Unit 4.2 The QR Method

Numerical Analysis

EE/NTHU

Mar. 27, 2017

Matrix QR Factorization

- Given a matrix $\mathbf{A}$, the QR factorization assumes there is a orthonormal matrix $\mathbf{Q}$ and an upper triangular matrix $\mathbf{R}$ such that

$$\mathbf{A} = \mathbf{QR}. \tag{4.2.1}$$

- Note that in general case, the dimension of matrix $\mathbf{A}$ is $m \times n$, $m \geq n$. In the case of $m > n$, $\mathbf{Q}$ is $m \times m$ and orthonormal, and $\mathbf{R}$ is $m \times n$ with bottom $m - n$ rows all 0's.
- In this course, we have the dimension of $\mathbf{A}$ as an $n \times n$, so are that of matrices $\mathbf{Q}$ and $\mathbf{R}$.

$$\begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \cdots & \cdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{bmatrix} = \begin{bmatrix} q_{11} & q_{12} & \cdots & q_{1n} \\ q_{21} & q_{22} & \cdots & q_{2n} \\ \cdots & \cdots & \ddots & \vdots \\ q_{n1} & q_{n2} & \cdots & q_{nn} \end{bmatrix} \begin{bmatrix} r_{11} & r_{12} & \cdots & r_{1n} \\ 0 & r_{22} & \cdots & r_{2n} \\ \cdots & \cdots & \ddots & \vdots \\ 0 & 0 & \cdots & r_{nn} \end{bmatrix} \tag{4.2.2}$$

Matrix QR Factorization, II

- Let the column vectors of matrix $\mathbf{A}$ be $\{\mathbf{a}_1, \mathbf{a}_2, \ldots, \mathbf{a}_n\}$, and the corresponding column vectors of $\mathbf{Q}$ be $\{\mathbf{q}_1, \mathbf{q}_2, \ldots, \mathbf{q}_n\}$.
- Since $\mathbf{Q}$ is orthonormal

$$(\mathbf{q}_i)^T\mathbf{q}_j = \begin{cases} 1, & \text{if } i = j, \\ 0, & \text{if } i \neq j. \end{cases} \tag{4.2.3}$$

- Due to $\mathbf{A} = \mathbf{QR}$,

$$\mathbf{a}_1 = r_{11}\mathbf{q}_1, \tag{4.2.4}$$

$$\mathbf{a}_2 = r_{12}\mathbf{q}_1 + r_{22}\mathbf{q}_2, \tag{4.2.5}$$

$$\cdots$$

$$\mathbf{a}_j = \sum_{i=1}^{j} r_{i,j}\mathbf{q}_i, \qquad j = 1, \ldots, n. \tag{4.2.6}$$

- Thus, column vectors, $\mathbf{a}_i$ are linear combinations of column vectors $\mathbf{q}_j$. The linear space spanned by $\{\mathbf{a}_i\}$ can also be spanned by $\{\mathbf{q}_j\}$.

The Gram-Schmidt Orthogonalization Process

- From Eqs (4.2.3) and (4.2.4), we have

$$r_{11} = \sqrt{(\mathbf{a}_1)^T\mathbf{a}_1}, \tag{4.2.7}$$

$$\mathbf{q}_1 = \frac{\mathbf{a}_1}{r_{11}}. \tag{4.2.8}$$

- Multiply $(\mathbf{q}_1)^T$ to Eq. (4.2.5), we have

$$r_{12} = (\mathbf{q}_1)^T\mathbf{a}_2, \tag{4.2.9}$$

$$r_{22}\mathbf{q}_2 = \mathbf{a}_2 - r_{12}\mathbf{q}_1. \tag{4.2.10}$$

Thus,

$$r_{22} = \sqrt{(\mathbf{a}_2 - r_{12}\mathbf{q}_1)^T(\mathbf{a}_2 - r_{12}\mathbf{q}_1)}, \tag{4.2.11}$$

$$\mathbf{q}_2 = \frac{\mathbf{a}_2 - r_{12}\mathbf{q}_1}{r_{22}}. \tag{4.2.12}$$

Using the same process and Eq. (4.2.6), we have for $i < j$

$$r_{ij} = (\mathbf{q}_i)^T\mathbf{a}_j, \tag{4.2.13}$$

$$r_{jj} = \sqrt{(\mathbf{a_j} - \sum_{i=1}^{j-1} r_{ij}\mathbf{q}_i)^T(\mathbf{a_j} - \sum_{i=1}^{j-1} r_{ij}\mathbf{q}_i)}, \tag{4.2.14}$$

$$\mathbf{q}_j = \frac{\mathbf{a_j} - \sum_{i=1}^{j-1} r_{ij}\mathbf{q}_i}{r_{jj}}. \tag{4.2.15}$$

Matrix QR Decomposition, III

Algorithm 4.2.1. Matrix QR Decomposition.

