Matrix-less spectral approximation for large structured matrices

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Abstract

Sequences of structured matrices of increasing size arise in many scientific applications and especially in the numerical discretization of linear differential problems; for example by using Finite Differences (FD), Finite Elements (FE), Finite Volumes (FV), Discontinuous Galerkin (DG), Isogreometric Analysis (IgA). The eigenvalues $\lambda_j(A_n)$ of matrices A_n, belonging to such a sequence $\{A_n\}_n$, can often be approximated by a regular expansion:

$$\lambda_j(A_n) = \sum_{k=0}^{\alpha} c_k(\theta_{j,n})h^k + E_{j,n,\alpha}, \qquad j = 1,\dots,n \qquad \theta_{j,n} = \frac{j\pi}{n+1}, \tag{1}$$

where $c_k : [-\pi,\pi] \to \mathbb{C}$ (c_0 is called the *spectral symbol* and $c_k, k > 0$ are called *higher order symbols*) and the errors $E_{j,n,\alpha} = \mathcal{O}(h^{\alpha+1})$.

Hence, if we know these functions $c_k(\theta)$, or approximate them since they are often not known analytically, we can accurately (and very fast) approximate some (or all) of the eigenvalues of any matrix A_n simply by evaluating (1).

It was previously shown (under appropriate assumptions, [4, 5]) [1, 7, 8, 9, 10] that for Hermitian sequences $\{A_n\}_n$, where c_0 is known, that we can approximate $c_k(\theta_{j,n_0}), k = 1,\dots,\alpha$ at specified grid points θ_{j,n_0} using so-called *matrix-less* methods. The name is derived from the fact that the spectrum for any matrix A_n in the sequence $\{A_n\}_n$ can be approximated by (1) *without ever constructing the matrix*; only the spectrum of a few small matrices have to be computed. That is, we have equality in (1), up to machine precision, for some chosen $n = n_0$ and α. These approximations $c_k(\theta_{j,n_0})$ can then be used for interpolation-extrapolation to any grid $\theta_{j,n}$ (for any n) to approximate $\lambda_j(A_n)$.

In the current presentation, mainly inspired by [3], but also [6, 11], we extend the previous algorithms with two important features:

1. The function c_0 is not needed as an input and is approximated; this is necessary for most non-Hermitian matrix sequences, but also for discretizations of problems with variable coefficients.
2. The algorithm can handle discretizations of variable coefficient problems, e.g., $(a(x)u'(x))'$.

We here briefly present these two new features.

1. No knowledge of c_0 necessary.

We begin by presenting two simple but representative pure Toeplitz matrix sequences; one Hermitian $\{T_n(f_1)\}_n$ and one non-Hermitian $\{T_n(f_2)\}_n$.

$$f_1(\theta)=6-8\cos(\theta)+2\cos(2\theta) \qquad T_n(f_1) = \begin{bmatrix} 6 & -4 & 1 & & & \\ -4 & 6 & -4 & 1 & & \\ 1 & -4 & 6 & -4 & 1 & \\ & \ddots & \ddots & \ddots & \ddots & \ddots \\ & & 1 & -4 & 6 & -4 & 1 \\ & & & 1 & -4 & 6 & -4 \\ & & & & 1 & -4 & 6 \end{bmatrix}$$

$$f_2(\theta)=-e^{\mathbf{i}\theta}+3-3e^{-\mathbf{i}\theta}+e^{-2\mathbf{i}\theta} \qquad T_n(f_2)= \begin{bmatrix} 3 & -3 & 1 & & & \\ -1 & 3 & -3 & 1 & & \\ & -1 & 3 & -3 & 1 & \\ & & \ddots & \ddots & \ddots & \ddots \\ & & & -1 & 3 & -3 & 1 \\ & & & & -1 & 3 & -3 \\ & & & & & -1 & 3 \end{bmatrix}$$

For matrices in the Hermitian sequence $\{T_n(f_1)\}_n$, we have that the eigenvalues can be approximated by $\lambda_j(T_n(f_1)) \approx c_0(\theta_{j,n}) = f_1(\theta_{j,n})$ where $\theta_{j,n} = j\pi/(n+1)$; the spectral symbol c_0 is known and equal to f_1.

