Extension of Tom Booth's Modified Power Method for Higher Eigen Modes

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1. Introduction

The power iteration method is commonly used to get the fundamental eigenmode (0^{th} mode). Recent years a modified power iteration method was proposed by Tom Booth [1-8] and it can be applied to get the second smallest eigenmode (1^{st} mode) [9-10]. A possible technique to get the even higher modes is suggested, but it is difficult to be applied practically. In this paper, a general solution strategy is proposed, which can extend Tom Booth's modified power method to get the higher eigenmodes and there is no limitation about the number of eigenmodes that can be obtained with this method.

2. Theory

In this section the modified power iteration method and the general solution strategy are presented.

2.1 The modified power iteration method to get the 1st eigenmode

Supposing that after many times of power iterations, only the first two smallest eigenmodes exist and the higher eigenmodes are negligible. The eigenfunctions can be written as:

$$\begin{aligned}\psi_1 &= a_0\phi_0 + a_1\phi_1,\\ \psi_2 &= b_0\phi_0 + b_1\phi_1,\end{aligned} \tag{1}$$

where ψ_1 and ψ_2 are resulted from different initial sources. Considering the linear combination of ψ_1 and ψ_2,

$$\begin{aligned}\psi &= \psi_1 + x\psi_2\\ &= (a_0 + b_0 x)\phi_0 + (a_1 + b_1 x)\phi_1.\end{aligned} \tag{2}$$

If $x = -a_1/b_1$, ψ will be the 0^{th} eigenmode; while if $x = -a_0/b_0$, ψ will be the 1^{st} eigenmode. The corresponding eigenvalue:

$$\lambda = \frac{\int \psi^n dr}{\int \psi^{n-1} dr} = \frac{\int A\psi^{n-1} dr}{\int \psi^{n-1} dr} \tag{3}$$

will be the 0^{th} and 1^{st} eigenvalues, k_0 and k_1, respectively.

It is then observed that the integration of ψ in any subregion of the system will produce the same eigenvalue. Typically, choose two subregions R1 and R2:

$$\lambda = \frac{\int_{R1} \psi^n dr}{\int_{R1} \psi^{n-1} dr} = \frac{\int_{R2} \psi^n dr}{\int_{R2} \psi^{n-1} dr}. \tag{4}$$

If we denote:

$$\int_{Rj} \psi_i dr = W_{ij}, \int_{Rj} A\psi_i dr = AW_{ij}, \tag{5}$$

then Eq. (4) will become:

$$\lambda = \frac{AW_{11} + xAW_{21}}{W_{11} + xW_{21}} = \frac{AW_{12} + xAW_{22}}{W_{12} + xW_{22}}, \tag{6}$$

which will then leads to $c_2x^2 + c_1x + c_0 = 0$ with

$$\begin{aligned}c_2 &= AW_{21}\cdot W_{22} - AW_{22}\cdot W_{21},\\ c_1 &= AW_{21}\cdot W_{12} + AW_{11}\cdot W_{22}\\ &\quad - AW_{22}\cdot W_{11} - AW_{12}\cdot W_{21},\\ c_0 &= AW_{11}\cdot W_{12} - AW_{12}\cdot W_{11}.\end{aligned} \tag{7}$$

If two real solutions of the quadratic equation exist, they will certainly be $x_1 = -a_1/b_1$ and $x_2 = -a_0/b_0$. The corresponding eigenvalues and eigenfunctions will be:

$$\begin{aligned}\lambda_{1,2} &= \frac{AW_{1i} + x_{1,2}AW_{2i}}{W_{1i} + x_{1,2}W_{2i}},\\ \psi'_{1,2} &= \psi_1 + x_{1,2}\psi_2.\end{aligned} \tag{8}$$

The strategy is to apply A repeatedly to ψ_1 and ψ_2, and continue updating $\lambda_{1,2}$ and $\psi'_{1,2}$. (λ_1, ψ'_1) and (λ_2, ψ'_2) will finally converge to (k_0, ϕ_0) and (k_1, ϕ_1).