Given an $n \times n$ matrix $\mathbf{A}$, the QR decomposition constructs an orthonormal matrix $\mathbf{Q}$ and an upper triangle matrix $\mathbf{R}$ as

$r_{11} = \sqrt{(\mathbf{a}_1)^T \mathbf{a}_1}$,
$\mathbf{q}_1 = \dfrac{\mathbf{a}_1}{r_{11}}$,
for $(j = 2;\ j \le n;\ j = j + 1\ )$ {
    $\mathbf{q}_j = \mathbf{a}_j$,
    for $(i = 1;\ i < j;\ i = i + 1\ )$ {
        $r_{ij} = (\mathbf{q}_i)^T \mathbf{q}_j$,
        $\mathbf{q}_j = \mathbf{q}_j - r_{ij}\mathbf{q}_i$,
    }
    $r_{jj} = \sqrt{(\mathbf{q}_j)^T \mathbf{q}_j}$.
}

where $\mathbf{a}_i$ is the i-th column vector or matrix $\mathbf{A}$, and $\mathbf{q}_j$ is the j-th column vector of $\mathbf{Q}$.

- It can be observed that the matrices $\mathbf{Q}$ and $\mathbf{R}$ are both unique.
- Note this process is the modified Gram-Schmidt process which results in smaller round-off errors.

QR Iterations

- The inverse power method with shift is an effective method to find an eigenvalue and the associated eigenvector.
- To find all the eigenvalues, however, takes some effort using power method based approach.
- The QR iteration method can be used to find all eigenvalues simultaneously.

Algorithm 4.2.2. QR Iteration

Given a real $n \times n$ matrix $\mathbf{A}$, let $\mathbf{T}^{(0)} = \mathbf{A}$ and iterate for $k \ge 0$

$$\mathbf{T}^{(k)} = \mathbf{Q}^{(k)}\mathbf{R}^{(k)}, \tag{4.2.16}$$

$$\mathbf{T}^{(k+1)} = \mathbf{R}^{(k)}\mathbf{Q}^{(k)}. \tag{4.2.17}$$

- If $\mathbf{A}$ is diagonalizable then the diagonal elements $t_{ii}, i = 1, \ldots, n$ of the converged matrix $\mathbf{T}$ are the eigenvalues of $\mathbf{A}$.
- Note that Eq. (4.2.16) is the matrix QR decomposition.
- And Eq. (4.2.17) is simply matrix multiplication.

QR Iterations, II

- In QR iterations

$$\begin{aligned}
\mathbf{T}^{(k+1)} &= \mathbf{R}^{(k)}\mathbf{Q}^{(k)} \\
&= \left[(\mathbf{Q}^{(k)})^T\mathbf{Q}^{(k)}\right]\mathbf{R}^{(k)}\mathbf{Q}^{(k)} \\
&= (\mathbf{Q}^{(k)})^T\left[\mathbf{Q}^{(k)}\mathbf{R}^{(k)}\right]\mathbf{Q}^{(k)} \\
&= (\mathbf{Q}^{(k)})^T\mathbf{T}^{(k)}\mathbf{Q}^{(k)} \\
&= (\mathbf{Q}^{(k)})^T\cdots(\mathbf{Q}^{(0)})^T\mathbf{T}^{(0)}\mathbf{Q}^{(0)}\cdots\mathbf{Q}^{(k)} \\
&= (\mathbf{Q}^{(0)}\cdots\mathbf{Q}^{(k)})^T\mathbf{A}\mathbf{Q}^{(0)}\cdots\mathbf{Q}^{(k)}
\end{aligned}$$

- Thus, the QR iterations algorithm is simply applying similar transformations to matrix $\mathbf{A}$

QR Iterations, III

Theorem 4.2.3.

