Finding The Rightmost Eigenvalues of Large Sparse Non-Symmetric Parameterized Eigenvalue Problem

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Introduction

Consider the eigenvalue problem

$$A_S x = \lambda B_S x \qquad (1)$$

where A_S and B_S are large sparse non-symmetric real $N \times N$ matrices and S is a set of parameters given by the underlying partial differential equation (PDE).

I am primarily interested in computing the rightmost eigenvalues (namely, eigenvalues of the largest real parts) of (1). The motivation lies in the stability analysis of steady state solutions of systems of PDEs of the form:

$$B\frac{du}{dt} = f(u) \quad f: R^N \to R^N, \quad u \in R^N \qquad (2)$$

Introduction

$$B\frac{du}{dt} = f(u) \quad f : R^N \to R^N, \quad u \in R^N \qquad (2)$$

Define the Jacobian matrix for the steady state u^* by $A = \partial f / \partial u\left(u^*\right)$, then u^* is stable if the eigenvalues of (1) all have negative real parts.

Typically, f arises from the spatial discretization of a PDE. When finite differences are used to discretize a PDE, then often $B = I$ and (1) is called a standard eigenproblem. If the equations are discretized by finite elements, $B \neq I$ and (1) is called a generalized eigenvalue problem.

Introduction

Beside the numerical algorithm of computing rightmost eigenvalues, another interesting problem is how the stability of steady state solution will change as the parameters vary.

Example: Olmstead Model (Nonlinear Diffusion Equation)

Rayleigh Number

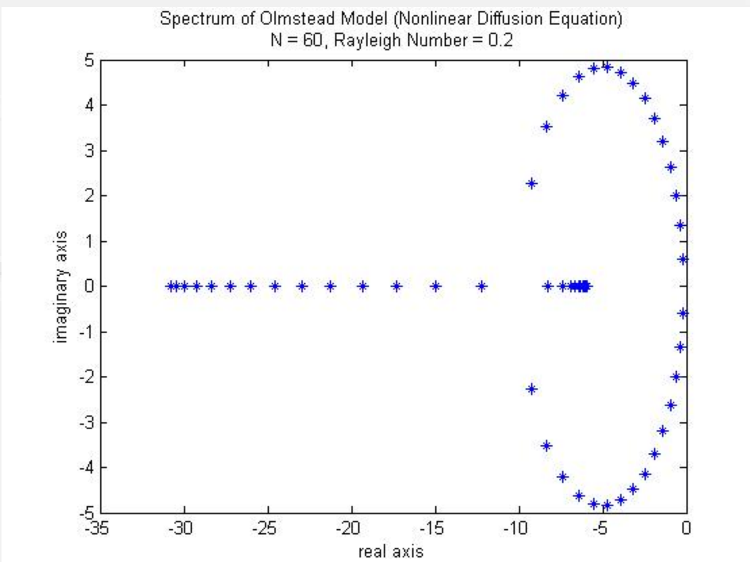


Fig 1. steady state solution is stable

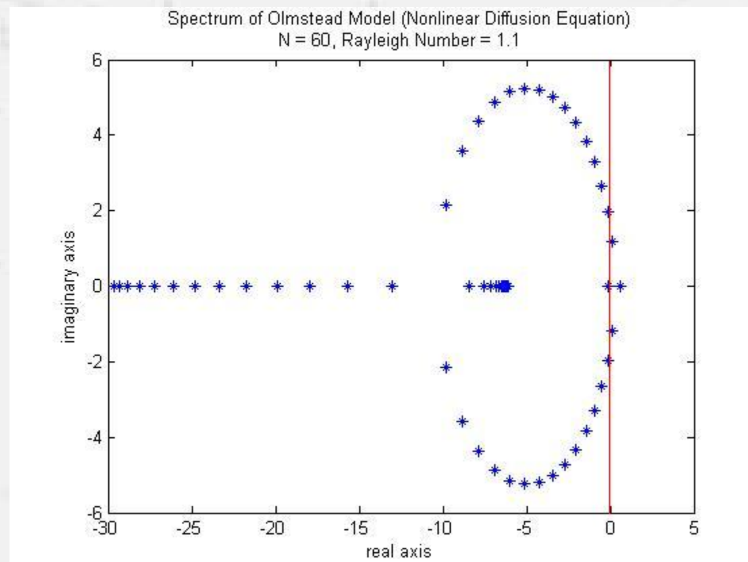


Fig 2. steady state solution is NOT stable

Major Computational Difficulties

- **A and B are large, sparse and non-symmetric**

    Iterative methods must be used.

