Using Complex Shifts in Rayleigh Quotient Iteration to Compute Close Eigenvalues

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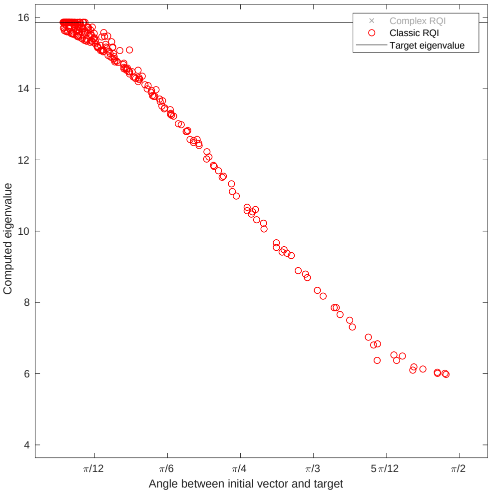
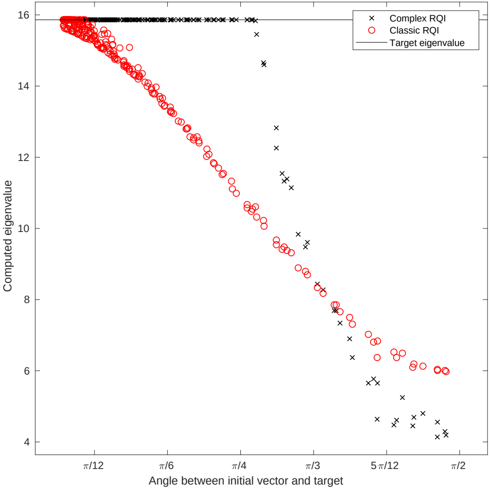

Complex RQI
Classic RQI
Target eigenvalue
Computed eigenvalue
Angle between initial vector and target
16
14
12
10
8
6
4
π/12
π/6
π/4
π/3
5 π/12
π/2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Compute one eigenpair $(\lambda, \mathbf{v})$ of symmetric matrix $\boldsymbol{A}$, i. e.,

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

Properties

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 $k = 1, 2, \ldots$ **until convergence do**

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

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

Converges linearly to $\mathbf{v}_n$ with rate

$$\rho = \frac{|\lambda_{n-1}|}{|\lambda_n|}.$$

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Eigenvalues of $\boldsymbol{A}^{-1}$ are $\dfrac{1}{\lambda_i}$.

Eigenvalues of $\boldsymbol{A} - \mu \boldsymbol{I}$ are $\lambda_i - \mu$.

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

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Algorithm: Shifted Inverse Iteration

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

for $k = 1, 2, \ldots$ **until convergence do**

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

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

Converges linearly to with rate

$$\rho = \frac{|\mu_1 - \sigma|}{|\mu_2 - \sigma|}.$$

Algorithm: Shifted Inverse Iteration

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for $k = 1, 2, \ldots$ **until convergence do**

- Solve $(\boldsymbol{A} - \sigma \boldsymbol{I})\mathbf{x}^{(k)} = \mathbf{x}^{(k-1)}$
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Eigenvector approximation from eigenvalue approximation?

Eigenvalue approximation from eigenvector approximation?

Shifted Inverse Iteration

Rayleigh Quotient

$$\mathcal{R}_A(\mathbf{x}) = \frac{\mathbf{x}^\top A \mathbf{x}}{\mathbf{x}^\top \mathbf{x}}$$

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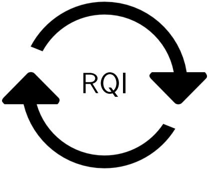

$$\mathcal{R}_{\boldsymbol{A}}(\mathbf{x}) = \arg\min_{\mu \in \mathbb{C}} \|\boldsymbol{A}\mathbf{x} - \mu\mathbf{x}\|$$

