Using Complex Shifts in Rayleigh Quotient Iteration to Compute Close Eigenvalues

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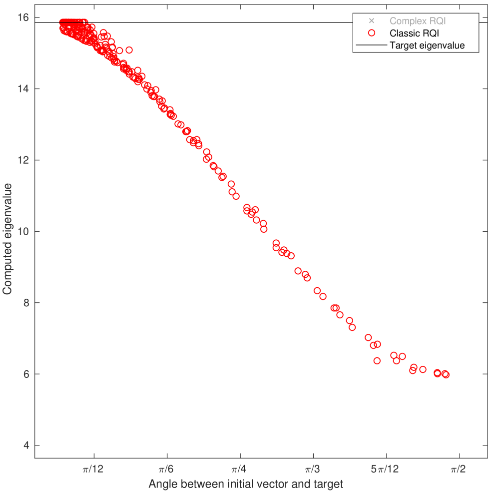
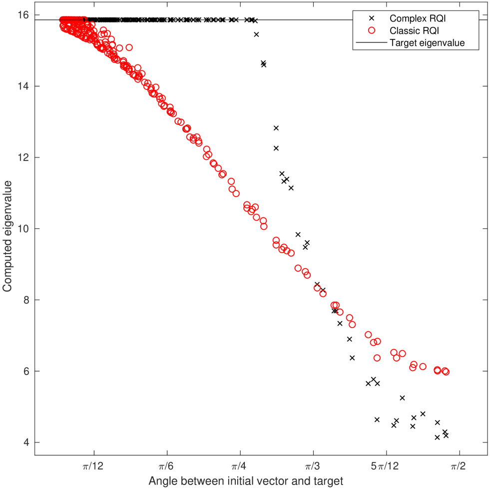
Contents



Complex RQI
Classic RQI
Target eigenvalue
16
14
12
10
8
6
4
Computed eigenvalue
π/12
π/6
π/4
π/3
5π/12
π/2
Angle between initial vector and target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Compute one eigenpair $(\lambda, \mathbf{v})$ of symmetric matrix $\boldsymbol{A}$, i. e.,

$$\boldsymbol{A}\mathbf{v} = \lambda \mathbf{v}\,.$$

Theorem

- *The eigenvalues $\lambda_1, \ldots, \lambda_n$ of $\boldsymbol{A}$ are real.*
- *The eigenvectors $\mathbf{v}_1, \ldots, \mathbf{v}_n$ of $\boldsymbol{A}$ are real.*
- *The eigenvectors form an orthogonal basis of $\mathbb{R}^n$.*

Algorithm: Power method

Input: Nonzero unit vector $\mathbf{x}^{(0)}$

for $k = 0, 1, \ldots$ **until convergence do**

$\mathbf{x}^{(k+1)} \leftarrow \boldsymbol{A}\mathbf{x}^{(k)}$

Normalise $\mathbf{x}^{(k+1)}$

Theorem

- *The eigenvalues of* $\boldsymbol{A}^{-1}$ *are* $\dfrac{1}{\lambda_i}$.
- *The eigenvalues of* $\boldsymbol{A} - \mu \boldsymbol{I}$ *are* $\lambda_i - \mu$.
- *The eigenvalues of* $(\boldsymbol{A} - \mu \boldsymbol{I})^{-1}$ *are* $\dfrac{1}{\lambda_i - \mu}$.

Algorithm: Shifted Inverse Iteration

Input: Nonzero unit vector $\mathbf{x}^{(0)}$

for $k = 0, 1, \ldots$ **until convergence do**

Solve $(\boldsymbol{A} - \mu \boldsymbol{I})\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)}$

Normalise $\mathbf{x}^{(k+1)}$

Rayleigh Quotient

$$\mathcal{R}_{\boldsymbol{A}}(\mathbf{x}) = \frac{\mathbf{x}^\mathsf{T} \boldsymbol{A}\mathbf{x}}{\mathbf{x}^\mathsf{T}\mathbf{x}} = \arg\min_{\mu \in \mathbb{C}} \| \boldsymbol{A}\mathbf{x} - \mu\mathbf{x} \|$$

Rayleigh Quotient

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Eigenvector approximation from eigenvalue approximation?

- Shifted Inverse Iteration

Eigenvalue approximation from eigenvector approximation?

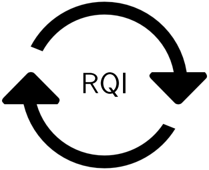
- Rayleigh Quotient

Eigenvector approximation from eigenvalue approximation?

