A multilevel Jacobi-Davidson method for pde eigenvalue problems

Eigenvalue equation of physical interest

In the magnetic confinement fusion device Tokamak, drift instabilities cause a strong anomalous transport, i.e. losses. The linearized transport model [3] yields the following pde eigenvalue equation for the electric field perturbation envelope \( \phi \) as a subproblem in a fixed point iteration:

\[
\frac{\partial^2 \phi}{\partial t^2} + \mathbf{a}(t) \frac{\partial \phi}{\partial t} + \mathbf{b}(t) \phi + \mathbf{c}(t, \omega, \theta) \phi = 0, \tag{1}
\]

The most dominant eigenpair is of interest, which is the eigenpair \((\omega, \theta)\), where \(\omega\) is a \(2\pi\)-periodic smooth function and \(\text{Im}(\omega)\) is maximal. An accurate discretization requires a number of at least thousand grid points. The rational (1) can be transformed into a polynomial eigenvalue equation and solved by standard software, i.e. the QZ algorithm after linearization. In [2, 4] a more efficient technique, the multilevel Jacobi-Davidson method (MJD), was developed and is presented on this poster.

In the advanced physical model the condition

\[
\frac{\partial^2 \phi}{\partial t^2} + \mathbf{a}(t) \frac{\partial \phi}{\partial t} + \mathbf{b}(t) \phi + \mathbf{c}(t, \omega, \theta) \phi = 0,
\]

becomes worse if the number of grid points \(N\) is large. On coarse grids \((N\text{ small})\) the standard software is applicable to the matrix polynomial of (1). The extension of the MJD to the rational eigenvalue equation (1) is explained on this poster, too.

Jacobi-Davidson method

Let \(R(\omega)\phi = 0\) be the discretized (1).

(0.) Use prolongated coarse grid solution as initial space vector \(V_0\).

(1.) Orthonormalize \(V\).

(2.) Compute eigenpairs \((\nu, \psi)\) of \(V^\dagger R(\nu)V\).

(3.) Select Ritz pair \((\nu, \psi) \rightarrow V_0\).

(4.) Compute residual \(r := R(\nu)\psi\). It holds \(r \perp V\).

If forward error estimate \(e = 0\) is sufficiently small then Stop if \(\|r\| < \epsilon\).

(5.) Solve (approximately)

\[
t = \frac{u^H Q(r)}{u^H Q(r) R(\nu) u} R(\nu) u, \quad \lambda := \frac{u^H Q(r)}{u^H Q(r) R(\nu) u}.
\]

(6.) Expand search space \([V, t]\).

(2.) compute eigenpairs via linearization and QZ algorithm (polynomial) or inverse iteration (rational), apply spectral discretization for high accuracy.

(3.) selection of Ritz pair (polynomial) by similarity measure

\[
\tilde{\phi} = \phi(t, \nu, \psi) \approx \frac{\|\mathbf{b}(t)\phi(t, \nu, \psi)\|}{\|\mathbf{a}(t)\phi(t, \nu, \psi)\|} \quad \text{sim}(\nu, \psi, \phi). \tag{3}
\]

Forward error estimate [5] for (approximate) eigentriple \(( \nu, \psi, \phi)\)

\[
\tilde{\phi} = \phi(t, \nu, \psi) \approx \frac{\mathbf{b}(t)\phi(t, \nu, \psi)}{\mathbf{a}(t)\phi(t, \nu, \psi)} \tag{4}
\]

Correction equation (5) is equivalent to one Newton step for

\[
F(\lambda, x) := \frac{R(\lambda) x}{x^H x - 1} = 0
\]

starting at the current approximation \((\nu, \psi)\). The Newton step can be written as one step approximation

\[
t = \frac{\mathbf{u}^H Q(r)}{\mathbf{u}^H Q(r) R(\nu) u - Q(r)} R(\nu) u, \quad \mathbf{Q}(\nu) R(\nu) = I. \tag{6}
\]

Computational cost: solution of two linear systems.

Approximative solution is sufficient, thus discretize by finite differences here (linear effort in 1d, multigrid methods in \(\geq 2d\)).

Scaling and linearization in multilevel procedure

Approximately optimal scaling [1] requires

- block symmetric linearization to transfer the structure in the left eigenvector to the generalized eigenvalue equation.
- approximation to left and right eigenvectors \(\rightarrow\) prolonged solution from next coarser grid.
- Scaling is improved at each restart.
- Left and right eigenvectors allow two-sided Rayleigh quotients.

Numerical results for a polynomial eigenvalue equation

Figure: \(\nu = -0.0008825 + 0.1353370 i\) first (solid), second (dashed) companion linearization and (dash-dotted), (dotted) block symmetric linearizations.

Numerical results for a rational eigenvalue equation

\[
\text{dim } V \leq 16 \text{ limited}
\]

Desired accuracy in stopping condition \(\epsilon \leq 10^{-9}\)

Two-sided Rayleigh quotients

Displayed is the total number of Jacobi-Davidson cycles and in brackets the number of restarts (limited to 3)

\[
\begin{array}{cccccc}
N & \text{EP 1} & \text{EP 2} & \text{EP 3} & \text{EP 4} \\
\hline
4096 & 64(3) & 5(0) & 8(0) & 5(0) & 64(3) & 7(0) & 14(0) & 8(0) \\
2048 & 64(3) & 5(0) & 7(0) & 4(0) & 19(1) & 6(0) & 12(0) & 9(0) \\
1024 & 9(0) & 6(0) & 9(0) & 6(0) & 14(0) & 30(1) & 14(0) & 12(0) \\
512 & 12(0) & 7(0) & 8(0) & 6(0) & 24(1) & 64(3) & 55(3) & 25(1) \\
256 & 12(0) & 9(0) & 11(0) & 9(0) & 64(3) & 64(3) & 64(3) & 64(3) \\
128 & 16(0) & 13(0) & 14(0) & 13(0) & 64(3) & 64(3) & 64(3) & 64(3) \\
64 & 11(0) & 22(1) & 10(0) & 10(0) & 22(1) & 25(1) & 27(1) & 45(2)
\end{array}
\]

References