

Unit 4.2 The QR Method

Numerical Analysis

Apr. 9, 2015

Matrix QR Factorization

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

$$\mathbf{A} = \mathbf{QR}. \quad (4.2.1)$$

- 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 orthogonal, 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} .

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

Matrix QR Factorization, II

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

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

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

$$\mathbf{a}_1 = r_{11} \mathbf{q}_1, \quad (4.2.4)$$

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

...

$$\mathbf{a}_j = \sum_{i=1}^j r_{ij} \mathbf{q}_i, \quad j = 1, \dots, n. \quad (4.2.6)$$

- 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

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

$$\mathbf{q}_1 = \frac{\mathbf{a}_1}{r_{11}}. \quad (4.2.8)$$

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

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

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

Thus,

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

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

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

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

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

$$\mathbf{q}_j = \frac{\mathbf{a}_j - \sum_{i=1}^{j-1} r_{ij} \mathbf{q}_i}{r_{jj}}. \quad (4.2.15)$$

Matrix QR Decomposition, III

Algorithm 4.2.1. Matrix QR Decomposition.

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

$$\begin{aligned} r_{11} &= \sqrt{(\mathbf{a}_1)^T \mathbf{a}_1}, \\ \mathbf{q}_1 &= \frac{\mathbf{a}_1}{r_{11}}, \\ \text{for } (j = 2; j \leq n; j = j + 1) \{ \\ &\quad \text{for } (i = 1; i \leq j; i = i + 1) \ r_{ij} = (\mathbf{q}_i)^T \mathbf{a}_j, \\ &\quad r_{jj} = \sqrt{(\mathbf{a}_j - \sum_{i=1}^{j-1} r_{ij} \mathbf{q}_i)^T (\mathbf{a}_j - \sum_{i=1}^{j-1} r_{ij} \mathbf{q}_i)}, \\ &\quad \mathbf{q}_j = \frac{\mathbf{a}_j - \sum_{i=1}^{j-1} r_{ij} \mathbf{q}_i}{r_{jj}}. \\ &\} \end{aligned}$$

where \mathbf{a}_i is the i -th column vector of 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.
- To reduce roundoff error, the vector $\mathbf{a}_j - \sum_{i=1}^{j-1} r_{ij} \mathbf{q}_i$ should be formed by repeatedly subtracting $r_{ij} \mathbf{q}_i$ from \mathbf{a}_j rather than forming the series sum first then subtracting it from \mathbf{a}_j .

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 $k \geq 0$

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

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

- If \mathbf{A} is diagonalizable then the diagonal elements $t_{ii}, i = 1, \dots, n$ 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.

- In QR iterations

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

- 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 orthogonal and real matrix \mathbf{Q} such that

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

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

$$\mathbf{Q} = \lim_{k \rightarrow \infty} [\mathbf{Q}^{(0)} \mathbf{Q}^{(1)} \dots \mathbf{Q}^{(k)}] \quad (4.2.19)$$

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

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

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

As for the convergence rate, we have

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

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: **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: **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: **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: **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: **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 IR 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 $k \geq 0$

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

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

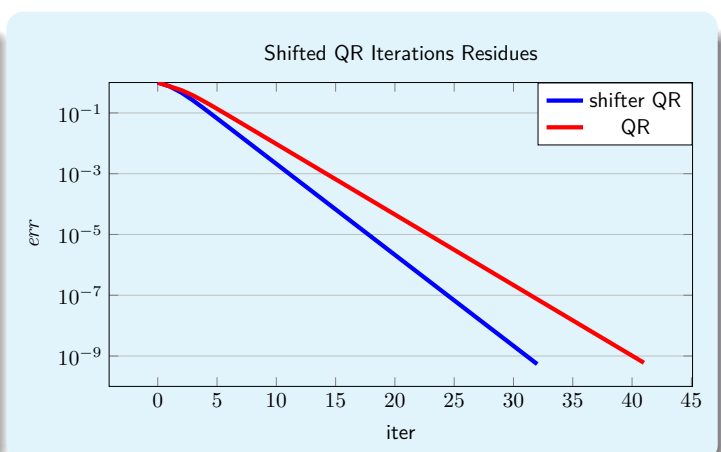
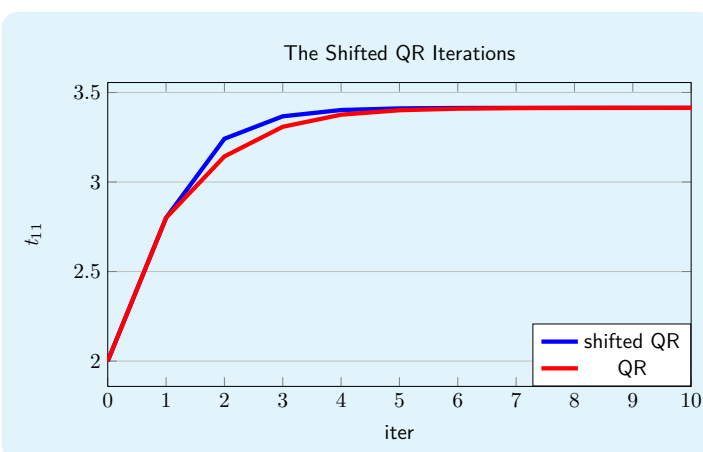
- Note that

