Unit 4.2 The QR Method

Numerical Analysis

EE/NTHU

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Numerical Analysis (EE/NTHU)

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Matrix QR Factorization

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

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

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

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

Matrix QR Factorization, II

- Let the column vectors of matrix A be $\{a_1, a_2, \dots, a_n\}$, and the corresponding column vectors of \mathbf{Q} be $\{\mathbf{q}_1,\mathbf{q}_2,\ldots,\mathbf{q}_n\}$.
- Since Q is orthonormal

$$(\mathbf{q}_i)^T \mathbf{q}_j = 1,$$
 if $i = j,$
 $0,$ if $i \neq j.$ (4.2.3)

lacktriangle Due to $\mathbf{A}=\mathbf{Q}\mathbf{R}$,

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

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

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

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

Numerical Analysis (Eigenvalues)

The Gram-Schmidt Orthogonalization Process

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

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

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

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

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

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

Thus,

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

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

$$\mathbf{q}_2 = \frac{\mathbf{a}_2 - r_{12}\mathbf{q}_1}{r_{22}}.$$
(4.2.11)

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

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

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

$$r_{jj} = \sqrt{(\mathbf{a}_j - \sum_{i=1}^{j-1} r_{ij} \mathbf{q}_i)^T (\mathbf{a}_j - \sum_{i=1}^{j-1} r_{ij} \mathbf{q}_i)},$$
(4.2.13)

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

Numerical Analysis (Eigenvalues)

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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

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egin{aligned} r_{11} &= \sqrt{(\mathbf{a}_1)^T}\mathbf{a}_1, \ \mathbf{q}_1 &= \frac{\mathbf{a}_1}{r_{11}}, \ \mathbf{for} \; (j=2;\; j \leq n;\; j=j+1\;) \; \{ \ \mathbf{q}_j &= \mathbf{a}_j, \ \mathbf{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. \ \} \end{aligned}
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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} .

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

Numerical Analysis (Eigenvalues)

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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 **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 A is diagonalizable then the diagonal elements t_{ii} , i = 1, ..., n of the converged matrix T are the eigenvalues of 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

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

$$= [(\mathbf{Q}^{(k)})^T \mathbf{Q}^{(k)}] \mathbf{R}^{(k)} \mathbf{Q}^{(k)}$$

$$= (\mathbf{Q}^{(k)})^T [\mathbf{Q}^{(k)} \mathbf{R}^{(k)}] \mathbf{Q}^{(k)}$$

$$= (\mathbf{Q}^{(k)})^T \mathbf{T}^{(k)} \mathbf{Q}^{(k)}$$

$$= (\mathbf{Q}^{(k)})^T \cdots (\mathbf{Q}^{(0)})^T \mathbf{T}^{(0)} \mathbf{Q}^{(0)} \cdots \mathbf{Q}^{(k)}$$

$$= (\mathbf{Q}^{(0)} \cdots \mathbf{Q}^{(k)})^T \mathbf{A} \mathbf{Q}^{(0)} \cdots \mathbf{Q}^{(k)}$$

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

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QR Iterations, III

Theorem 4.2.3

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

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

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

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

 $\mathbf{Q}^{(k)}$ being the orthonormal 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 **A** has real eigenvalues such that

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

Then

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

As for the convergence rate, we have

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

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

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QR Iterations, Example

ullet Given a 3×3 matrix ${f A}$ and perform QR iterations to get the following:

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

lter 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: 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 ${\bf A}$ and a real number μ , let ${\bf T}^{(0)} = {\bf A}$ and iterate for $k \ge 0$

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

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

• 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} .

Numerical Analysis (Eigenvalues)

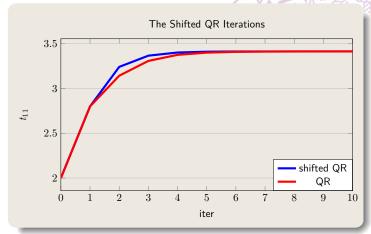
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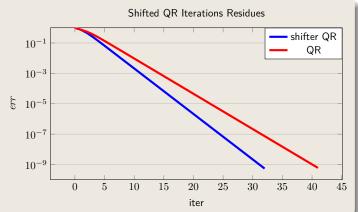
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Shifted QR Iterations, II

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

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

Theorem 4.2.7.

