Matrix functions and solutions to fractional differential equations: new contributions to their numerical approximation

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The numerical approximation of matrix functions and the numerical solution of differential equations of fractional order are important and challenging topics which recover a fundamental role in several branches of applied sciences as biology, physics, engineering and many others [2,7].

Matrix functions arise for example in control theory, when continuous-time systems need to be converted into discrete-time state-space systems and the matrix exponential comes into play. Analogously, the Solomon equations for the nuclear magnetic resonance can be solved by means of matrix functions. However, the most common application field is the solution of systems of ordinary or partial differential equations.

In recent years the attention to fractional differential equations has reached new and relevant levels. They are generalization of ordinary differential equations to arbitrary (noninteger) order; their strength is in capturing the nonlocal relations in space and time with power law memory kernels. This aspect makes them very effective to model problems with "memory" or anomalous diffusion; on the other hand it is hard to tackle from a numerical point of view thus to motivate the active research devoted to the subject in the last period.

Matrix functions and differential equations of fractional order are related to each other since, as widely described in [3], the solution of a linear system of fractional differential equations can be often written in terms of the Mittag–Leffler function evaluated in a suitable matrix argument.

In the context of matrix functions' approximation we have recently focused on a *restarted* version of the *Shift-and-Invert* Krylov subspace methods, as introduced in [8] and deepened in [10]. The key issue of our work [9] are the new error estimates for the Krylov subspace methods: such estimates give insights into the selection of the shift parameter and lead to a simple and effective restart procedure, with relevant saving in terms of computational time and memory requirement. In particular, we applied it to the class of Mittag–Leffler functions, typical of the fractional calculus, with very nice results.

The numerical approximation of the Mittag–Leffler function itself represents an important topic for the scientific research; more precisely, for the numerical solution of fractional differential equations, a class of functions generalizing the Mittag-Leffler plays a fundamental role. Unfortunately, the numerical approximation of these functions presents some difficulties, even for scalar arguments. In [6] we tackled this problem, with a deep analysis to identify the optimal parameters to describe the contour used to define the generalized Mittag-Leffler functions by means of the Cauchy integral. The recovered parameters work very well, with good results also when the evaluation on matrix arguments is required.

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