$$\begin{aligned} \mathbf{T}^{(k+1)} &= \mathbf{R}^{(k)} \mathbf{Q}^{(k)} + \mu \mathbf{I} \\ &= [(\mathbf{Q}^{(k)})^T \mathbf{Q}^{(k)}] [\mathbf{R}^{(k)} \mathbf{Q}^{(k)} + \mu \mathbf{I}] \\ &= (\mathbf{Q}^{(k)})^T [\mathbf{Q}^{(k)} \mathbf{R}^{(k)} \mathbf{Q}^{(k)} + \mu \mathbf{Q}^{(k)}] \\ &= (\mathbf{Q}^{(k)})^T [\mathbf{Q}^{(k)} \mathbf{R}^{(k)} + \mu \mathbf{I}] \mathbf{Q}^{(k)} \\ &= (\mathbf{Q}^{(k)})^T \mathbf{T}^{(k)} \mathbf{Q}^{(k)} \\ &= (\mathbf{Q}^{(0)} \mathbf{Q}^{(1)} \dots \mathbf{Q}^{(k)})^T \mathbf{T}^{(0)} \mathbf{Q}^{(0)} \mathbf{Q}^{(1)} \dots \mathbf{Q}^{(k)} \end{aligned}$$

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

Shifted IR 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 $\left| \frac{\lambda_i - \mu}{\lambda_{i-1} - \mu} \right|$.
- 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 $k \rightarrow \infty$.
- 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

$$\|\mathbf{A}\mathbf{x}\| \leq \|\mathbf{A}\| \|\mathbf{x}\|, \quad \forall \mathbf{x} \in \mathbb{R}^n. \quad (4.2.24)$$

Theorem 4.2.7.

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

$$|\lambda| \leq \|\mathbf{A}\|, \quad \forall \lambda \in \sigma(\mathbf{A}), \quad (4.2.25)$$

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

This is due to

$$\|\mathbf{A}\| \|\mathbf{x}\| \geq \|\mathbf{A}\mathbf{x}\| = \|\lambda\mathbf{x}\| = |\lambda| \|\mathbf{x}\| \quad (4.2.26)$$

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 of 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

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

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 $\mathbf{x} \neq \mathbf{0}$. Thus,

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

Gershgorin Circles, II

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

$$\begin{aligned}\|\mathbf{x}\|_\infty &\leq \|(\mathbf{D} - \lambda\mathbf{I})^{-1}\mathbf{E}\|_\infty \|\mathbf{x}\|_\infty, \\ 1 &\leq \|(\mathbf{D} - \lambda\mathbf{I})^{-1}\mathbf{E}\|_\infty,\end{aligned}$$

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

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

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

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

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

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

□

Gershgorin Circles, Example

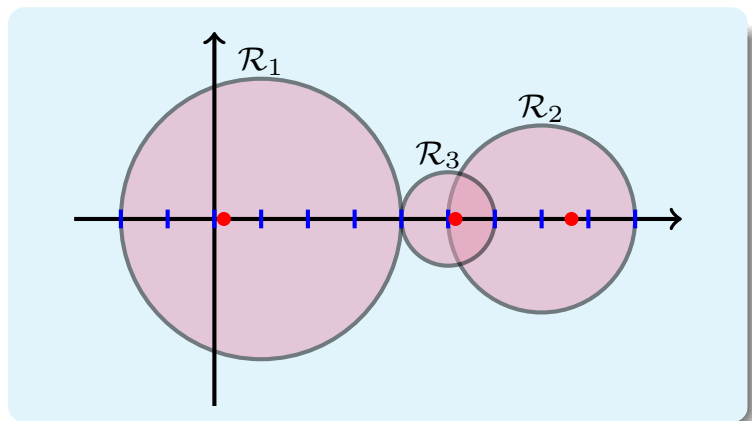
- Given a matrix \mathbf{A} as below, the Gershgorin circles and the eigenvalues are plotted on the right.