- **Iterative methods cannot solve generalized eigenvalue problems**

    Matrix transformation $Ax = \lambda Bx \rightarrow Tz = \theta z$ is necessary.

- **Rightmost eigenvalues are often hard to find by eigensolvers**

    Matrix transformation must map rightmost eigenvalues to well-separated extremal eigenvalues.

- **Rightmost eigenvalues can be complex**

    Complex arithmetic should be considered.

Methodology

- **Eigensolver**
- **Matrix Transformation**

Eigensolver: Arnoldi Type Algorithm

- The standard Arnoldi Algorithm:

  It builds the Krylov subspace $K_k(A,v_1) = span\{v_1, Av_1, A^2 v_1, \ldots, A^{k-1} v_1\}.$

$procedure\ \{(\lambda_i, x_i), i = 1,\ldots,k; V_k, H_k\} = Arnoldi(A, v_1, k)$

(1) $Normalize\ v_1.$

(2) $for\ i = 1\ to\ k\ do:$

(2.1) $Form\ w_i = Av_i.$

(2.2) $Form\ h_{ji} = v_j^H w_i,\ j = 1,\ldots,i.$

(2.3) $Compute\ w_i \leftarrow w_i - \sum_{j=1}^{i} h_{ji} v_j.\ (QR - Gram - Schmidt)$

(2.4) $Form\ h_{i+1,i} = \|w_i\|_2.$

(2.5) $Form\ v_{i+1} = w_i / h_{i+1,i}.\ (Normalization)$

(3) $Let\ H_k = [h_{ji}]_{i,j=1}^{k}\ where\ h_{ji} = 0\ for\ j > i+1\ and\ V_k = [v_1,\ldots,v_k].$

(4) $Compute\ the\ eigenpairs\ (\lambda_i, z_i), i = 1,\ldots,k\ of\ H_k\ by\ the\ QR - method$

(5) $Compute\ the\ approximate\ eigenvectors\ x_i = V_k z_i, i = 1,\ldots,k.$

Eigensolver: Arnoldi Type Algorithm

- The Convergence Behavior of the Arnoldi Algorithm

  The Arnoldi algorithm converges to well-separated extremal eigenvalues.

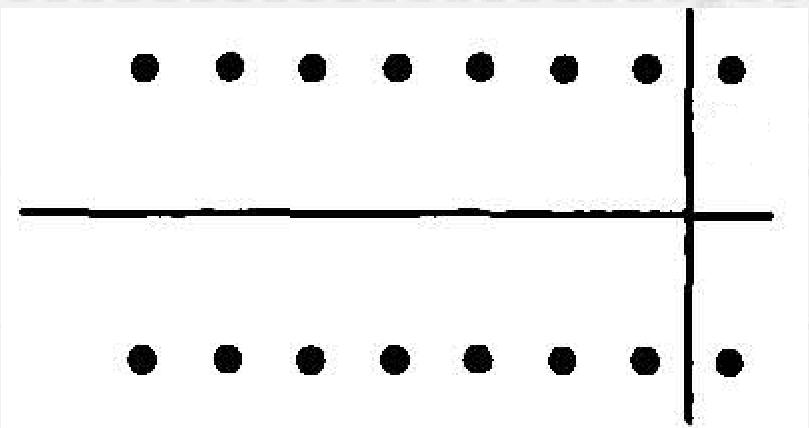


Fig 3. Equally-spaced Eigenvalues

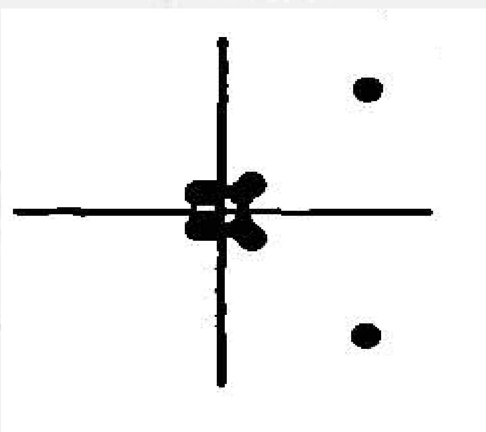


Fig 4. Well Separated Eigenvalues

Eigensolver: Arnoldi Type Algorithm

- The Convergence Behavior of the Arnoldi Algorithm

Theorem. Consider λ_i and $\theta_i = T(\lambda_i)$ $i = 1, \ldots, N$ simple and

