

Towards model reduction of the WTC and a FORTRAN version of LYAPACK for large scale second order systems.

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March 25th, 2006

1 The Problem

Let M , B , and K be positive definite real symmetric n by n matrices and consider the 2nd order linear dynamical system

$$\begin{aligned} M\ddot{x} + D\dot{x} + Sx &= Bu(t) \\ y &= Cx \end{aligned}$$

where C^T , and B are tall matrices. Our task is to compute the transfer function

$$T(s) = C(s^2M + sD + S)^{-1}B$$

which relates the Laplace transform U of the input u to the Laplace of the output Y

$$Y(s) = T(s)U(s)$$

For the World Trade Center simulation n is larger than 3 million. We are writing a FORTRAN code that will reduce such models.

2 The Method

First we note that the 2nd order system is equivalent to

$$\begin{aligned} \begin{bmatrix} \dot{x} \\ \ddot{x} \end{bmatrix} &= \underbrace{\begin{bmatrix} 0 & I \\ -M^{-1}S & -M^{-1}D \end{bmatrix}}_{\bar{A}} \begin{bmatrix} x \\ \dot{x} \end{bmatrix} + \underbrace{\begin{bmatrix} 0 \\ M^{-1}B \end{bmatrix}}_{\bar{B}} u(t) \\ y &= \underbrace{\begin{bmatrix} C & 0 \end{bmatrix}}_{\bar{C}} \begin{bmatrix} x \\ \dot{x} \end{bmatrix}, \end{aligned}$$

i.e. a 1st order system of size $2n$ by $2n$:

$$\begin{aligned}\dot{\bar{x}} &= \bar{A}\bar{x} + \bar{B}u(t) \\ y &= \bar{C}\bar{x}\end{aligned}$$

For simplicity, we change the notation from $(\bar{A}, \bar{B}, \bar{C})$ to (A, B, C) .

We solve the associated Lyapunov equations

$$\begin{aligned}AP + PA^T + BB^T &= 0 \\ A^TQ + QA + C^TC &= 0\end{aligned}$$

for P, Q using the low rank Smith(l) iteration due to T. Penzl [?], with the modifications made by S. Gugercin, D.C. Sorensen, and A.C. Antoulas [?]. Then we use the balancing free square root method by T. Penzl [?] to compute small and dense matrices $\hat{A}, \hat{B}, \hat{C}$ s.t.

$$T(s) \approx \hat{C}(sI - \hat{A})^{-1}\hat{B}$$

3 How to solve the Lyapunov equations

The low rank Smith iteration is given by

$$\begin{aligned}Z_1 &= \sqrt{-2p_1}(A + p_1I)^{-1}F \\ Z_i &= [(A - p_iI)(A + p_iI)^{-1}Z_i, \sqrt{-2p_i}(A + p_iI)^{-1}F]\end{aligned}$$

If the shift parameters p_i are selected carefully, then $Z_i Z_i^T \rightarrow X$ where X solves the Lyapunov equation

$$AX + XA^T + FF^T = 0.$$

Theoretically the selection of optimal parameters requires full knowledge of the spectrum of A , but there are at least two alternatives:

1. Apply the heuristic algorithm developed by T. Penzl [?] using Arnoldi's method to estimate the eigenvalues of A with the smallest and the largest magnitudes, or
2. Reduce the WTC to a single column. Select the shift parameters among the eigenvalues for this extremely small system.

We would like to thank Prof. Ayhan Irfanoglu, Purdue, for providing such small models of the WTC as well as estimating the damping matrix.

4 Details

4.1 Overview

The main loop requirements are

1. Compute $Y = (A + pI)X$.
2. Solve $(A + pI)X = Y$ for X .
3. Evaluate the residual norm

$$\|AZZ^T + ZZ^T A^T + FF^T\|.$$

Arnoldi's algorithm requires that we can:

- compute $Y = AX$ and
- solve $AX = Y$.

