Matrix-Less Methods for Computing Eigenvalues of Structured Matrices

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Eigenvalues (and singular values) of matrices are of great importance in applications, both in themselves (e.g., generalized eigenvalue problems) and as tools for designing fast solvers (e.g., preconditioning). When we discretize partial differential equations (PDE), or fractional differential equations, by standard methods (FDM, FVM, FEM, DGM, IgA, etc.) we obtain structured matrices, specifically **Toeplitz-like** matrices [6]. In the simplest case, we find Toeplitz matrices of the form

$$T_n(f) = \left[\hat{f}_{i-j}\right]_{i,j=1}^{n}, \qquad f(\theta) = \sum_{k=-\infty}^{\infty} \hat{f}_k \mathrm{e}^{k\mathbf{i}\theta}, \qquad \hat{f}_k = \frac{1}{2\pi}\int_{-\pi}^{\pi} f(\theta)\mathrm{e}^{-k\mathbf{i}\theta}\mathrm{d}\theta, \qquad k \in \mathbb{Z},$$

where $f(\theta)$ is a 2π-periodic function, called the **symbol** of the sequence $\{T_n(f)\}_n$. Assuming that the symbol f is real and smooth, the Szegő first limit theorem intuitively says that

$$E_{j,n} = \lambda_j(T_n(f)) - f(\theta_{j,n}) = \mathcal{O}(h),$$

where $\{\theta_{j,n} : j = 1,\ldots,n\}$ is a uniform grid in the domain of f. In a series of papers (see [1, 2] and the references therein), and under suitable assumptions, Böttcher et al. derived an asymptotic expansion of the form

$$E_{j,n} = \sum_{k=1}^{\alpha} c_k(\theta_{j,n})h^k + E_{j,n,\alpha}, \qquad E_{j,n,\alpha} = \mathcal{O}(h^{\alpha+1}). \tag{1}$$

Typically the functions $c_k(\theta)$ in (1) are not known, and knowing them would yield extremely accurate and fast approximations of $\lambda_j(T_n(f))$ for any matrix size n.

In a number of papers (see [3, 4, 5] and [7] for all references and co-authors) we developed the so-called **matrix-less** methods (not to be confused with matrix-free methods) to find approximations $\tilde{c}_k(\theta_{j,n_0})$ of $c_k(\theta_{j,n_0})$ on a coarse grid θ_{j,n_0} for all $k = 0,\ldots,\alpha$. These approximations can then be interpolated–extrapolated [5] to a finer grid $\theta_{j,n}$ in order to obtain fast and accurate approximations of the eigenvalues

$$\lambda_j(T_n(f)) \approx \sum_{k=0}^{\alpha} \tilde{c}_k(\theta_{j,n})h^k = \sum_{k=0}^{\alpha} \left(\tilde{c}_k^{\Re}(\theta_{j,n}) + \mathbf{i}\tilde{c}_k^{\Im}(\theta_{j,n})\right) h^k. \tag{2}$$

The proposed interpolation–extrapolation algorithm works even if the simple Toeplitz matrix $T_n(f)$ in (2) is replaced by a more general Toeplitz-like matrix (such as a preconditioned or block Toeplitz matrix, a PDE discretization matrix, a generalized locally Toeplitz matrix, etc.). Moreover, the algorithm is applicable even if the symbol f is not known or does not describe the eigenvalue distribution of $\{T_n(f)\}_n$.

We show examples where matrix-less methods yield machine precision accuracy "instantaneously" (i.e., seconds vs. days for standard solvers) when approximating eigenvalues. The necessity for high precision computations, as opposed to double precision, will also be demonstrated with multiple examples.

In future research, we will focus on matrices with non-monotone, multivariate, non-Hermitian, and diagonal sampling symbols. Developing the same techniques for eigenvectors is also an interesting extension. Collaborations for the use of matrix-less methods for solving real-world physical problems are welcome.

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