A RAYLEIGH QUOTIENT FIXED POINT METHOD FOR ALPHA-EIGENVALUE PROBLEMS

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Outline

Introduction

- Modern nuclear reactor designs and experiments require both robust and simple numerical methods for modeling.
- What works well for some problems might not work at all for other problems (no silver bullet).
- While the physics of the problem might give us hints on how to solve a problem, the mathematics also gives us clues (structure).

Motivation: The Alpha-Eigenvalue Problem

- Applications of the alpha-eigenvalue have increased substantially in the past decade.

- Research into accelerator-driven subcritical reactors and pulsed neutron experiments has led to renewed interest in the alpha-eigenvalue problem of neutron transport as it helps to predict reactor kinetic parameters and the time necessary to establish the asymptotic neutron flux distribution.

- Subcritical assembly experiments used in non-proliferation research and cross section evaluation can be evaluated using the alpha-eigenvalue as it exists even for systems without fissile material.

The Alpha-Eigenvalue Problem

$$\left[\frac{\alpha}{v(E)} + \hat{\Omega}\cdot\nabla + \sigma(\vec{r},E)\right]\psi(\vec{r},E,\hat{\Omega}) = \frac{\chi(E)}{4\pi}\int_{4\pi} d\hat{\Omega}' \int_0^\infty dE'\,\nu(E)\sigma_f(\vec{r},E')\psi(\vec{r},E',\hat{\Omega}') + \int_{4\pi} d\hat{\Omega}' \int_0^\infty dE'\,\sigma_s(\vec{r},E'\to E,\hat{\Omega}'\to\hat{\Omega})\psi(\vec{r},E',\hat{\Omega}')$$

- The sign of the algebraically largest eigenvalue determines the criticality of a system:

$$\alpha_0 \begin{cases} > 0, & \text{supercritical,} \\ = 0, & \text{critical,} \\ < 0, & \text{subcritical.} \end{cases}$$

- Eigenvalues ordered by their real parts with α_0 being the *algebraically dominant* eigenvalue

$$\alpha_0 > \text{Re }\alpha_1 \geq \text{Re }\alpha_2 \geq \cdots \geq \text{Re }\alpha_m.$$

Objectives of this Work

Consider the discretized eigenvalue transport equation

$$\left[\mathbf{H} + \alpha\mathbf{V}^{-1}\right]\mathbf{\Psi} = \left[\mathbf{\Sigma_s^*} + \mathbf{\Sigma_f^*}\right]\mathbf{\Psi} \tag{1}$$

- Derive a fixed point method capable of solving subcritical/critical/supercritical alpha-eigenvalue problems for Cartesian geometry. diamond differencing in space, multigroup in energy, isotropic scattering, and discrete ordinates in angle approximation transport problem (these restrictions are relaxed).

The Discretized Eigenvalue Equations

- Consider the following fixed point formulation:

$$\mathbf{\Psi} = \mathbf{H}^{-1}\big[-\alpha\mathbf{V}^{-1} + \mathbf{\Sigma}_{\mathbf{s}}^{*} + \mathbf{\Sigma}_{\mathbf{f}}^{*}\big]\mathbf{\Psi} \equiv \mathbf{A}(\alpha)\mathbf{\Psi} \qquad (2)$$

- Why this form? Only requires inversion of $\mathbf{H}$ (A *transport sweep*).

- The matrix $\mathbf{A}(\alpha)$ is primitive. We can assure it has a positive eigenvector.

- This positive eigenvector solves the discretized multigroup criticality eigenvalue equations when we also have the dominant eigenvalue.

Primitive Matrices [?]

Definition

Let $\mathbf{B} \geq \mathbf{0}$ be an irreducible $n \times n$ matrix, if there is some $m > 0$ such that $\mathbf{B}^m > 0$, then $\mathbf{B}$ is *primitive*.