Given an $n \times n$ matrix **A**, then

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

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

This is due to

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

for any eigenvalue λ of **A** and **x** is the associated eigenvector.

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

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Gershgorin Circles

Theorem 4.2.8. Gershgorin circles

Given an $n \times n$ complex matrix **A**, then

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

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

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

$$(\mathbf{D} + \mathbf{E} - \lambda \mathbf{I})\mathbf{x} = \mathbf{0},$$

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

Gershgorin Circles, II

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

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

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, $1 \le k \le n$, 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

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

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Gershgorin Circles, Example

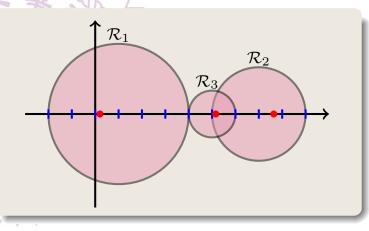
• Given a matrix A as below, the Gershgorin circles and the eigenvalues are plotted on the right.

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

$$\lambda_1 = 7.63897,$$

$$\lambda_2 = 5.15799,$$

$$\lambda_3 = 0.203037$$



First Gershgorin Theorem

ullet Since old A and $old A^T$ have the same eigenvalues, we also have

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

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

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First Gershgorin Theorem, Example

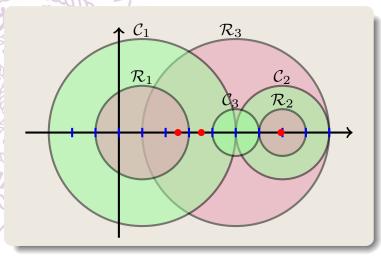
• Given a matrix A as below, the Gershgorin circles and the eigenvalues are plotted on the right.

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

$$\lambda_1 = 6.93543,$$

$$\lambda_2 = 3.5374,$$

$$\lambda_3 = 2.52717$$



• Note that circle C_3 contains no eigenvalues.

Second Gershgorin Theorem

Theorem 4.2.10. Second Gershgorin theorem.

Given an $n \times n$ complex matrix **A**, if

$$S_1 = \bigcup_{i=1}^m \mathcal{R}_i, \qquad S_2 = \bigcup_{i=m+1}^n \mathcal{R}_i,$$
 (4.2.30)

and $S_1 \cap S_2 = \emptyset$, then S_1 contains exactly m eigenvalues of A, each one being accounted for with its algebraic multiplicity, while the remaining eigenvalues are contained in S_2 .

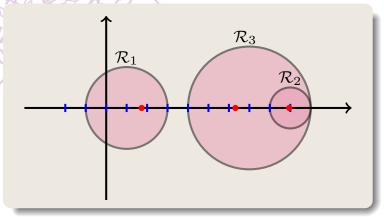
Example

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

$$\lambda_1 = 8.94583,$$

$$\lambda_2 = 6.53081,$$

$$\lambda_3 = 1.52336.$$



Numerical Analysis (Eigenvalues)

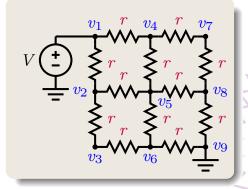
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Resistor Network Example

• The resistor network example can be formulated as



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

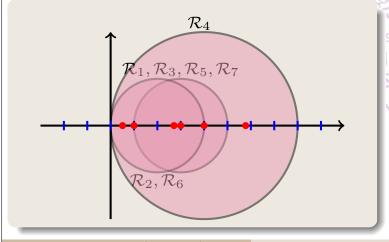
The matrix can be rewritten as

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

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, $\forall k, \lambda_k \in [0, 8]$.

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Summary

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