2.2 The modified power iteration method to get the 2nd eigenmode

Similar to the previous section, we can write 3 different eigenfunctions as:

$$\begin{aligned}\psi_1 &= a_0\phi_0 + a_1\phi_1 + a_2\phi_2,\\ \psi_2 &= b_0\phi_0 + b_1\phi_1 + b_2\phi_2,\\ \psi_3 &= c_0\phi_0 + c_1\phi_1 + c_2\phi_2.\end{aligned} \tag{9}$$

The linear combination of the three functions can be:

$$\begin{aligned}\psi &= \psi_1 + x\psi_2 + y\psi_3 \\ &= \left(a_0 + b_0 x + c_0 y\right)\phi_0 \\ &+ \left(a_1 + b_1 x + c_1 y\right)\phi_1 \\ &+ \left(a_2 + b_2 x + c_2 y\right)\phi_2 .\end{aligned} \tag{10}$$

Then, it is integrated over three different subregions to get the same eigenvalue:

$$\lambda = \frac{\int_{R1}\psi^n dr}{\int_{R1}\psi^{n-1}dr} = \frac{\int_{R2}\psi^n dr}{\int_{R2}\psi^{n-1}dr} = \frac{\int_{R3}\psi^n dr}{\int_{R3}\psi^{n-1}dr}. \tag{11}$$

Substitute Eq. (5) into Eq. (11) we can get:

$$\begin{aligned}\lambda &= \frac{AW_{11} + xAW_{21} + yAW_{31}}{W_{11} + xW_{21} + yW_{31}} \\ &= \frac{AW_{12} + xAW_{22} + yAW_{32}}{W_{12} + xW_{22} + yW_{32}} \\ &= \frac{AW_{13} + xAW_{23} + yAW_{33}}{W_{13} + xW_{23} + yW_{33}}.\end{aligned} \tag{12}$$

This will result in a nonlinear equation system to get the unknown variables λ, x, and y. There should be three different sets of solutions which lead to the 0th, 1st and 2nd eigenmodes, respectively. To solve such nonlinear equation system may be difficult, so it is not practical to get the 2nd and even higher eigenmodes with this solution strategy.

2.3 Another solution strategy to get the 1st eigenmode

We concentrate on the solution of Eq. (6) at this section. It can be rewritten as:

$$x = \frac{\lambda W_{11} - AW_{11}}{AW_{21} - \lambda W_{21}} = \frac{\lambda W_{12} - AW_{12}}{AW_{22} - \lambda W_{22}}. \tag{13}$$

This will leads to $c_2\lambda^2 + c_1\lambda + c_0 = 0$ with

$$\begin{aligned}c_2 &= W_{11}W_{22} - W_{12}W_{21}, \\ c_1 &= -W_{11}\cdot AW_{22} - W_{22}\cdot AW_{11} \\ &\quad + W_{12}\cdot AW_{21} + W_{21}\cdot AW_{12}, \\ c_0 &= AW_{11}\cdot AW_{22} - AW_{12}\cdot AW_{21}.\end{aligned} \tag{14}$$

We can first get the two solutions of $\lambda_{1,2}$, and then substitute them to Eq. (13) to get $x_{1,2}$.

Now we consider the transfer matrix $\overline{\overline{P}}$, which is defined as:

$$\begin{aligned}\overline{\overline{AW}} &= \overline{\overline{P}}\cdot\overline{\overline{W}}, \\ \begin{pmatrix} AW_{11} & AW_{21} \\ AW_{12} & AW_{22}\end{pmatrix} &= \overline{\overline{P}}\cdot\begin{pmatrix} W_{11} & W_{21} \\ W_{12} & W_{22}\end{pmatrix}.\end{aligned} \tag{15}$$