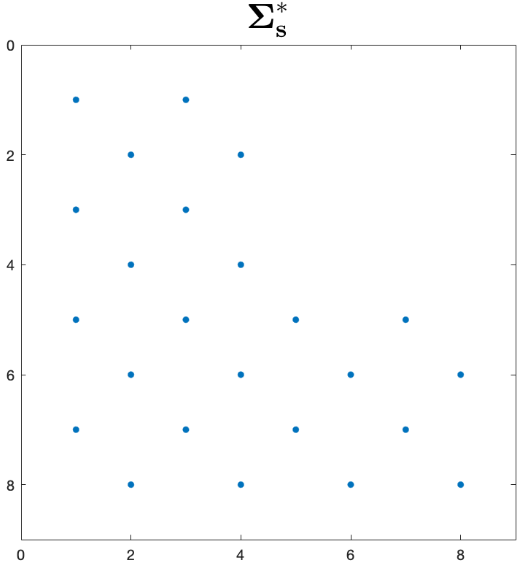
Theorem

The Perron-Froebenius Theorem for Primitive Matrices

Let $\mathbf{B} \geq \mathbf{0}$ be a primitive $n \times n$ matrix. Then,

1. $\mathbf{B}$ *has a positive real eigenvalue, λ_1, equal to its spectral radius, and which is greater than (in absolute value) all other eigenvalues.*
2. *For $\rho(\mathbf{B})$ there is a corresponding eigenvector $x > 0$.*
3. $\rho(\mathbf{B})$ *is a simple eigenvalue of $\mathbf{B}$.*

Primitivity of the Matrix $\mathbf{A}(\alpha)$



What Has Been Done Before?–Critical Search

$$\left(\mathbf{H} + \alpha^{\ell}\mathbf{V}^{-1}\right)\mathbf{\Psi}^{\ell} = \left(\mathbf{\Sigma}^{*}_{\mathbf{s}} + \frac{1}{k^{\ell}}\mathbf{\Sigma}^{*}_{\mathbf{f}}\right)\mathbf{\Psi}^{\ell} \tag{3}$$

Algorithm 1 Critical Search Method [?]

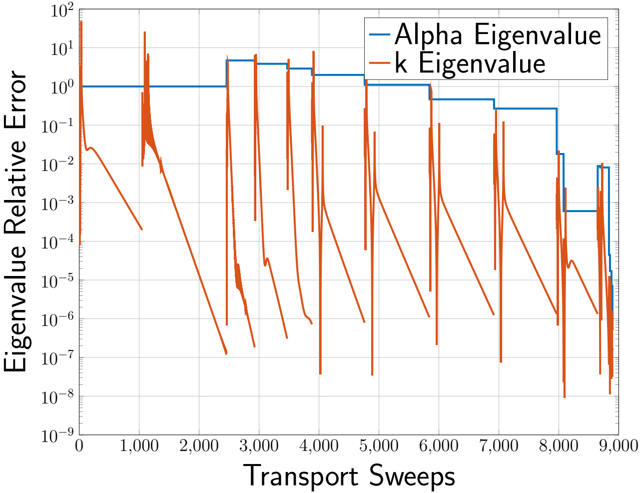
1: Make an initial guess for α^0.
2: Solve Eq. 3 for k^0.
3: Obtain a second guess α^1 by adjusting α^0 by some eigenvalue modifier value: $\alpha^1 = \alpha^0 + \text{EMV}$.
4: Solve Eq. 3 for k^1.
5: Using $(\alpha^{\ell}, k^{\ell})$ and $(\alpha^{\ell-1}, k^{\ell-1})$, perform a linear extrapolation of $k(\alpha)$ to find $\alpha^{\ell+1}$ such that $k^{\ell+1}(\alpha^{\ell+1}) = 1$.
6: Solve Eq. 3 for $k^{\ell+1}$.
7: Repeat until $k^{\ell+1} = 1$.

What Has Been Done Before?–Critical Search

- This method struggles for subcritical problems as the negative eigenvalue introduces negative absorption which can cause instability in the transport sweep [**?**].
- The method requires an eigenvalue modifier that is usually selected by the user. Bad modifiers might slow down convergence or prevent it entirely.
- Method incredibly slow for problems close to critical. Requires many k-eigenvalue calculations.
- Requires fissile material in system (non-multiplying problems are not possible).

Critical Search Convergence

Figure 1. Critical Search Convergence Behavior



A Fixed Point Method

$$\mathbf{\Psi} = \mathbf{H}^{-1}\Big[-\alpha\mathbf{V}^{-1} + \mathbf{\Sigma_s^*} + \mathbf{\Sigma_f^*}\Big]\mathbf{\Psi} \equiv \mathbf{A}(\alpha)\mathbf{\Psi}$$

- Given the limitations of the previous algorithm, we instead derive a fixed point method.
- For the fixed point equation above, we see that the fixed point to these equations is the positive eigenvector we are looking for.
- Given an approximate eigenvector, we need to derive an update for the eigenvalue.