suppose that there is a ζ such that

$$|\theta_1 - \zeta| > |\theta_2 - \zeta| \geq \cdots \geq |\theta_N - \zeta|.$$

Then $|\lambda_1 - \hat{\lambda}_1| \leq c \left(\dfrac{|\theta_2 - \zeta|}{|\theta_1 - \zeta|} \right)^{k-1}.$

Matrix Transformation: Cayley Transformation

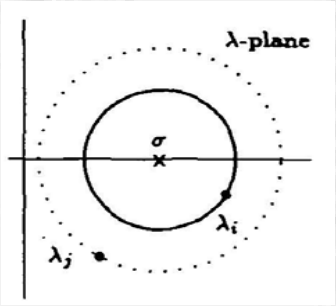
- Motivation of Matrix Transformation

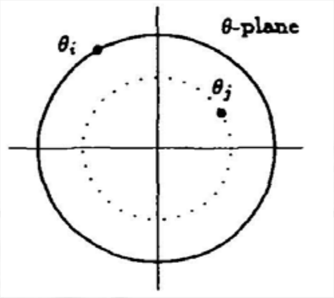
  - iterative method cannot solve generalized eigenvalue problems
  - eigensolvers prefer well-separated extremal eigenvalues

- Shift-invert Transformation

$$T_{SI}(A,B;\sigma)=(A-\sigma B)^{-1}B \quad \sigma\in R$$

$$\lambda\rightarrow\theta=\frac{1}{\lambda-\sigma}$$





The generalized eigenvalue problem $Ax=\lambda Bx$ becomes a standard eigenvalue problem $T_{SI}x=\theta x$. σ is called the shift.

Matrix Transformation: Cayley Transformation

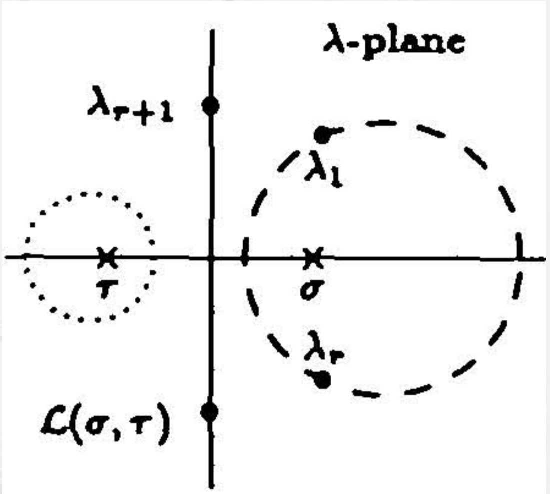
- Cayley Transformation

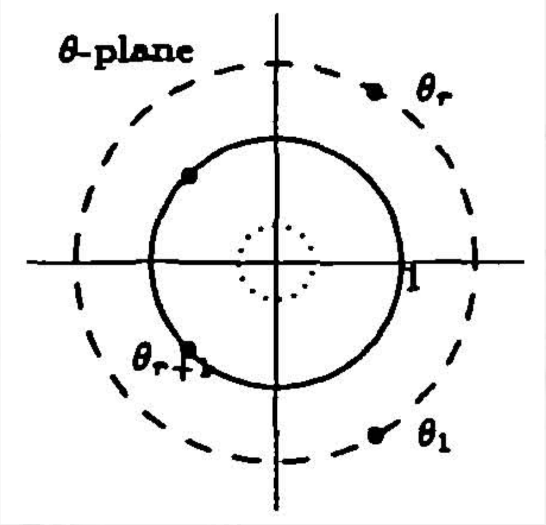
$$T_C(A,B;\sigma,\tau) = I + (\sigma-\tau)T_{SI}$$
$$= (A-\sigma B)^{-1}(A-\tau B)$$

$$\lambda \to \theta = \frac{\lambda-\tau}{\lambda-\sigma}$$

$\sigma : shift \quad \tau : anti-shift$

$$L(\sigma,\tau) = \left\{\lambda : \mathrm{Re}(\lambda) = \frac{1}{2}(\sigma+\tau)\right\}$$





Implementation

- All the algorithms will be coded in Matlab

- Available software packages (also written in Matlab)
  - IFISS ("Incompressible Fluid Iterative Solution Software")
  - Implicitly Restarted Arnoldi Code

Test and Validation

All test problems have been solved in the literature.