The solution of $\overline{\overline{P}}$ is:

$$\begin{aligned}\overline{\overline{P}} &= \begin{pmatrix} AW_{11} & AW_{21} \\ AW_{12} & AW_{22}\end{pmatrix}\cdot\frac{1}{W_{11}W_{22} - W_{21}W_{12}}\begin{pmatrix} W_{22} & -W_{21} \\ -W_{12} & W_{11}\end{pmatrix} \\ &= \frac{1}{W_{11}W_{22} - W_{21}W_{12}}\cdot \\ &\begin{pmatrix} AW_{11}\cdot W_{22} - AW_{21}\cdot W_{12} & -AW_{11}\cdot W_{21} + AW_{21}\cdot W_{11} \\ AW_{12}\cdot W_{22} - AW_{22}\cdot W_{12} & -AW_{12}\cdot W_{21} + AW_{22}\cdot W_{11}\end{pmatrix}.\end{aligned} \tag{16}$$

We are interested in the eigenvalues of the transfer matrix $\overline{\overline{P}}$, so we need to solve the equation:

$$\begin{vmatrix} p_{11} - \lambda & p_{12} \\ p_{21} & p_{22} - \lambda\end{vmatrix} = 0. \tag{17}$$

If we substitute the elements of $\overline{\overline{P}}$ into Eq. (7), we can get the quadratic equation $q_2\lambda^2 + q_1\lambda + q_0 = 0$ with

$$\begin{aligned}q_2 &= W_{11}\cdot W_{22} - W_{12}\cdot W_{21}, \\ q_1 &= -W_{11}\cdot AW_{22} - W_{22}\cdot AW_{11} \\ &\quad + W_{12}\cdot AW_{21} + W_{21}\cdot AW_{12}, \\ q_0 &= AW_{11}\cdot AW_{22} - AW_{12}\cdot AW_{21}.\end{aligned} \tag{18}$$

The coefficients are the same as that given in Eq. (14). Thus, the solutions of $\lambda_{1,2}$ is exactly the eigenvalus of the transfer matrix.

Now let's look at the solution of $x_{1,2}$, which can be written in matrix form:

$$\begin{aligned}&\begin{pmatrix} AW_{11} & AW_{21} \\ AW_{12} & AW_{22}\end{pmatrix}\begin{pmatrix} 1 & 1 \\ x_1 & x_2\end{pmatrix} \\ &= \begin{pmatrix} W_{11} & W_{21} \\ W_{12} & W_{22}\end{pmatrix}\begin{pmatrix} 1 & 1 \\ x_1 & x_2\end{pmatrix}\begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2\end{pmatrix}.\end{aligned} \tag{19}$$

Substitute Eq. (15) into Eq. (19), we can get:

$$\begin{aligned}&\overline{\overline{P}}\begin{pmatrix} W_{11} & W_{21} \\ W_{12} & W_{22}\end{pmatrix}\begin{pmatrix} 1 & 1 \\ x_1 & x_2\end{pmatrix} \\ &= \begin{pmatrix} W_{11} & W_{21} \\ W_{12} & W_{22}\end{pmatrix}\begin{pmatrix} 1 & 1 \\ x_1 & x_2\end{pmatrix}\begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2\end{pmatrix}.\end{aligned} \tag{20}$$

If we can get the eigenvalues and corresponding eigenvectors of $\overline{\overline{P}}$:

$$\begin{aligned}&\overline{\overline{P}}\cdot\overline{\overline{V}} = \overline{\overline{V}}\cdot\overline{\overline{D}} \\ &\overline{\overline{D}} = \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2\end{pmatrix}, \overline{\overline{V}} = \begin{pmatrix} V_{11} & V_{21} \\ V_{12} & V_{22}\end{pmatrix}.\end{aligned} \tag{21}$$