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

$$\lambda_1 = 7.63897,$$

$$\lambda_2 = 5.15799,$$

$$\lambda_3 = 0.203037$$



First Gershgorin Theorem

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

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

- The circles \mathcal{R}_i in the complex plane are called **row circles**, and \mathcal{C}_j **column circles**.
- Since all eigenvalues must be 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} ,

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

First Gershgorin Theorem, Example

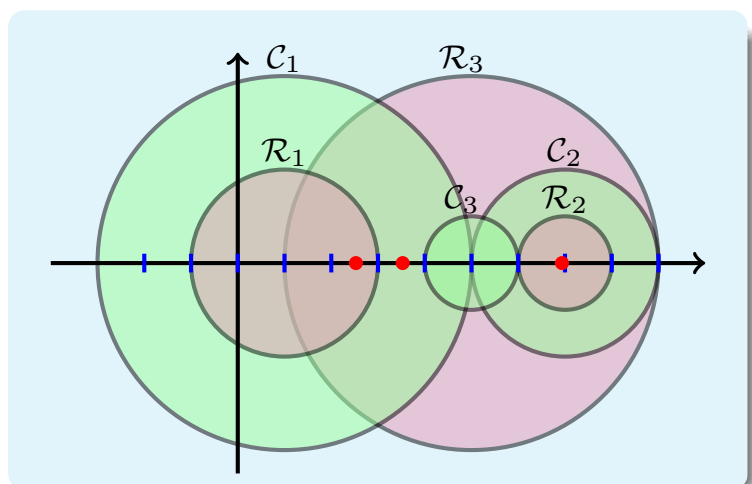
- Given a matrix \mathbf{A} as below, the Gershgorin circles and the eigenvalues are plotted on the right.

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

$$\lambda_1 = 6.93543,$$

$$\lambda_2 = 3.5374,$$

$$\lambda_3 = 2.52717$$



- 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

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

and $\mathcal{S}_1 \cap \mathcal{S}_2 = \emptyset$, 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 .

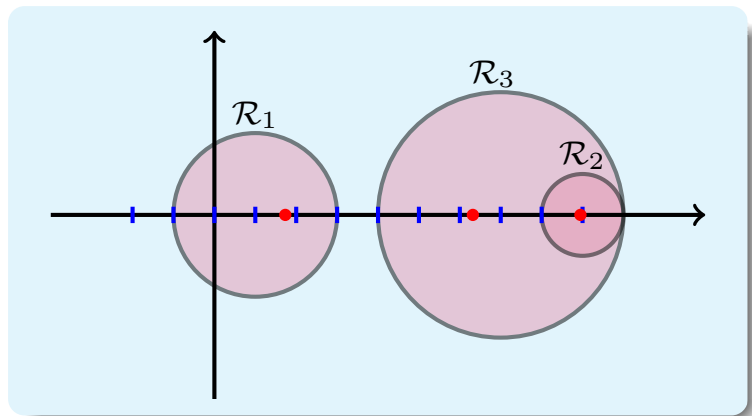
• Example

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

$$\lambda_1 = 8.94583,$$

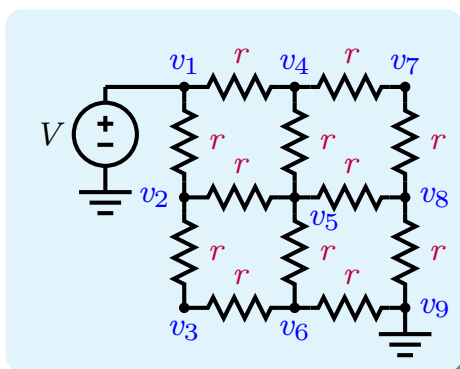
$$\lambda_2 = 6.53081,$$

$$\lambda_3 = 1.52336.$$



Resistor Network Example

• The resistor network example can be formulated as



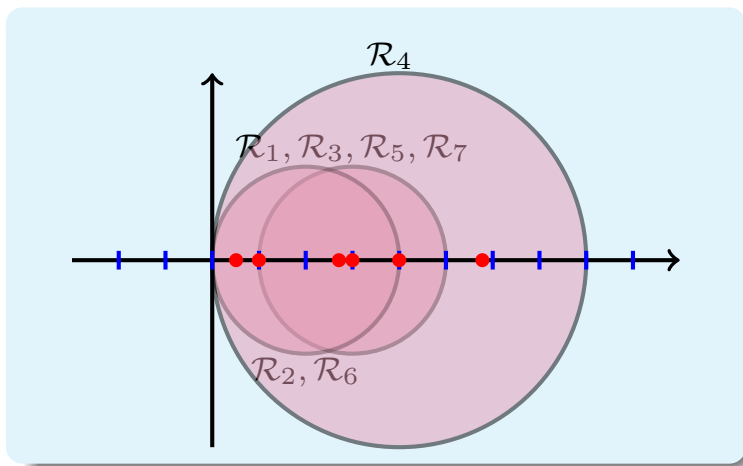
$$\begin{bmatrix} 3g & -g & & -g & & & \\ -g & 2g & & & & & \\ & & 3g & -g & & -g & \\ -g & & -g & 4g & -g & & -g \\ & -g & & -g & 3g & & \\ & & -g & & & 2g & -g \\ & & & -g & & -g & 3g \end{bmatrix} \begin{bmatrix} v_2 \\ v_3 \\ v_4 \\ v_5 \\ v_6 \\ v_7 \\ v_8 \end{bmatrix} = \begin{bmatrix} gV \\ 0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

• The matrix can be rewritten as

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

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