Deriving the Eigenvalue Updates

- If $(\mathbf{\Psi}, \lambda)$ are an eigenpair, then

$$\|\mathbf{A}(\alpha_*)\mathbf{\Psi} - \lambda\mathbf{\Psi}\|_2^2 = 0.$$

- Suppose instead we have some approximate eigenvector, $\mathbf{\Psi}_i$. We find the corresponding best approximate eigenvalue λ_i by minimizing the residual in the least squares sense with respect to some parameter μ,

$$\lambda_i = \arg\min_{\mu} \|\mathbf{A}(\alpha_i)\mathbf{\Psi} - \mu\mathbf{\Psi}\|_2 . \quad (4)$$

- The previous equation is minimized when μ equals the Rayleigh quotient [**?**].

Deriving the Eigenvalue Updates–Continued

- The positive eigenvector corresponds to eigenvalue equal to one. We set the Rayleigh quotient equal to one and solve for the α_i:

$$1 = \frac{\mathbf{\Psi}_i^T \mathbf{A}(\alpha_i)\mathbf{\Psi}_i}{\mathbf{\Psi}_i^T \mathbf{\Psi}_i} = \frac{-\alpha_i \mathbf{\Psi}_i^T \mathbf{H}^{-1}\mathbf{V}^{-1}\mathbf{\Psi}_i + \mathbf{\Psi}_i^T \mathbf{H}^{-1}(\mathbf{\Sigma}_{\mathbf{s}}^* + \mathbf{\Sigma}_{\mathbf{f}}^*)\mathbf{\Psi}_i}{\mathbf{\Psi}_i^T \mathbf{\Psi}_i}$$

$$\rightarrow \alpha_i = \frac{\mathbf{\Psi}_i^T \mathbf{H}^{-1}(\mathbf{\Sigma}_{\mathbf{s}}^* + \mathbf{\Sigma}_{\mathbf{f}}^*)\mathbf{\Psi}_i - \mathbf{\Psi}_i^T \mathbf{\Psi}_i}{\mathbf{\Psi}_i^T \mathbf{H}^{-1}\mathbf{V}^{-1}\mathbf{\Psi}_i}.$$

The Rayleigh Quotient Fixed Point Method I

Algorithm 2 One-Sweep Rayleigh Quotient Fixed Point Method

while residual $>$ tolerance **do**

if $i = 0$ **then**

$$\alpha_{(i)} = \frac{\boldsymbol{\Psi}_{(i)}^{T}\left(\boldsymbol{\Sigma}_{\mathbf{s}}^{*} + \boldsymbol{\Sigma}_{\mathbf{f}}^{*}\right)\boldsymbol{\Psi}_{(i)}}{\boldsymbol{\Psi}_{(i)}^{T}\mathbf{V}_{\mathbf{z}}^{-1}\boldsymbol{\Psi}_{(i)}}.$$

$$\mathbf{q}_{(i)} = \Bigg(- \alpha_{(i)}\mathbf{V}_{\mathbf{z}}^{-1} + \boldsymbol{\Sigma}_{\mathbf{s}}^{*} + \boldsymbol{\Sigma}_{\mathbf{f}}^{*}\Bigg)\boldsymbol{\Psi}_{(i)}$$

$$\boldsymbol{\Psi}_{(i+1)} = \mathbf{H}_{\mathbf{z}}^{-1}\mathbf{q}_{(i)}$$

else

The Rayleigh Quotient Fixed Point Method II

$$\alpha_{(i)} = \frac{\boldsymbol{\Psi}_{(i)}^T \big(\boldsymbol{\Sigma}_{\mathbf{s}}^* + \boldsymbol{\Sigma}_{\mathbf{f}}^*\big) \boldsymbol{\Psi}_{(i)} - \boldsymbol{\Psi}_{(i)}^T \mathbf{q}_{(i-1)}}{\boldsymbol{\Psi}_{(i)}^T \mathbf{V}_{\mathbf{z}}^{-1} \boldsymbol{\Psi}_{(i)}}.$$