Then, we can solve $x_{1,2}$ with

$$\begin{aligned}&\begin{pmatrix} W_{11} & W_{21} \\ W_{12} & W_{22}\end{pmatrix}\begin{pmatrix} 1 & 1 \\ x_1 & x_2\end{pmatrix} = \begin{pmatrix} C_1 & 0 \\ 0 & C_2\end{pmatrix}\begin{pmatrix} V_{11} & V_{21} \\ V_{12} & V_{22}\end{pmatrix}, \\ &\overline{\overline{W}}\cdot\overline{\overline{X}} = \overline{\overline{C}}\cdot\overline{\overline{V}},\end{aligned} \tag{22}$$

where $\overline{\overline{C}}$ contains the constants that are just used to scale the eigenvectors. Considering the normalization operation during every iteration of the power method, we can simplify the solution of $x_{1,2}$ as:

$$\begin{pmatrix} W_{11} & W_{21} \\ W_{12} & W_{22} \end{pmatrix}\begin{pmatrix} 1 & x_2 \\ x_1 & 1 \end{pmatrix}=\begin{pmatrix} V_{11} & V_{21} \\ V_{12} & V_{22} \end{pmatrix}, \quad (23)$$

and update the eigenfunctions as:

$$\begin{bmatrix} \psi'_1 & \psi'_2 \end{bmatrix}=\begin{bmatrix} \psi_1 & \psi_2 \end{bmatrix}\begin{pmatrix} 1 & x_2 \\ x_1 & 1 \end{pmatrix}. \quad (24)$$

2.4 The general solution strategy to get the higher eigenmodes

Similarly, in order to get the first *N* eigenmodes, we should define *N* regions and get the integration of *N* different eigenfunctions in these *N* regions. The general solution strategy is as following.

(1) During each power iteration, get

$$\overline{\overline{W}}=\begin{pmatrix} W_{11} & \cdots & W_{N1} \\ \vdots & \ddots & \vdots \\ W_{1N} & \cdots & W_{NN} \end{pmatrix},$$
$$\overline{\overline{AW}}=\begin{pmatrix} AW_{11} & \cdots & AW_{N1} \\ \vdots & \ddots & \vdots \\ AW_{1N} & \cdots & AW_{NN} \end{pmatrix}, \quad (25)$$

where W_{ij} and AW_{ij} are defined as in Eq. (5).

(2) Get the transfer matrix

$$\overline{\overline{P}}=\overline{\overline{AW}}\cdot\overline{\overline{W}}^{-1}. \quad (26)$$

(3) Get the eigenvalues and eigenvectors of transfer matrix:

$$\overline{\overline{P}}\cdot\overline{\overline{V}}=\overline{\overline{V}}\cdot\overline{\overline{D}}. \quad (27)$$

(4) The eigenvalues contained in $\overline{\overline{D}}$ are sorted to be from the largest to the smallest, and the eigenvectors contained in $\overline{\overline{V}}$ are changed accordingly.

(5) Get the correction matrix $\overline{\overline{X}}$:

$$\overline{\overline{X}}=\overline{\overline{AW}}^{-1}\cdot\overline{\overline{V}}. \quad (28)$$

And set the diagonal elements of $\overline{\overline{X}}$ to 1. That is,

$$for\ i=1,N$$
$$\overline{\overline{X}}(:,i)=\overline{\overline{X}}(:,i)\Big/\overline{\overline{X}}(i,i) \quad (29)$$
$$end$$

With the diagonal elements to be 1, the shape of the eigenfunctions can be kept the same.

(6) Update the *N* eigenfunctions:

$$\begin{pmatrix} \psi'_1 & \cdots & \psi'_N \end{pmatrix}=\begin{pmatrix} \psi_1 & \cdots & \psi_N \end{pmatrix}\cdot\overline{\overline{X}}. \quad (30)$$

And then renormalize each eigenfunction.

3. Numerical Tests

In this section the deterministic and Monte Carlo results for 1D slab problems are given to show the performance of the method.

3.1 Demonstration of the method with FDM

A 1D1G slab problem is tested to show the ability of the general solution strategy for higher eigenmodes. The first four eigenmodes are considered.

