(U) Time-Eigenvalue Estimation using the Dynamic Mode Decomposition

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Abstract

We consider a sequence of vectors that are solutions to a discretized neutron transport problem:

$$\frac{\partial \psi}{\partial t} = A\psi(t),$$

where ψ is a vector of length N containing the spatial, energy, and angle degrees of freedom, and A is the transport operator:

$$A = v(E)(-\Omega \cdot \nabla + -\sigma_{\rm t} + \mathcal{S} + \mathcal{F}),$$

with $\mathcal{S}$ and $\mathcal{F}$ the scattering and fission operators. In our notation, the α eigenvalues and eigenvectors satisfy this equation:

$$A\hat{\psi} = \alpha\hat{\psi}.$$

The vectors are the solutions at particular times separated by time steps of size Δt. We define $\psi_k \equiv \psi(k\Delta t)$ and the vectors are related by the matrix exponential:

$$\psi_{k+1} = e^{A\Delta t}\psi_k.$$

We take $K+1$ of these vectors to form the $N \times K$ *data matrices* Y_+ and Y_-,

$$Y_+ = \begin{pmatrix} | & | & & | \\ \psi_1 & \psi_2 & \dots & \psi_K \\ | & | & & | \end{pmatrix} \qquad Y_- = \begin{pmatrix} | & | & & | \\ \psi_0 & \psi_1 & \dots & \psi_{K-1} \\ | & | & & | \end{pmatrix}.$$

These matrices are related as

$$Y_+ = e^{A\Delta t}Y_-. \tag{1}$$

the thin singular value decomposition (SVD) of Y_- to write

$$Y_- = U\Sigma V^{\mathrm{T}},$$

where U is a $N \times K$ orthogonal matrix, Σ is a diagonal $K \times K$ matrix with non-negative entries on the diagonal, and V is a $K \times K$ orthogonal matrix. Using properties of orthogonal matrices we can substitute the SVD into Eq. (1) to approximate the matrix exponential:

$$U^{\mathrm{T}} e^{A\Delta t} U = U^{\mathrm{T}} Y_+ V \Sigma^{-1}.$$

The estimation of an approximate operator using the SVD of data is called the dynamic mode decomposition (DMD) in the computational fluid dynamics literature [1].

One can show the following: (1) The eigenvalues of $U^{\mathrm{T}} e^{A\Delta t} U$ are also eigenvalues of $e^{A\Delta t}$. (2) If α is an eigenvalue of A, then $e^{\alpha\Delta t}$ is an eigenvalue of $e^{A\Delta t}$. (3) The eigenvectors of A are the same as those from $e^{A\Delta t}$.

Therefore, if we estimate the eigenvalues λ of the $K \times K$ matrix $U^{\mathrm{T}} e^{A\Delta t} U$, we can compute the alpha eigenvalues of the system as

$$\alpha = \frac{\log \lambda}{\Delta t}.$$

This requires no specialized α-eigenvalue solver: we only need to evolve the system in time from an initial condition and use the time-dependent solution to estimate eigenvalues/vectors.

If the time discretization used in the time dependent transport solve is backward Euler (as is common), then a better approximation is

$$\alpha = \frac{\lambda - 1}{\Delta t \lambda},$$

because this method makes the approximation $e^{A\Delta t} \approx (I - A\Delta t)^{-1}$.

As an example calculation we consider a 12-group calculation of an infinite medium of Pu-239 with a buckling approximation to simulate a finite sphere. We set the radius in the buckling approximation to make $k_{\text{eff}} = 0.95$. The eigenvalues we get from the full transport operator for this system are in the first column of Table I.

Using an initial condition of only neutrons in the group containing 14.1 MeV, we run a time dependent problem to a specified final time. We then use the last 10 time steps to estimate the α eigenvalues. The values of α estimated are shown in Table I and the eigenvectors are show in Fig. 1. Early in time the modes corresponding to the spike at 14.1 MeV are found by the DMD calculation, late in time we relax to the fundamental, slowly decaying mode. The $\alpha = -29.1318\ \mu\mathrm{s}^{-1}$ eigenmode is not present because it has a larger number of thermal neutrons than our system does and was not excited by our initial condition.

Our observation using this method is that it finds the eigenvalues/vectors that have the most neutrons in them over the course of the time steps used. This can be useful for calculating what eigenvalues one should expect to observe in an experiment.

Table I: Eigenvalues of the 12-group subcritical sphere as estimated by a direct calculation and from a DMD calculation using 10 times steps before t_{final}.