- Shifted Inverse Iteration

Eigenvalue approximation from eigenvector approximation?

- Rayleigh Quotient



Algorithm: Rayleigh Quotient Iteration

Input: Nonzero unit vector $\mathbf{x}^{(0)}$

$\mu^{(0)} \leftarrow \left(\mathbf{x}^{(0)}\right)^{\mathsf{T}} \boldsymbol{A}\mathbf{x}^{(0)}$

for $k = 0, 1, \ldots$ **until convergence do**

Solve $\left(\boldsymbol{A} - \mu^{(k)}\boldsymbol{I}\right)\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)}$ for $\mathbf{x}^{(k+1)}$

Normalise $\mathbf{x}^{(k+1)}$

$\mu^{(k+1)} \leftarrow \left(\mathbf{x}^{(k+1)}\right)^{\mathsf{T}} \boldsymbol{A}\mathbf{x}^{(k+1)}$

$\mathcal{R}_{\boldsymbol{A}}(\mathbf{x}) = \frac{\mathbf{x}^{\mathsf{T}}\boldsymbol{A}\mathbf{x}}{\mathbf{x}^{\mathsf{T}}\mathbf{x}}$

- Cubic convergence
- Converges for almost all starting vectors

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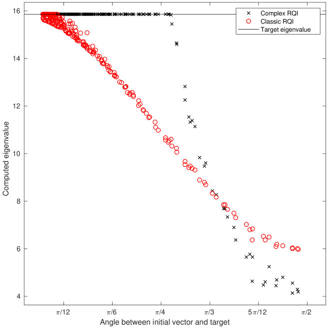
Convergence behaviour can be erratic



Observation

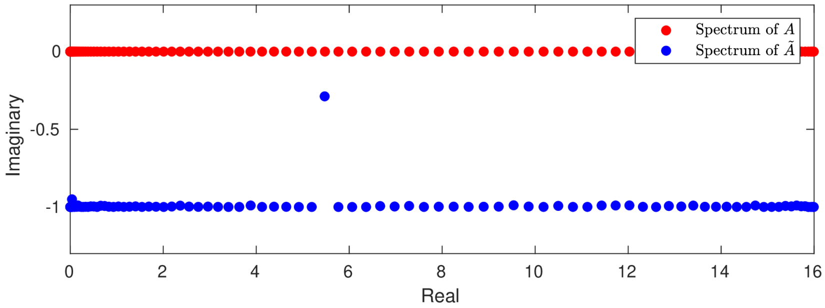
Convergence depends on initial shift but **not** initial vector

Suppose $\mathbf{u} \approx \mathbf{v}_k$.

$$\boldsymbol{A} \quad \longrightarrow \quad \boldsymbol{A} - i\gamma(\boldsymbol{I} - \mathbf{u}\mathbf{u}^\mathsf{T}) =: \tilde{\boldsymbol{A}}$$

Suppose $\mathbf{u} \approx \mathbf{v}_k$.

$$\boldsymbol{A} \quad \longrightarrow \quad \boldsymbol{A} - i\gamma(\boldsymbol{I} - \mathbf{u}\mathbf{u}^\mathsf{T}) =: \tilde{\boldsymbol{A}}$$



Algorithm: Complex RQI (first version)

for $k = 0, 1, \ldots$ **until convergence do**

  Solve $\left(\boldsymbol{A} - i\gamma\left(\boldsymbol{I} - \mathbf{u}\mathbf{u}^{\mathsf{T}}\right) - \mu^{(k)}\boldsymbol{I}\right)\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)}$

  Normalise $\mathbf{x}^{(k+1)}$

  $\mu^{(k+1)} \leftarrow \left(\mathbf{x}^{(k+1)}\right)^{*}\boldsymbol{A}\mathbf{x}^{(k+1)}$

Algorithm: Complex RQI (first version)

for $k = 0, 1, \ldots$ **until convergence do**

- Solve $\left(\boldsymbol{A} - i\gamma^{(k)}\left(\boldsymbol{I} - \mathbf{x}^{(k)}(\mathbf{x}^{(k)})^*\right) - \mu^{(k)}\boldsymbol{I}\right)\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)}$
- Normalise $\mathbf{x}^{(k+1)}$
- $\mu^{(k+1)} \leftarrow (\mathbf{x}^{(k+1)})^* \boldsymbol{A}\mathbf{x}^{(k+1)}$
- $\gamma^{(k+1)} \leftarrow \|(\boldsymbol{A} - \mu^{(k+1)}\boldsymbol{I})\mathbf{x}^{(k+1)}\|$