Given a real $n \times n$ matrix $\mathbf{A}$, there exists an orthonormal and real matrix $\mathbf{Q}$ such that

$$\mathbf{Q}^T\mathbf{A}\mathbf{Q} = \begin{bmatrix} \mathbf{R}_{11} & \mathbf{R}_{12} & \cdots & \mathbf{R}_{1m} \\ 0 & \mathbf{R}_{22} & \cdots & \mathbf{R}_{2m} \\ \cdots & \cdots & \ddots & \vdots \\ 0 & 0 & \cdots & \mathbf{R}_{mm} \end{bmatrix}, \tag{4.2.18}$$

where each block $\mathbf{R}_{ii}$ is either a real number or a matrix of order 2 having complex conjugate eigenvalues, and

$$\mathbf{Q} = \lim_{k\to\infty}\left[\mathbf{Q}^{(0)}\mathbf{Q}^{(1)}\cdots\mathbf{Q}^{(k)}\right] \tag{4.2.19}$$

$\mathbf{Q}^{(k)}$ being the orthonormal matrix generated by the k-th decomposition step of the QR iterations.

QR Iterations, IV

Theorem 4.2.4. Convergence of QR iterations

If the real $n \times n$ matrix $\mathbf{A}$ has real eigenvalues such that

$$|\lambda_1| > |\lambda_2| > \cdots > |\lambda_n|.$$

Then

$$\lim_{k\to\infty} \mathbf{T}^{(k)} = \begin{bmatrix} \lambda_1 & t_{12} & t_{13} & \cdots & t_{1n} \\ 0 & \lambda_2 & t_{23} & \cdots & t_{2n} \\ \dots & \dots & \dots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & \lambda_n \end{bmatrix}. \tag{4.2.20}$$

As for the convergence rate, we have

$$|t^{(k)}_{i,i-1}| = \mathcal{O}\left(\left|\frac{\lambda_i}{\lambda_{i-1}}\right|^k\right), i = 2, \dots, n, \text{ for } k \to \infty. \tag{4.2.21}$$

Under the additional assumption that $\mathbf{A}$ is symmetric, the sequence $\{\mathbf{T}^{(k)}\}$ tends to a diagonal matrix.

QR Iterations, Example

- Given a 3×3 matrix $\mathbf{A}$ and perform QR iterations to get the following:

Matrix $\mathbf{A}$

$$\begin{bmatrix} 2 & 1 & 0 \\ 1 & 2 & 1 \\ 0 & 1 & 2 \end{bmatrix}$$

Iter 1: $\mathbf{RQ}$

$$\begin{bmatrix} 2.8 & 0.748331 & -1.82065e-16 \\ 0.748331 & 2.34286 & 0.638877 \\ 0 & 0.638877 & 0.857143 \end{bmatrix}$$

Iter 2: $\mathbf{RQ}$

$$\begin{bmatrix} 3.14286 & 0.559397 & -3.83184e-16 \\ 0.559397 & 2.24845 & 0.187848 \\ 0 & 0.187848 & 0.608696 \end{bmatrix}$$

Iter 3: $\mathbf{RQ}$

$$\begin{bmatrix} 3.30841 & 0.372193 & -2.45016e-16 \\ 0.372193 & 2.10395 & 0.052177 \\ 0 & 0.052177 & 0.587642 \end{bmatrix}$$

Iter 10: $\mathbf{RQ}$

$$\begin{bmatrix} 3.4141 & 0.0095149 & -1.5355e-16 \\ 0.0095149 & 2.0001 & 9.2925e-06 \\ 0 & 9.2925e-06 & 0.58579 \end{bmatrix}$$

Iter 20: $\mathbf{RQ}$

$$\begin{bmatrix} 3.4142 & 4.5271e-05 & -1.5102e-16 \\ 4.5271e-05 & 2 & 4.3174e-11 \\ 0 & 4.3173e-11 & 0.58579 \end{bmatrix}$$

- The eigenvalues are 3.41421, 2, 0.585786

Shifted QR Iterations

- The QR iterations method can be accelerated using the same technique as the inverse power method with shifting.

Algorithm 4.2.5. Shifted QR Iterations.