$$\mathbf{q}_{(i)} = \Bigg(- \alpha_{(i)} \mathbf{V}_{\mathbf{z}}^{-1} + \boldsymbol{\Sigma}_{\mathbf{s}}^* + \boldsymbol{\Sigma}_{\mathbf{f}}^* \Bigg) \boldsymbol{\Psi}_{(i)}$$

$$\boldsymbol{\Psi}_{(i+1)} = \mathbf{H}_{\mathbf{z}}^{-1} \mathbf{q}_{(i)}$$

end if

$$\text{residual} = \frac{\big\| \boldsymbol{\Psi}_{(i+1)} - \boldsymbol{\Psi}_{(i)} \big\|_2}{\big\| \boldsymbol{\Psi}_{(i+1)} \big\|_2}$$

end while

Results

1D Criticality Benchmark Problems

Table 1. Criticality Benchmark Problem List and Properties

Problem ID	Problem Properties: 1D Slab	1D Spherical	Infinite Medium	Reflected BC	Reference k_{eff}
PUa-1-0-IN			✓		2.612903
PUa-1-0-SL	✓				1.00
PUb-1-0-IN			✓		2.290323
PUa-H2O(1)-1-0-SL	✓			✓	1.00
PUa-H2O(0.5)-1-0-SL	✓			✓	1.00
PUb-1-0-SL	✓				1.00
PUb-1-0-SP		✓			1.00
Ua-1-0-SL	✓				1.00
Ua-1-0-IN			✓		2.25
Ub-1-0-IN			✓		2.330917
Uc-1-0-IN			✓		2.256083
Ud-1-0-IN			✓		2.232667

- Benchmark problems from the *Analytical Benchmark Test Set for Criticality Code Verification* [**?**].

Results

Alpha–Eigenvalue Sweep Comparison

Table 2. Alpha-Eigenvalue Sweep Comparisons

(a) Infinite Medium Sweeps

Problem ID	Sweeps: Rayleigh Quotient	Sweeps: Critical Search Method
Plutonium (a)	33	432
Plutonium(b)	21	391
Uranium(a)	24	472
Uranium(b)	24	464
Uranium(c)	24	474
Uranium(d)	24	472

(b) Critical System Sweeps

Problem ID	Sweeps: Rayleigh Quotient	Sweeps: Critical Search Method
Plutonium(a) Slab	26	64
Plutonium(a)/Water Slab	37	*
Plutonium(b)/Water Slab	23	*
Plutonium(b) Slab	24	*
Plutonium(b) Sphere	37	105
Uranium(a) Slab	27	*

* Did Not Converge

- Critical search requires multiple k-effective calculations.
- Rayleigh quotient method performed better than the critical search method for subcritical, critical, and supercritical systems.

Results

Alpha-Eigenvalue L_2 Convergence for Select Problems

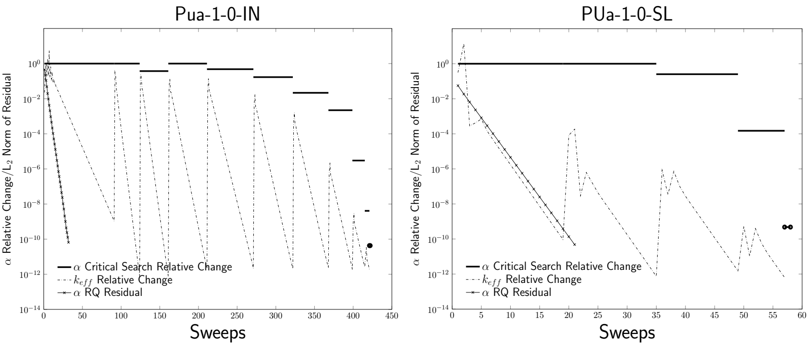
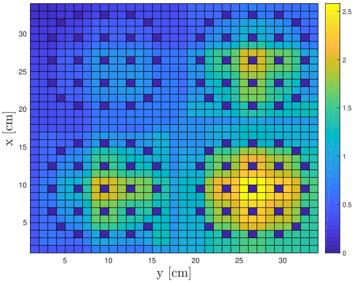


Figure 2. Eigenvalue Relative Change/Residual as a Function of Sweeps for α-Eigenvalue Problems

