(k-1)})$

QR-Decomposition: proof by induction

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

$$\boldsymbol{A}_{k+1} = \boldsymbol{Q}_k^{\mathrm{T}} \boldsymbol{A} \boldsymbol{Q}_k = \boldsymbol{Q}_k^{\mathrm{T}} \boldsymbol{Q}_k \boldsymbol{R}_k \boldsymbol{Q}_k = \boldsymbol{R}_k \boldsymbol{Q}_k$$

✓ Stopping criteria: $\max_{j} \left| \frac{\lambda_{j}^{k+1} - \lambda_{j}^{k}}{\lambda_{j}^{k}} \right| \leq \varepsilon$

QR-Decomposition: Algorithm

✓ For a given matrix A, formulate Q using Gram-Schmidt procedure (MTH 102) as follows:

✓ Initialize:
$$q^{(1)} = \frac{a^{(1)}}{\|a^{(1)}\|_2}$$
✓ $z^{(k+1)} = a^{(k+1)} - \sum_{i=1}^k \left(a^{(k+1)^T} q^{(i)}\right) q^{(i)}$
✓ $q^{(k+1)} = \frac{z^{(k+1)}}{\|z^{(k+1)}\|_2}$

 \checkmark Compute the elements of matrix \mathbf{R} as follows:

$$\checkmark r_{ij} = \boldsymbol{q}^{(i)^T} \boldsymbol{a}^{(j)}$$

Example: QR-Decomposition

$$A = \begin{bmatrix} 3 & 4 & 1 \\ 3 & 5 & 1 \\ 2 & 2 & 1 \end{bmatrix}$$

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

$$||x_1|| = \sqrt{3^2 + 3^2 + 2^2} = 4.6904$$

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

$$z_2 = x_2 - (x_2^T y_1) y_1 = \begin{bmatrix} -0.2273 \\ 0.7727 \\ -0.8182 \end{bmatrix}$$

$$z_{2} = x_{2} - (x_{2}^{T}y_{1})y_{1} = \begin{vmatrix} -0.2273 \\ 0.7727 \\ -0.8182 \end{vmatrix} = \begin{vmatrix} -0.1980 \\ |z_{2}|| = 1.1481, \quad y_{2} = \frac{z_{2}}{||z_{2}||} = \begin{vmatrix} -0.1980 \\ 0.6730 \\ -0.7126 \end{vmatrix}$$

Example: QR-Decomposition

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

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

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

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	$A_k = R_k Q_k$			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							