Theorem

It suffices to use

$$\tilde{\boldsymbol{A}} = \boldsymbol{A} - i\gamma^{(k)}\boldsymbol{I}$$

instead of

$$\tilde{\boldsymbol{A}} = \boldsymbol{A} - i\gamma^{(k)}\left(\boldsymbol{I} - \mathbf{x}^{(k)}\left(\mathbf{x}^{(k)}\right)^{*}\right).$$

Algorithm: Complex Rayleigh Quotient Iteration

Input: Nonzero unit vector $\mathbf{x}^{(0)}$

$\mu^{(0)} \leftarrow \left(\mathbf{x}^{(0)}\right)^{\mathsf{T}} \boldsymbol{A}\mathbf{x}^{(0)}$

$\gamma^{(0)} \leftarrow \|(\boldsymbol{A} - \mu^{(0)}\boldsymbol{I})\mathbf{x}^{(0)}\|$

$\sigma^{(0)} \leftarrow \mu^{(0)} + i\gamma^{(0)}$

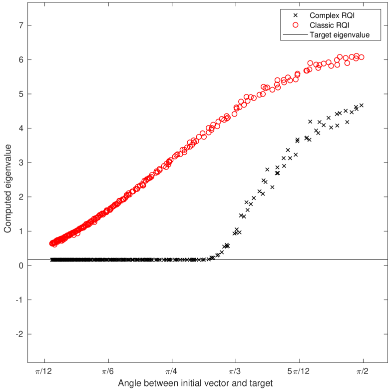
for $k = 0, 1, \ldots$ **until convergence do**

- Solve $(\boldsymbol{A} - \sigma^{(k)}\boldsymbol{I})\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)}$
- Normalise $\mathbf{x}^{(k+1)}$
- $\mu^{(k+1)} \leftarrow \left(\mathbf{x}^{(k+1)}\right)^{*} \boldsymbol{A}\mathbf{x}^{(k+1)}$
- $\gamma^{(k+1)} \leftarrow \|(\boldsymbol{A} - \mu^{(k+1)}\boldsymbol{I})\mathbf{x}^{(k+1)}\|$
- $\sigma^{(k+1)} \leftarrow \mu^{(k+1)} + i\gamma^{(k+1)}$

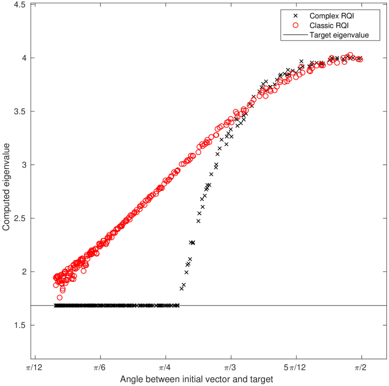
$\mathbf{x} \leftarrow \mathrm{Re}(\mathbf{x}^{(k+1)})$

$\mathbf{x} \leftarrow \mathbf{x}/\|\mathbf{x}\|$

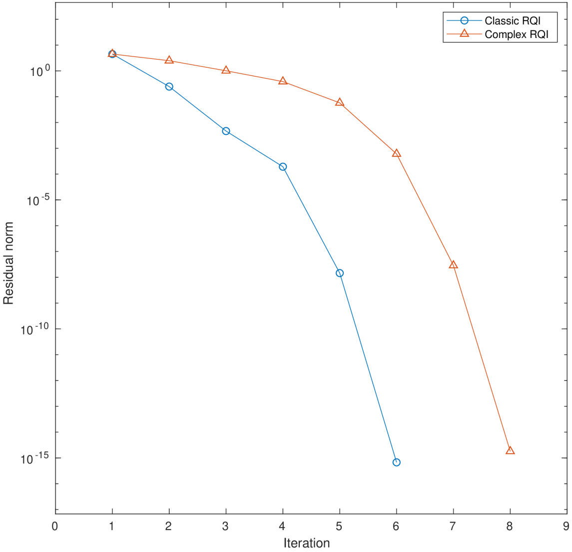
$\mu \leftarrow \mathbf{x}^{\mathsf{T}}\boldsymbol{A}\mathbf{x}$

