Rational Krylov sequences and orthogonal rational functions

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In this contribution we discuss the relationship between spectral decomposition, orthogonal rational functions (ORF) and the rational Lanczos algorithm (RLA), based on a simple identity for the rational Krylov sequences (RKS).

Suppose A is a large Hermitian $N \times N$ matrix and $v \in \mathbb{C}^N$. Then the space $K_n(A, v) = \text{span}\{v_0, \ldots, v_{n-1}\}$, with $n \ll N$, $v_0 = v$, $v_k = A(I - \alpha_k A)^{-1} v_{k-1}$ and $\alpha_k \in \mathbb{R}$, is called a rational Krylov subspace. Because of its construction we can also write v_k as $v_k = r_k(A)v$ with r_k a rational function of the form $p_k(z)/[(1 - \alpha_1 z) \cdots (1 - \alpha_k z)]$, where p_k is a polynomial of degree k at most. After orthogonalising v_k with respect to the previous vectors, we obtain a vector $q_k = \varphi_k(A)v$, where again φ_k is a rational function of the same form as r_k.

If $\alpha_k = 0$ for every $k > 0$, the rational functions r_k and φ_k reduce to respectively the polynomials p_k and ϕ_k, so that $v_k = p_k(A)v$ and $q_k = \phi_k(A)v$. The orthogonality of the vectors q_k is then equivalent with the orthogonality of the polynomials ϕ_k with respect to the inner product $\langle \phi_k, \phi_l \rangle = M(\phi_k \overline{\phi}_l)$, where the linear functional M is defined on the space of polynomials by its moments $M(z^k) = v^* A^k v$. Since the classical moment matrix has a Hankel structure, this theory will be related to the orthogonality of polynomials on the real line. Thus, in the classical Lanczos method for Hermitian matrices, the three-term recurrence relation for the orthogonal polynomials (OP) leads to a short recurrence between the successive vectors q_k, meaning that q_k can be computed from q_{k-1} and q_{k-2} without the need for a full Gram-Schmidt orthogonalisation.

ORF on the real line are a generalisation of OP on the real line in such a way that the OP return if all the poles α_k^{-1} are at infinity. Consequently, if the α_ks are arbitrarily real, it will be obvious that the orthogonality of the q_k will lead to the orthogonality of the rational functions φ_k, so that a simple recurrence of the ORF will lead to an efficient implementation of the RLA.

We prove this relationship between ORF and the RLA based on a simple identity for RKS.

Keywords: Numerical linear algebra, Ordinary differential equations, Partial differential equations, Rational Krylov sequences, orthogonal rational functions, rational Lanczos algorithm, three-term recurrence relation.