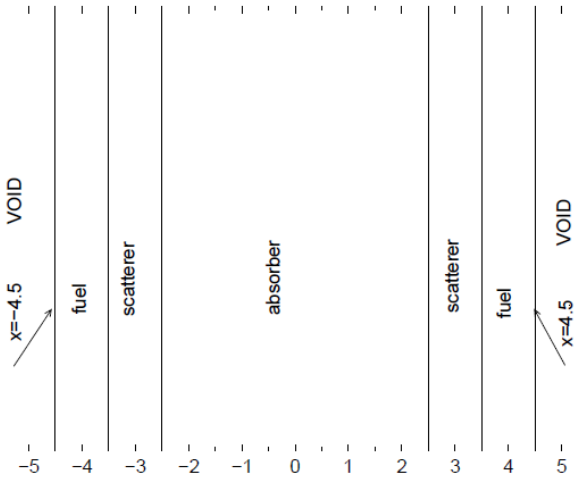

Fig. 1. Split fuel problem geometry

Table I. Cross Sections of Material

Material	Σ_a (1/cm)	$\nu\Sigma_f$ (1/cm)	D (cm)
Fuel	0.20	0.30	0.33
Scatterer	0.20	0.00	0.33
Absorber	0.90	0.00	0.33

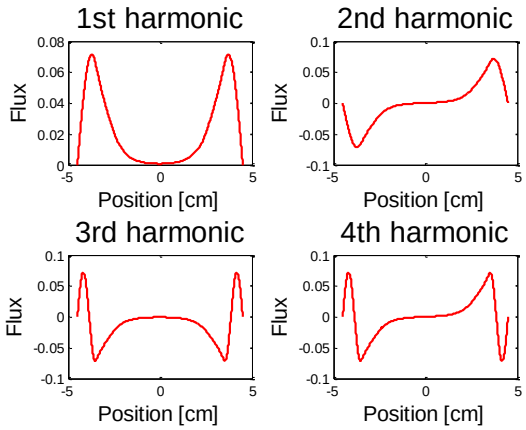

Fig. 2. The first 4 eigenmodes

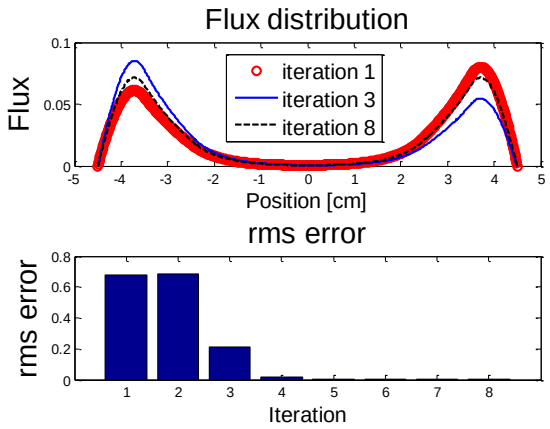

Fig. 3. Flux distribution and the RMS error of the flux (with 4 eigenmodes)

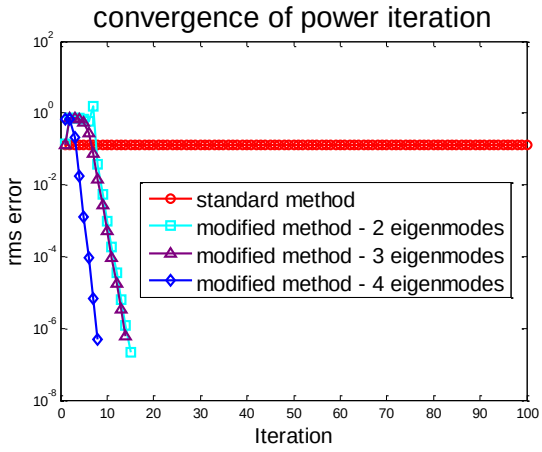

Fig. 4. Convergence analysis of the standard power method and the modified power method with different eigenmodes

Table II. Eigenvalue results

Parameter	Value
k_0	0.196417
k_1	0.196406
k_2	0.036654
k_3	0.036653
Convergence rate of the standard power method (~k_1/k_0)	0.999945
Convergence rate of the modified power method with 2 eigenmodes (~k_2/k_0)	0.186609
Convergence rate of the modified power method with 3 eigenmodes (~k_3/k_0)	0.186609
Convergence rate of the modified power method with 4 eigenmodes (~k_4/k_0)	0.071552

3.2 Implementation of the method in Continuous energy Monte Carlo code

A 1D fuel slab problem is chosen to test the implementation of the modified power method in continuous energy Monte Carlo code. The first four eigenmodes are considered.