4.2 Implementation

If

$$A = \begin{bmatrix} 0 & I \\ -M^{-1}S & -M^{-1}D \end{bmatrix}, \quad X = \begin{bmatrix} X_1 \\ X_2 \end{bmatrix}, \quad \text{and} \quad Y = \begin{bmatrix} Y_1 \\ Y_2 \end{bmatrix}$$

then

- $Y = (A + pI)X$ has

$$\begin{aligned} Y_1 &= X_2 \\ Y_2 &= -M^{-1}(SX_1 + DX_2) \end{aligned}$$

while

- $(A + pI)X = Y$ has

$$\begin{aligned} X_1 &= p^{-1}(Y_1 - X_2) \\ X_2 &= \underbrace{(p^2M - pD + S)^{-1}}_{\Omega_p} (pMY_2 + SY_1) \end{aligned}$$

We will use CG with incomplete Cholesky factorization as preconditioner to solve the first set of equations. The second set of equations is more complicated.

With $p = \alpha + i\beta$, Ω_p becomes

$$\Omega_p = \underbrace{(\alpha^2 - \beta^2)M - \alpha D + S}_A + i \underbrace{(2\alpha\beta M - \beta D)}_B$$

The complex system

$$(A + iB)(x + iy) = f + ig$$

is equivalent to

$$\begin{bmatrix} A & -B \\ B & A \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} f \\ g \end{bmatrix}$$

We will solve this system using preconditioned BiCGstab. We expect that

$$\begin{bmatrix} A & O \\ 0 & A \end{bmatrix},$$

will be a good preconditioner, because S is likely to dominate.

How to evaluate the preconditioner, i.e. solve $Ax = b$?

- A is likely to be SPD, so
- CG + incomplete Cholesky factorization can be used to evaluate the preconditioner

$$A \approx LL^T, \quad Ax = b \Leftrightarrow \underbrace{L^{-1}AL^{-T}}_{\text{SPD}}(L^T x) = L^{-1}b$$

Finally we need to evaluate the residual, i.e. compute

$$\|AZZ^T + ZZ^T A^T + FF^T\|.$$

Computing the residual is out of the question because it is a dense n by n matrix, but

$$AZZ^T + ZZ^T A^T + FF^T = [AZ, \quad Z, \quad F] \begin{bmatrix} Z^T \\ Z^T A^T \\ F^T \end{bmatrix},$$

i.e. it is just a product between a tall matrix and a wide matrix. Thus

$$\|AZZ^T + ZZ^T A^T + FF^T\|_2$$

can be computed using no more than

2 tall QR factorizations + 1 small SVD or just a few iterations of the power method.

After having solve two Lyapunov equations

$$\begin{aligned} AP + PA^T + BB^T &= 0 \\ A^T Q + QA + C^T C &= 0 \end{aligned}$$

approximately

$$P \approx Z_B Z_B^T, \quad Q \approx Z_C Z_C^T$$

the reduced model $(\hat{A}, \hat{B}, \hat{C})$ is computed as follows:

- Do a small SVD: $U_C \Sigma V_B = Z_C^T Z_B$

- Compute

$$S_B = Z_B V_B(:, 1:k) \Sigma(1:k, 1:k)^{-\frac{1}{2}}$$

$$S_C = Z_C U_C(:, 1:k) \Sigma(1:k, 1:k)^{-\frac{1}{2}}$$

- Compute

$$\hat{A} = S_C^T A S_B$$

$$\hat{B} = S_C^T B$$

$$\hat{C} = C S_B$$

This is the balancing free square root method developed by T. Penzl [?].

5 Summary of requirements and final goal

These are the operations that we need to do

- dense matrix arithmetic on tall, but narrow matrices,
- sparse matrix times dense vectors for CG and BiCGstab,
- incomplete Cholesky factorization of M, S and all Ω_p .
- small SVD

These operations are all well understood and implemented in HSL and LAPACK. Our task is to put them together and parallelize them as much as possible.

Our goal is to produce:

A parallel Fortran version of LYAPACK for large and sparse 2nd order systems.

References

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- [3] Penzl, T. “LYAPACK v. 1.0. User’s guide.”