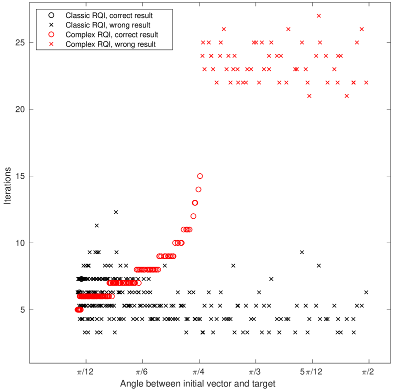


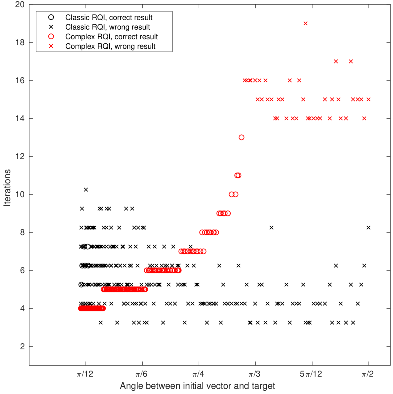
Complex RQI
Classic RQI
Target eigenvalue
Computed eigenvalue
Angle between initial vector and target
7
6
5
4
3
2
1
0
-1
-2
π/12
π/6
π/4
π/3
5π/12
π/2



Complex RQI
Classic RQI
Target eigenvalue
Computed eigenvalue
Angle between initial vector and target
4.5
4
3.5
3
2.5
2
1.5
π/12
π/6
π/4
π/3
5π/12
π/2


Classic RQI
Complex RQI
Residual norm
10^{0}
10^{-5}
10^{-10}
10^{-15}
0 1 2 3 4 5 6 7 8 9
Iteration


Classic RQI, correct result
Classic RQI, wrong result
Complex RQI, correct result
Complex RQI, wrong result
Iterations
5
10
15
20
25
π/12
π/6
π/4
π/3
5π/12
π/2
Angle between initial vector and target


Classic RQI, correct result
Classic RQI, wrong result
Complex RQI, correct result
Complex RQI, wrong result
Iterations
2
4
6
8
10
12
14
16
18
20
π/12
π/6
π/4
π/3
5π/12
π/2
Angle between initial vector and target

Summary

- Unpredictability of classic RQI
- Complex RQI succeeds for error angles below 45°
- More iterations than classic RQI but still fast

- Theoretical analysis
- Other test problems

Summary

- Unpredictability of classic RQI
- Complex RQI succeeds for error angles below 45°
- More iterations than classic RQI but still fast

- Theoretical analysis
- Other test problems

Write $\tilde{\boldsymbol{A}} = \boldsymbol{A} - i\gamma(\boldsymbol{I} - \mathbf{u}\mathbf{u}^\mathsf{T}) = \tilde{\boldsymbol{A}}_{(0)} + \tilde{\boldsymbol{A}}_{(1)}$ with

$$\tilde{\boldsymbol{A}}_{(0)} := \boldsymbol{A} - i\gamma(\boldsymbol{I} - \mathbf{v}_k\mathbf{v}_k^\mathsf{T})$$

$$\tilde{\boldsymbol{A}}_{(1)} := i\gamma(\mathbf{u}\mathbf{u}^\mathsf{T} - \mathbf{v}_k\mathbf{v}_k^\mathsf{T})$$

Theorem

$$\lambda_j(\tilde{\boldsymbol{A}}) = \lambda_j(\boldsymbol{A}) + i\gamma\left(\langle \mathbf{v}_j, \mathbf{u}\rangle^2 - 1\right) + \mathcal{O}\left(\left\|\tilde{\boldsymbol{A}}_{(1)}\right\|^2\right),$$

where

$$\left\|\tilde{\boldsymbol{A}}_{(1)}\right\| = \gamma\sqrt{1 - \langle \mathbf{u}, \mathbf{v}_k\rangle^2}.$$

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$$\tilde{\boldsymbol{A}}_{(0)} := \boldsymbol{A} - i\gamma(\boldsymbol{I} - \mathbf{v}_k\mathbf{v}_k^{\mathsf{T}})$$

$$\tilde{\boldsymbol{A}}_{(1)} := i\gamma(\mathbf{u}\mathbf{u}^{\mathsf{T}} - \mathbf{v}_k\mathbf{v}_k^{\mathsf{T}})$$

Theorem

$$\lambda_j(\tilde{\boldsymbol{A}}) = \lambda_j(\boldsymbol{A}) + i\gamma\left(\langle \mathbf{v}_j, \mathbf{u}\rangle^2 - 1\right) + \mathcal{O}\left(\left\|\tilde{\boldsymbol{A}}_{(1)}\right\|^2\right),$$

where

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