For matrices in the non-Hermitian sequence $\{T_n(f_2)\}_n$, we have that $\lambda_j(T_n(f_1)) \not\approx f_1(\theta_{j,n})$, we only know that the eigenvalues lie in the convex hull of the complex valued function f_2; the spectral symbol c_0 is not equal to f_2. For most non-Hermitian matrix sequences the c_0 is not known analytically, and the new matrix-less method presented in [3, 11] does not require it to be know. However, the matrix-less method is more efficient and accurate if it is provided.

Remark 1 *In the specific case of a non-Hermitian sequence $\{T_n(f_2)\}_n$ presented above we do know that the spectrum is real and the are many viable c_0, e.g. $c_0(\theta) = \sin^3(\theta)/(\sin(\theta/3)\sin^2(2\theta/3))$; see [13] for details.*

For clarity we show a Julia implementation below on how to compute a matrix $C = [c_k(\theta_{j,n_0})]_{k,j=1}^{\alpha+1,n_0}$; the inputs are n_0 (≈ 100), α (≈ 3) and `eigfun` (a function that returns an ordered set of eigenvalues $\lambda_j(A_n)$ for a matrix A_n in $\{A_n\}_n$).

```
function compute_C(n₀, α, eigfun)
    hs = zeros(α+1)
    E = zeros(α+1,n₀)
    for kk = 1:α+1
        nk = 2^(kk-1)*(n₀+1)-1
        jk = 2^(kk-1)*(1:n₀)
        hs[kk] = 1/(nk+1)
        E[kk,:] = eigfun(nk)[jk]
    end
    V=[hs[ii]^(jj-1) for ii=1:α+1, jj=1:α+1]
    return C=V\E
end
```

As is seen above, the algorithm relies on the computed spectrum for $\alpha+1$ small matrices (of sizes $n_k = 2^{k-1}(n_0+1)-1$, for $k = 1, \ldots, \alpha+1$) to compute the elements of C. Subesequently $c_k(\theta_{j,n})$ is approximated, using interpolation-extrapolation, for arbitrary n, and used in (1) to approximate $\lambda_j(A_n)$.

Remark 2 *If the spectral symbol is non-monotone (e.g., the stiffness matrix for IgA or $f(\theta) = 6-8\cos(\theta)+4\cos(2\theta)$), the matrix-less method does typically not work in the non-monotone region, since we usually do not know how to order the eigenvalues correctly.*

2. Variable coefficients.

The spectral symbol f of the 2nd order FD discretization of $(a(x)u'(x))'$ is two-dimensional, namely $f(x,\theta) = a(x)(2-2\cos(\theta))$, where $f : [0,1] \times [-\pi,\pi] \to \mathbb{C}$; e.g., see [12].

In [3] we show that we can use the rearranged symbol [2] to compute an expansion (1) for discretizations of variable coefficient problems; i.e., we map the function $f : [0,1] \times [-\pi,\pi] \to \mathbb{R}$ to a rearranged symbol $g : [0,1] \to \mathbb{R}$. In the new matrix-less method we have $c_0 = g$.

Remark 3 *We emphasize that the class of problems and matrices where this approach can be applied is extensive, e.g.,*

- *multi-dimensional problems (size of matrices are then $d_{\mathbf{n}}(\mathbf{n})$ and not n);*

- *block matrices (e.g., FE/FV/DG);*
- *boundary conditions (c_0 is the same, $c_k, k > 0$ changes);*
- *h-dependence, space-time, sums/inverses/products;*
- *eigenvectors, singular values, generalized eigenvaklue problems;*

and the approach could also be used to construct preconditioners and other solver techniques.

Apart from the two main points mentioned above, we will also discuss the current framework in detail, possible extension and current developments, and possible applications.

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