Eigenpair $(\lambda, \mathbf{v})$: $$|\mathcal{R}_{\boldsymbol{A}}(\mathbf{x}) - \lambda| = \mathcal{O}\left(\|\mathbf{x} - \mathbf{v}\|^2\right)$$

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 $k = 1, 2, \ldots$ **until convergence do**

- Solve $\left(\boldsymbol{A} - \mu^{(k)}\boldsymbol{I}\right)\mathbf{y}^{(k)} = \mathbf{x}^{(k-1)}$ for $\mathbf{y}^{(k)}$
- $\mathbf{x}^{(k)} \leftarrow \mathbf{y}^{(k)} / \left\|\mathbf{y}^{(k)}\right\|$
- $\mu^{(k)} \leftarrow \left(\mathbf{x}^{(k)}\right)^{\mathsf{T}} \boldsymbol{A}\mathbf{x}^{(k)}$

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

Converges locally cubically

- Correct digits triple

Converges for almost all starting vectors

- Impossible to fail in practice

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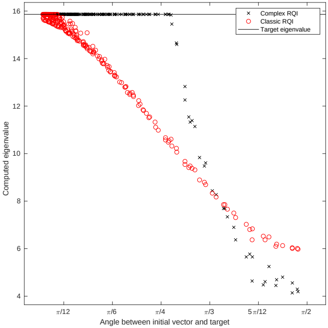
Convergence behaviour can be erratic



Observation

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

Idea: Perturb original problem to increase distance between eigenvalues.

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

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

Idea: Perturb original problem to increase distance between eigenvalues.

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

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

Suppose $\mathbf{u} \approx \mathbf{v}_k$. Set $\tilde{\boldsymbol{A}} = \boldsymbol{A} - i\gamma(\boldsymbol{I} - \mathbf{u}\mathbf{u}^\mathsf{T})$.

Vector $\mathbf{x}$ that is almost parallel to $\mathbf{u}$:

$$\tilde{\boldsymbol{A}}\mathbf{x} = \boldsymbol{A}\mathbf{x} - i\gamma(\mathbf{x} - \mathbf{u}\,\underbrace{\mathbf{u}^\mathsf{T}\mathbf{x}}_{\approx 1}) \approx \boldsymbol{A}\mathbf{x}\,.$$

Vector $\mathbf{y}$ that is almost perpendicular to $\mathbf{u}$:

$$\tilde{\boldsymbol{A}}\mathbf{y} = \boldsymbol{A}\mathbf{y} - i\gamma(\mathbf{y} - \mathbf{u}\,\underbrace{\mathbf{u}^\mathsf{T}\mathbf{y}}_{\approx 0}) \approx (\boldsymbol{A} - i\gamma\boldsymbol{I})\mathbf{y}\,.$$

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Eigenvectors and eigenvalues of $\tilde{\boldsymbol{A}}$:

$$\tilde{\boldsymbol{A}}\mathbf{v}_k \approx \boldsymbol{A}\mathbf{v}_k = \lambda_k \mathbf{v}_k$$

$$\tilde{\boldsymbol{A}}\mathbf{v}_j \approx (\boldsymbol{A} - i\gamma \boldsymbol{I})\mathbf{v}_j = (\lambda_j - i\gamma)\mathbf{v}_j$$

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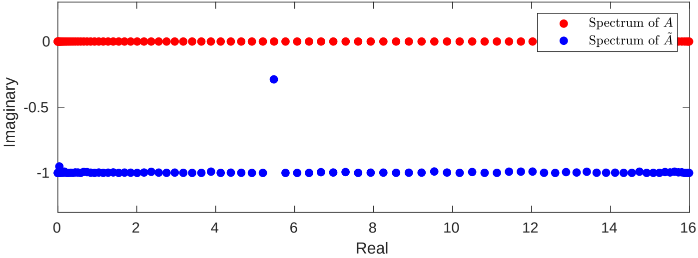

Write $\tilde{\boldsymbol{A}} = \tilde{\boldsymbol{A}}_{(0)} + \tilde{\boldsymbol{A}}_{(1)}$ with

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

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

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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