Exercise session II: Shifted linear systems

Numerical Linear Algebra

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1 Frequency response functions

The calculation of frequency response functions is one of the core operations of computational acoustics. The frequency response function (FRF) is the Fourier transform of the time dependent solution.

In vibration problems, including acoustics, many discretized problems take the form

$$(K - \omega^2 M)x = f \tag{1}$$

where f is the excitation as a function of the frequency ω and x the FRF.

In general, $x(\omega)$ is computed for a relatively large number of ω's. For each ω, the solution of (1) requires the solution of a linear system. Whether a direct or iterative linear solver is used does not really matter: the cost can be very high. Eq. (1) is a linear system with unknown x. It is solved frequency by frequency. To attack the problem from (1) we discuss the solution of

$$(I - \alpha A)x = b \tag{2}$$

by the Arnoldi method, which is already known to you as an eigenvalue solver or a method for reducing a nonsymmetric matrix to the upper Hessenberg form. Here we recall it:

Algorithm 1: Arnoldi algorithm for (partial) reduction to Hessenberg form

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Input: A ∈ ℝ^{n×n}, b ∈ ℝ^n, k ∈ ℕ;
Output: Q̃_k = [q_1 ··· q_k, q_{k+1}] ∈ ℝ^{n×(k+1)}, H̃_k ∈ ℝ^{(k+1)×k};
begin
    q_1 = b/‖b‖_2;
    /* k is the number of columns of Q and H to compute */
    for j = 1 : k do
        z = A q_j;
        for i = 1 : j do
            h_ij = q_i^T z;
            z = z − h_ij q_i;
        end
        h_{j+1,j} = ‖z‖_2;
        if h_{j+1,j} = 0 then
            exit;
        end
        q_{j+1} = z/h_{j+1,j};
    end
end
```

Recall that the columns of $Q_k = [q_1 \cdots q_k]$ form a basis of the Krylov subspace $\mathcal{K}_k$, H_k is the $k \times k$ upper Hessenberg matrix. (Q_k is $\tilde{Q}_k$ without the last column while H_k is $\tilde{H}_k$ without the last row.) From this algorithm we have $AQ_k = \tilde{Q}_k\tilde{H}_k$, which can be rewritten in the following form:

$$AQ_k - Q_kH_k = ze_k^*, \tag{3}$$

where ze_k^* is a rank-1 matrix formed by the product of the vector z of Algorithm 1 with the conjugate transpose of the kth column of the identity matrix of dimension $k \times k$, e_k^*.

To solve $Ax = b$ by Arnoldi's method, we project the space w.r.t. the subspace Q_k in the following way:

$$\begin{aligned}
b - Ax = 0 \Leftrightarrow & b - AQ_ky = 0, && x = Q_ky \\
\Leftrightarrow & b - Q_kH_ky - ze_k^*y = 0, && \text{By (3), } \textit{Arnoldi's Method} \\
\Leftrightarrow & Q_k^*b - Q_k^*Q_kH_ky - Q_k^*ze_k^*y = 0, && \text{Right multiplication for } Q_k* \\
\Leftrightarrow & \|b\|_2e_1 - H_ky = 0.
\end{aligned}$$

We started from a $n \times n$ linear system and we reduced it to a $k \times k$ linear system, which can be easily solved if k is small.

The residual norm can also be easily computed:

$$\begin{aligned}
\|Ax - b\|_2 &= \|AQ_ky - b\|_2 = \|Q_kH_ky + ze_k^*y - Q_kQ_k^*b\|_2 \\
&= \|Q_k\left(H_ky - Q_k^*b\right) + ze_k^*y\|_2 = \|z\|_2\left|e_k^*y\right| = h_{k+1,k}\left|e_k^*y\right|.
\end{aligned}$$

The Arnoldi method converges quickly when the eigenvalues of A are clustered near a value away from zero. When the spectrum is spread around and many eigenvalues are relatively close to zero, convergence is typically slow. The following theorem allows construction of an effective solver for several parametrized systems.

Theorem 1 (Shift Invariance Theorem)**.** *A Krylov space for A is the same as for $I - \alpha A$ with $\alpha \neq 0$. In addition, if (3) holds, then*

$$(I - \alpha A)Q_k - Q_k(I - \alpha H_k) = -\alpha ze_k^*. \tag{4}$$

Proof.

$$(I - \alpha A)Q_k = Q_k - \alpha AQ_k \underset{\text{By (3)}}{=} Q_k - \alpha Q_kH_k - \alpha ze_k^* = Q_k(I - \alpha H_k) - \alpha ze_k^*$$

□

2 Exercises

1. In the aforementioned text, two passages are left as exercise. The first one regards Arnoldi's method, which provides $AQ_k = \tilde{Q}_k \tilde{H}_k$, from this latter formula derive (3). The second one is the last passage of reducing the linear system $Ax = b$, namely

$$Q_k^* b - Q_k^* Q_k H_k - Q_k^* z e_k^* = 0 \Leftrightarrow \|b\|_2 e_1 - H_k y = 0.$$

2. In this exercise session you have seen how to reduce the linear system $Ax = b$ into $H_k y = \|b\|_2 e_1$ with a residual norm $h_{k+1,k} |e_k^* y|$, where $x = Q_k y$. Derive, in a analogous way, the reduced linear system for the shifted problem $(I - \alpha A)x = b$ and its residual norm.

3. Write an effective solver for the parametrized problem (2). You should be able to get the vector of parameters and return the vector of the solutions, each corresponding to one parameter value.

4. Take n equal to, e.g., 1000 and construct two testing matrices: one with the eigenvalues 1./(1:n), the second one with the eigenvalues $1./((1 \pm i)[1 : n/2])$. Do several steps (e.g., $k = 10, 20, 50, 100$) of your algorithm for $\alpha \in [0, 10]$. Experiment with different eigenvalue distributions.

5. Plot the norm of the solution and the norm of the error over α.

6. Compare with Arnoldi algorithm with full re-orthogonalization.

References

[1] K. Meerbergen, *Fast frequency response function computation by model reduction methods.* Computational Methods for Acoustics Problems, F. Magoulès, ed., Saxe-Cobourg, 2007.