- **Stage 1: Test the standard Arnoldi algorithm code, Shift-invert and Cayley transformation code**

Test problem 1: Olmstead model (Nonlinear Diffusion Equation)

$$\begin{cases} \dfrac{\partial u}{\partial t} = (1-C)\dfrac{\partial^2 v}{\partial X^2} + C\dfrac{\partial^2 u}{\partial X^2} + Ru - u^3 \\ b\dfrac{\partial v}{\partial t} = u - v \\ u(0) = u(\pi) = 0 \\ v(0) = u(\pi) = 0 \end{cases}$$

R: Rayleigh Number

Test and Validation

(Stage 1) Test problem 2: Tubular Reactor Model

$$\begin{cases} \dfrac{\partial y}{\partial t} = \dfrac{1}{Pe_m}\dfrac{\partial^2 y}{\partial X^2} - \dfrac{\partial y}{\partial X} - Dy\exp\left(\gamma - \gamma T^{-1}\right) \\ \dfrac{\partial T}{\partial t} = \dfrac{1}{Pe_h}\dfrac{\partial^2 T}{\partial X^2} - \dfrac{\partial T}{\partial X} - \beta\left(T - T_0\right) + BDy\exp\left(\gamma - \gamma T^{-1}\right) \\ y'(0) = Pe_m y(0), T'(0) = Pe_h T(0) \\ y'(1) = 0, T'(1) = 0 \end{cases}$$

D: Damköhler Number

Test and Validation

- **Stage 2: Modify and test the Implicitly Restarted Arnoldi (IRA) code**

  Test problem:

$$\begin{bmatrix} K & C \\ C^T & 0 \end{bmatrix} x = \lambda \begin{bmatrix} M & 0 \\ 0 & 0 \end{bmatrix} x$$

$$K, M \in R^{n\times n} \quad C \in R^{n\times m} \quad N = n + m$$

Since matrix B is singular, standard Arnoldi algorithm will produce spurious eigenvalues. IRA should be able to solve this problem.

Test and Validation

- **Stage 3: Solve the two-dimensional double diffusive convection equation**

$$\beta u_1 \frac{\partial u_1}{\partial x} - u_2 \frac{\partial u_1}{\partial y} + \beta \frac{\partial p}{\partial x} - \Pr\left\{\beta^2 \frac{\partial^2 u_1}{\partial x^2} + \frac{\partial^2 u_1}{\partial y^2}\right\} = \frac{\partial u_1}{\partial t}$$

$$\beta u_1 \frac{\partial u_2}{\partial x} + u_2 \frac{\partial u_2}{\partial y} + \frac{\partial p}{\partial y} - \Pr\left\{\beta^2 \frac{\partial^2 u_2}{\partial x^2} + \frac{\partial^2 u_2}{\partial y^2}\right\} = Ra \Pr T - Rs \Pr S + \frac{\partial u_2}{\partial t}$$

$$\beta \frac{\partial u_1}{\partial x} + \frac{\partial u_2}{\partial y} = 0$$

$$\beta u_1 \frac{\partial T}{\partial x} + u_2 \frac{\partial T}{\partial y} - u_2 - \left\{\beta^2 \frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2}\right\} = \frac{\partial T}{\partial t}$$

$$\frac{\partial S}{\partial t} + \beta u_1 \frac{\partial S}{\partial x} + u_2 \frac{\partial S}{\partial y} - u_2 - \tau\left\{\beta^2 \frac{\partial^2 S}{\partial x^2} + \frac{\partial^2 S}{\partial y^2}\right\} = 0$$

Project Schedule

- **Before November:**
  solve the Olmstead Model; explore the effect of Rayleigh number
- **November:**
  solve the Tubular Reactor Model; explore the effect of Damköhler Number
- **December:**
  modify and test IRA code; write midterm report; give mid-term presentation
- **January to March:**
  Solve the Two-dimensional Double Diffusive Convection problem
- **April:**
  write final report
- **May:**
  write final report; give final presentation

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