Given a real $n \times n$ matrix $\mathbf{A}$ and a real number μ, let $\mathbf{T}^{(0)} = \mathbf{A}$ and iterate for $k \geq 0$

$$\mathbf{T}^{(k)} - \mu\mathbf{I} = \mathbf{Q}^{(k)}\mathbf{R}^{(k)}, \tag{4.2.22}$$

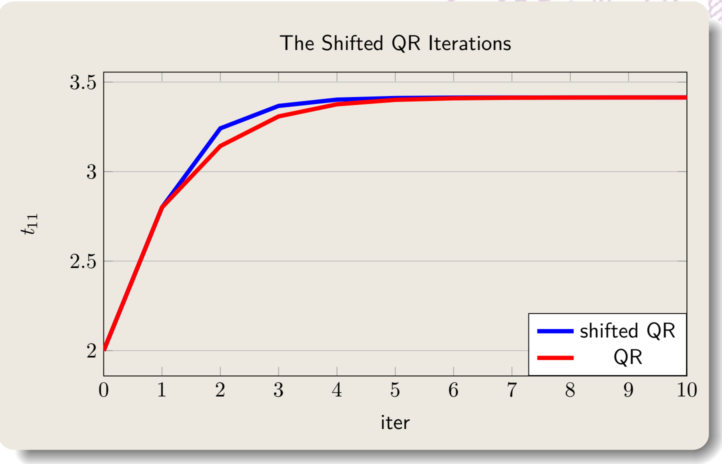
$$\mathbf{T}^{(k+1)} = \mathbf{R}^{(k)}\mathbf{Q}^{(k)} + \mu\mathbf{I}. \tag{4.2.23}$$

- Note that
$$\begin{aligned}
\mathbf{T}^{(k+1)} &= \mathbf{R}^{(k)}\mathbf{Q}^{(k)} + \mu\mathbf{I} \\
&= \left[(\mathbf{Q}^{(k)})^T\mathbf{Q}^{(k)}\right]\left[\mathbf{R}^{(k)}\mathbf{Q}^{(k)} + \mu\mathbf{I}\right] \\
&= (\mathbf{Q}^{(k)})^T\left[\mathbf{Q}^{(k)}\mathbf{R}^{(k)}\mathbf{Q}^{(k)} + \mu\mathbf{Q}^{(k)}\right] \\
&= (\mathbf{Q}^{(k)})^T\left[\mathbf{Q}^{(k)}\mathbf{R}^{(k)} + \mu\mathbf{I}\right]\mathbf{Q}^{(k)} \\
&= (\mathbf{Q}^{(k)})^T\mathbf{T}^{(k)}\mathbf{Q}^{(k)} \\
&= (\mathbf{Q}^{(0)}\mathbf{Q}^{(1)}\cdots\mathbf{Q}^{(k)})^T\mathbf{T}^{(0)}\mathbf{Q}^{(0)}\mathbf{Q}^{(1)}\cdots\mathbf{Q}^{(k)}
\end{aligned}$$

  Thus, $\mathbf{T}^{(k)}$ is an orthonormal similar transformation of $\mathbf{A}$.

Shifted QR Iterations, II

- Note also that the shift value μ needs to be equal in Eqs. (4.2.22) and (4.2.23), but it can be changed from iteration to iteration.
- The shifted QR iterations change the convergence rate from Eq. (4.2.21) to $\left|\dfrac{\lambda_i - \mu}{\lambda_{i-1} - \mu}\right|$.
- If the value of the numerator becomes smaller, the convergence rate improves.
- Thus one choice of the shift is $\mu = t_{nn} + \epsilon$, where $t_{nn}$is approaching λ_n as $k \to \infty$.
- A small number ϵ should be chosen to avoid significant roundoff error in r_{nn} which appears in the denominator in calculating $\mathbf{q}_n$ in the the QR decomposition step.



Eigenvalues and Matrix Norms

Definition 4.2.6.

A matrix norm $\|\cdot\|$ is said to be compatible or consistent with a vector norm $\|\cdot\|$ if

$$\|\mathbf{Ax}\| \le \|\mathbf{A}\|\|\mathbf{x}\|, \qquad \forall \mathbf{x} \in \mathbb{R}^n. \tag{4.2.24}$$

Theorem 4.2.7.

Given an $n \times n$ matrix $\mathbf{A}$, then

$$|\lambda| \le \|\mathbf{A}\|, \qquad \forall \lambda \in \sigma(\mathbf{A}), \tag{4.2.25}$$

for any consistent matrix norm $\|\cdot\|$.