Results

2D MOX Fuel Assembly-Transport Sweep Comparison

Figure 3. NEA MOX Fuel Benchmark

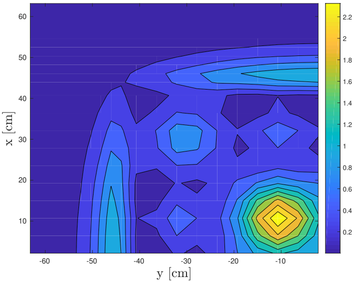


$$k_{\text{eff}} = 1.186550$$
$$\alpha_0 = 1.4930 \times 10^5\ \text{s}^{-1}$$

Table 3. Transport Sweeps for Convergence

α Rayleigh Quotient
1332

α Critical Search
8896



Results

2D MOX Fuel Assembly-Scalar Fluxes

Figure 4. Scalar Flux ϕ_g, $g = 4$

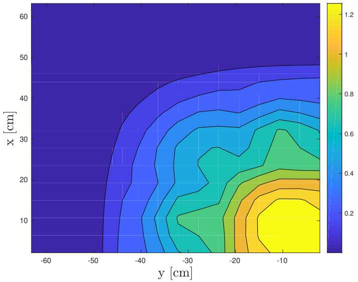
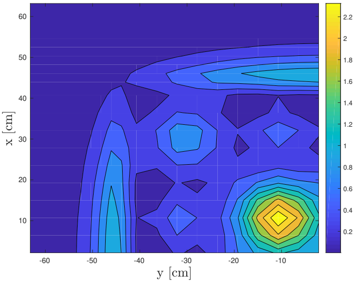


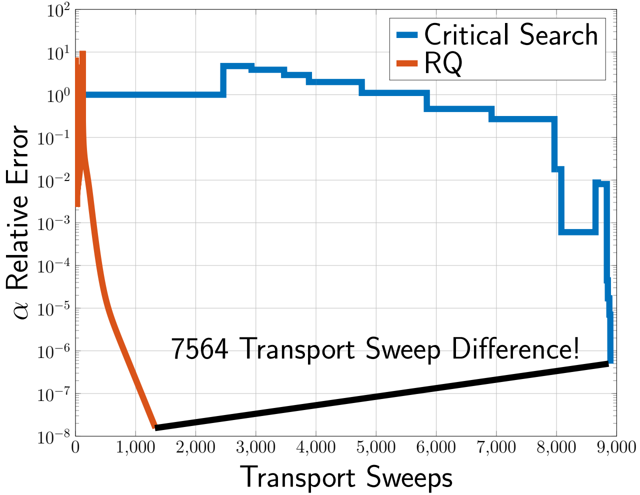
Figure 5. Scalar Flux ϕ_g, $g = 6$



Results

2D MOX Fuel Assembly-Scalar Fluxes

Figure 6. Relative Error Comparison



Results

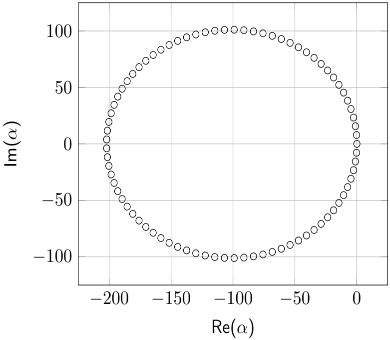
Failures-81 Group Infinite Medium Analytical Alpha-Eigenvalue Problem (Betzler)

$$\frac{\alpha_n}{v} = -(\sigma_g - \sigma_f) + \sigma_{sg,g+1}\left[\bar{\nu}^{G-1}\exp\left(\frac{2\pi i n}{G}\right) - 1\right], \text{ for } n = 0, \ldots, G-1.$$

- The Rayleigh Quotient method fails for certain test problems.
- Sometimes occurs when the irreducibility/primitivity condition is not met.

Table 4. Infinite Medium 81-Group Problem Cross Sections (cm^{-1})

g	σ	σ_f	$\sigma_{sg,g+1}$	χ	v_g [cm/s]
1	101.0	0.0	100.0	1.0	1.0
2-80	101.0	0.0	100.0	0.0	1.0
81	101.0	100.0	0.0	0.0	1.0



Conclusion

- We have developed an alpha-eigenvalue Rayleigh quotient fixed point method that is able to obtain the eigenpair for subcritical/critical/supercritical systems.
- We showed that the discretized transport eigenvalue problems form a primitive system of linear equations.
- Using primitivity, we are able to guarantee the existence of a simple, dominant eigenvalue with a corresponding unique, positive eigenvector.

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- Thank you! Questions?