Exact (μs^{-1})	$t_{\text{final}} = 0.0001$ μs	0.002 μs	0.02 μs	0.2 μs
-17.9734			-18.2064	-17.9802
-29.1318				
-34.6882			-34.6326	-34.6946
-48.783				
-75.6007			-73.261	
-133.304	-140.235		-150.13	
-264.032			-259.257	
-552.353		-531.228		
-900.368	-765.929	-760.506		
-1379.38				
-1746.03				
-1972.14	-1972.12	-1971.39		

We also present results from a slab-geometry system comprised of ^{239}Pu and high-density polyethylene (HDPE) where the material layout is given by

$$\text{material}(x) = \begin{cases} \text{HDPE} & x \in (0\,\text{cm}, 1.42\,\text{cm}) \\ ^{239}\text{Pu} & x \in (1.42\,\text{cm}, 2.334\,\text{cm}) \\ \text{HDPE} & x \in (2.334\,\text{cm}, 22.696\,\text{cm}) \\ ^{239}\text{Pu} & x \in (22.696\,\text{cm}, 23.8\,\text{cm}) \\ \text{HDPE} & x \in (23.8\,\text{cm}, 25.25\,\text{cm}) \end{cases} .$$

The initial condition for the system has 14.1 MeV neutrons incident at $x = 0$ and $25.25\,\text{cm}$. We solve this problem with 70 groups, diamond difference in space, S_8 in angle, and a time step of 0.0001 μs. The estimated k_{eff} for the system is 0.97004. The neutron density as a function of space and the spectrum at two points are shown in Fig. 2.

Early in time, at 0.0005 μs, the rightmost eigenvalue estimated by DMD is -660.87 μs^{-1}. Later, at 0.1 μs, the rightmost eigenvalue estimated is -9.306495 μs^{-1}. Near 1 μs the rightmost eigenvalue estimated is -0.448908 μs^{-1}.

References

[1] Schmid, P. J. Dynamic mode decomposition of numerical and experimental data. *Journal of Fluid Mechanics*, 656, 5–28 (2010).

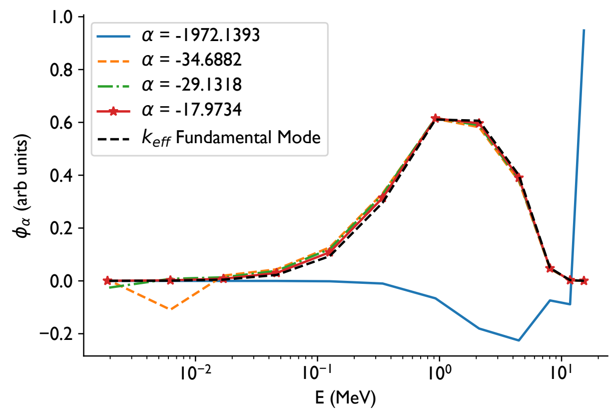

Figure 1: Comparison of scalar flux for the fundamental k eigenmode with 4 α eigenmodes for the subcritical sphere.

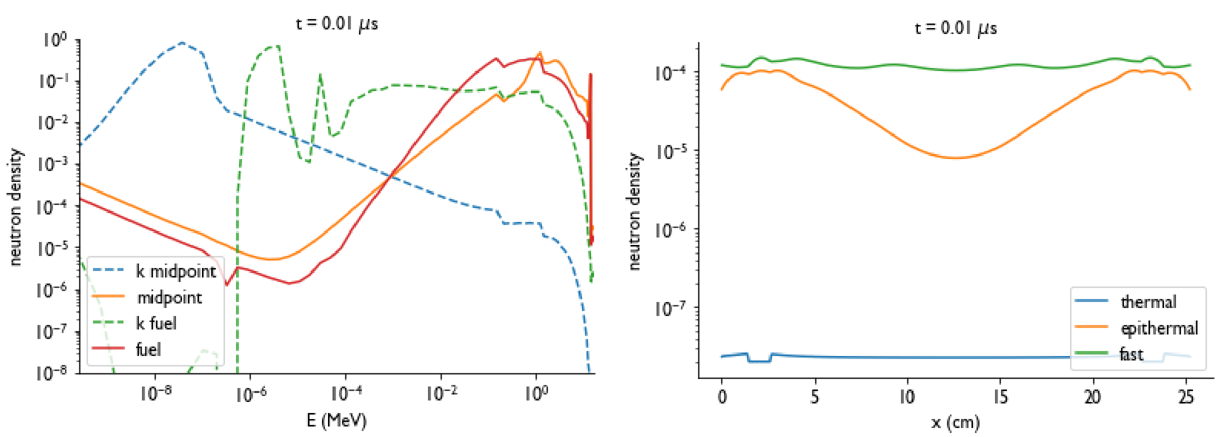

Figure 2: Spatial profile for neutron density and spectrum the center of the fuel and at the midpoint of the problem at 0.01 μs.