This is due to

$$\|\mathbf{A}\|\|\mathbf{x}\| \ge \|\mathbf{Ax}\| = \|\lambda \mathbf{x}\| = |\lambda|\|\mathbf{x}\| \tag{4.2.26}$$

for any eigenvalue λ of $\mathbf{A}$ and $\mathbf{x}$ is the associated eigenvector.

- Thus all eigenvalues of $\mathbf{A}$ are contained in a circle or radius $R = \|\mathbf{A}\|$ centered at the origin of the complex plane.
- Also, any consistent norm $\|\cdot\|$ is bounded below by the largest eigenvalue λ_1.

Gershgorin Circles

Theorem 4.2.8. Gershgorin circles

Given an $n \times n$ complex matrix $\mathbf{A}$, then

$$\sigma(\mathbf{A}) \subseteq \mathcal{S}_{\mathcal{R}} = \bigcup_{i=1}^{n} \mathcal{R}_i, \qquad \mathcal{R}_i = \{z \in \mathbb{C} : |z - a_{ii}| \le \sum_{j=1, j\ne i}^{n} |a_{ij}|\}. \tag{4.2.27}$$

The sets $\mathcal{R}_i$ are called Gershgorin circles.

Proof. Decompose $\mathbf{A}$ as $\mathbf{A} = \mathbf{D} + \mathbf{E}$, where $\mathbf{D}$ is the diagonal matrix and $\mathbf{E}$ has all diagonal elements equal to 0. For a $\lambda \in \sigma(\mathbf{A})$, $(\mathbf{A} - \lambda\mathbf{I})\mathbf{x}$ has nontrivial solution $\mathbf{x} \ne \mathbf{0}$. Thus,

$$\begin{aligned}
(\mathbf{D} + \mathbf{E} - \lambda\mathbf{I})\mathbf{x} &= \mathbf{0}, \\
(\mathbf{D} - \lambda\mathbf{I})\mathbf{x} + \mathbf{Ex} &= \mathbf{0}, \\
(\mathbf{D} - \lambda\mathbf{I})\mathbf{x} &= -\mathbf{Ex}, \\
\mathbf{x} &= -(\mathbf{D} - \lambda\mathbf{I})^{-1}\mathbf{Ex},
\end{aligned}$$

Gershgorin Circles, II

Taking norm $\|\cdot\|_\infty$,

$$\|\mathbf{x}\|_\infty \le \|(\mathbf{D}-\lambda\mathbf{I})^{-1}\mathbf{E}\|_\infty \|\mathbf{x}\|_\infty,$$
$$1 \le \|(\mathbf{D}-\lambda\mathbf{I})^{-1}\mathbf{E}\|_\infty,$$

Note that matrix $\|\mathbf{A}\|_\infty$ is defined as

$$\|\mathbf{A}\|_\infty = \max_{1\le i\le n}\sum_{j=1}^{n}|a_{ij}|.$$

Thus, there is a k, $1 \le k \le n$, such that

$$1 \le \sum_{j=1, j\ne k}^{n}\frac{|a_{kj}|}{|a_{kk}-\lambda|} = \frac{1}{|a_{kk}-\lambda|}\sum_{j=1, j\ne k}^{n}|a_{kj}|.$$

And, for any eigenvalue λ there is a k such that

$$|\lambda - a_{kk}| \le \sum_{j=1, j\ne k}^{n}|a_{kj}|.$$

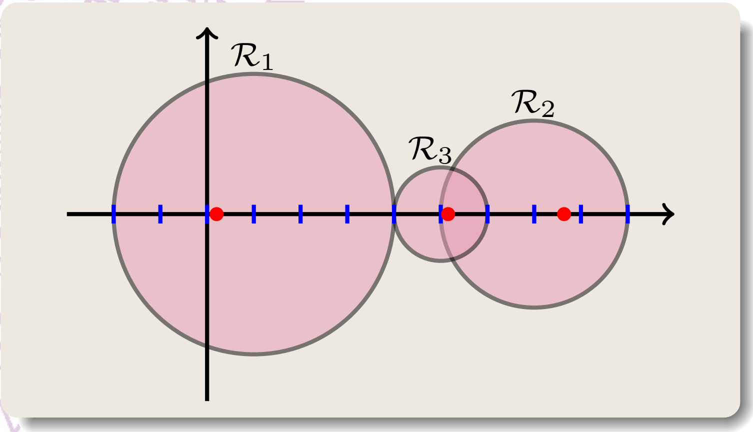
$\square$

Gershgorin Circles, Example

- Given a matrix A as below, the Gershgorin circles and the eigenvalues are plotted on the right.