The Monte Carlo simulations with both original and modified power method are done with 200 inactive cycles / 1000 active cycles / 5,000 histories per cycle. Parallel computing with 7 threads is adopted with the typical desktop computer.

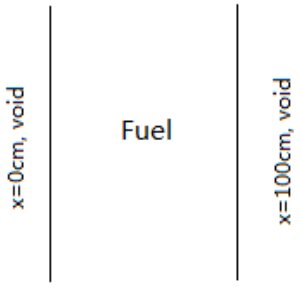

Fig. 5. 1D slab problem geometry

Table III. Composition of the fuel (units: atoms/barn-cm)

Nuclide	Density
H-1	5.9347E-02
N-14	2.1220E-03
O-16	3.7258E-02
U-235	7.6864E-05
U-238	6.8303E-04

Table IV. Eigenvalue results

Parameter	Value
k_0 (original)	1.25797±0.00018
k_0	1.25845±0.00015
k_1	1.15626±0.00059
k_2	1.01823±0.00070
k_3	0.86440±0.00082

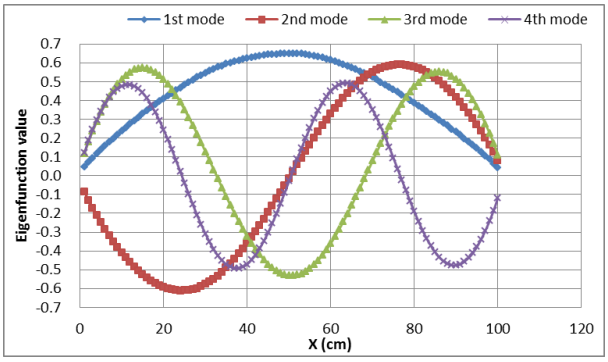

Fig. 6. The first 4 eigenmodes

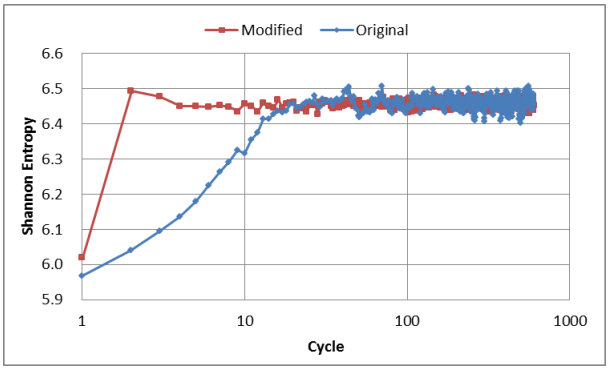

Fig. 7. The Shannon Entropy results of the original and modified power method

It can be seen that the fundamental eigenvalue result of the modified power method is consistent with the original power method, the difference is within 3σ. As shown with the Shannon Entropy results, the source convergence rate is significantly increased with the modified power method. The computing times for the original and modified power method are 22.38 and 26.98 minutes respectively, which show that the implementation of the modified power method with Monte Carlo code doesn't require obviously more simulation time.

4. Conclusions

In this paper, a general solution strategy is proposed, which can extend Tom Booth's modified power method to get the higher eigenmodes and there is no limitation about the number of eigenmodes that can be obtained with this method. It is more practical than the original solution strategy that Tom Booth proposed. The implementation of the method in Monte Carlo code shows significant advantages comparing to the original power method.

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