$$\mathbf{A} = \begin{bmatrix} 1 & 2 & -1 \\ 2 & 7 & 0 \\ -1 & 0 & 5 \end{bmatrix}$$

$$\lambda_1 = 7.63897,$$
$$\lambda_2 = 5.15799,$$
$$\lambda_3 = 0.203037$$



First Gershgorin Theorem

- Since $\mathbf{A}$ and $\mathbf{A}^T$ have the same eigenvalues, we also have

$$\sigma(\mathbf{A}) \subseteq \mathcal{S}_{\mathcal{C}} = \bigcup_{i=1}^{n} \mathcal{C}_i, \qquad \mathcal{C}_i = \{z \in \mathbb{C} : |z - a_{jj}| \leq \sum_{i=1, i\neq j}^{n} |a_{ij}|\}. \tag{4.2.28}$$

- The circles $\mathcal{R}_i$ in the complex plane are called row circles, and $\mathcal{C}_j$ column circles.
- Since all eigenvalues must located in the union of row circles and the union of column circles, we have the following theorem.

Theorem 4.2.9. First Gershgorin theorem.

Given an $n \times n$ complex matrix $\mathbf{A}$,

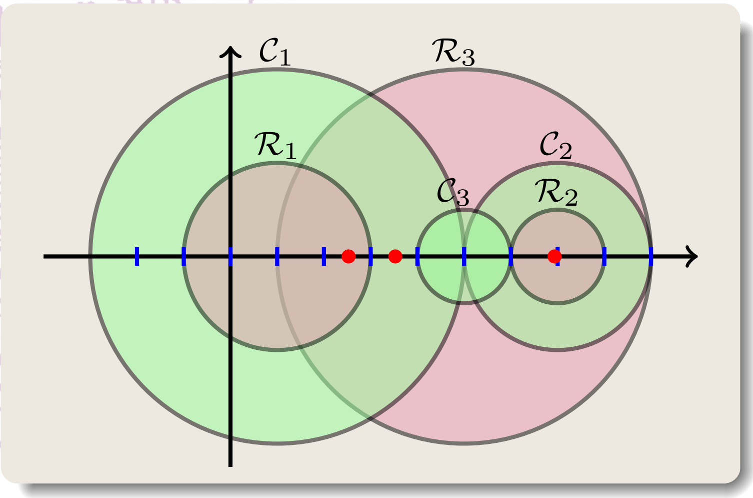
$$\forall \lambda \in \sigma(\mathbf{A}), \qquad \lambda \in \mathcal{S}_{\mathcal{R}} \bigcap \mathcal{S}_{\mathcal{C}}. \tag{4.2.29}$$

First Gershgorin Theorem, Example

- Given a matrix A as below, the Gershgorin circles and the eigenvalues are plotted on the right.

$$\mathbf{A} = \begin{bmatrix} 1 & 1 & -1 \\ -1 & 7 & 0 \\ 3 & 1 & 5 \end{bmatrix}$$

$$\lambda_1 = 6.93543, \quad \lambda_2 = 3.5374, \quad \lambda_3 = 2.52717$$



- Note that circle $\mathcal{C}_3$ contains no eigenvalues.

Second Gershgorin Theorem

Theorem 4.2.10. Second Gershgorin theorem.

Given an $n \times n$ complex matrix $\mathbf{A}$, if

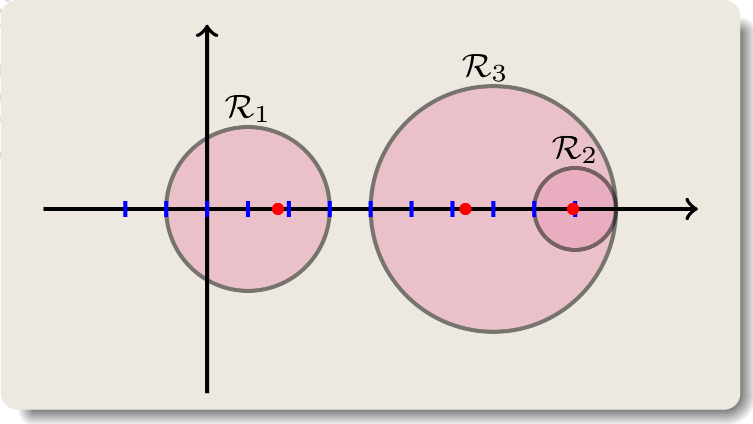
$$\mathcal{S}_1 = \bigcup_{i=1}^{m} \mathcal{R}_i, \qquad \mathcal{S}_2 = \bigcup_{i=m+1}^{n} \mathcal{R}_i, \tag{4.2.30}$$

and $\mathcal{S}_1 \bigcap \mathcal{S}_2 = \emptyset$, then $\mathcal{S}_1$ contains exactly m eigenvalues of $\mathbf{A}$, each one being accounted for with its algebraic multiplicity, while the remaining eigenvalues are contained in $\mathcal{S}_2$.

- Example

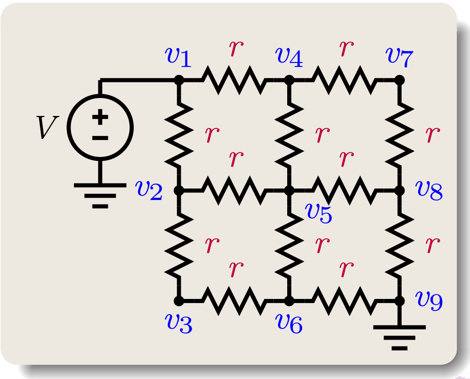
$$\mathbf{A} = \begin{bmatrix} 1 & 1 & -1 \\ -1 & 9 & 0 \\ 2 & 1 & 7 \end{bmatrix}$$

$$\lambda_1 = 8.94583,$$
$$\lambda_2 = 6.53081,$$
$$\lambda_3 = 1.52336.$$



Resistor Network Example

- The resistor network example can be formulated as



$$\begin{bmatrix} 3g & -g & & -g & & & \\ -g & 2g & & & -g & & \\ & & 3g & -g & & -g & \\ -g & & -g & 4g & -g & & -g \\ & -g & & -g & 3g & & \\ & & -g & & & 2g & -g \\ & & & -g & & -g & 3g \end{bmatrix} \begin{bmatrix} v_2 \\ v_3 \\ v_4 \\ v_5 \\ v_6 \\ v_7 \\ v_8 \end{bmatrix} = \begin{bmatrix} gV \\ 0 \\ gV \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}.$$

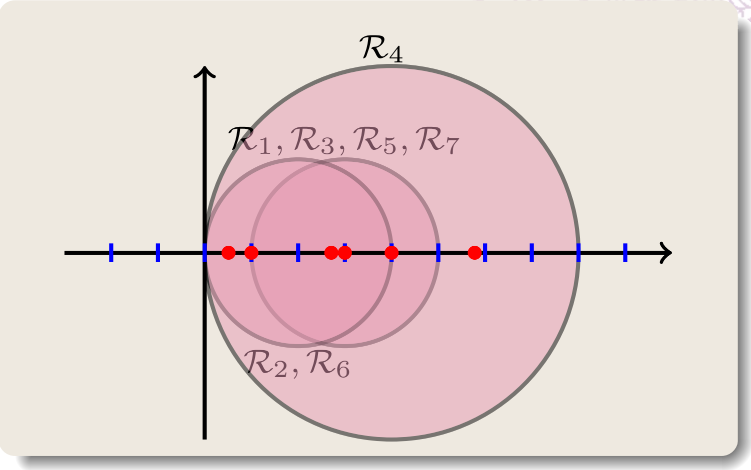
- The matrix can be rewritten as

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

Resistor Network Example

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

$$\sigma_{\mathbf{A}} = \{5.77846, 4, 3, 3, 2.71083, 1, 0.510711\}.$$



- For resistor network problems, there are 3 circles
- $\mathcal{R}_1$ with radius of 2 and centered at (3,0),
- $\mathcal{R}_2$ with radius of 2 and centered at (2,0),
- $\mathcal{R}_3$ with radius of 4 and centered at (4,0),
- For resistor network arranged in a mesh structure, there are only these three Gershgorin circles possible.
- Thus, $\forall k, \lambda_k \in [0, 8]$.

Summary

- Matrix QR decomposition
- QR method
- Shifted QR method
- Gershgorin theorems and locations of eigenvalues