Numerical linear algebra tools for data driven computational analysis of nonlinear dynamical systems

Zlatko Drmač
Department of Mathematics, Faculty of Science, University of Zagreb

In this talk, we discuss several themes from computational analysis of nonlinear dynamical systems in data driven scenarios. We show how to deploy state of the art numerical linear algebra to curb ill-conditioning that precludes successful numerical implementation of sophisticated methods in applications. As case studies we use selected computational tasks from the Koopman operator based spectral analysis and identification/learning of nonlinear dynamical systems accessible through a sequence of data snapshots. In particular, in the framework of data driven Koopman spectral analysis, we study the numerics of the Dynamic Mode Decomposition (DMD) and the Koopman mode decomposition.
In particular, the DMD can be enhanced with data driven formula for the residuals, thus allowing for a selection of accurate Ritz pairs that provide more precise spectral information of the underlying Koopman operator. For instance, we show that a numerically robust DMD type algorithm can be constructed also by following the natural formulation via the Krylov decomposition with the Frobenius companion matrix, and by using its eigenvectors explicitly - these are defined as the inverse of the notoriously ill-conditioned Vandermonde matrix. The key step to curb ill-conditioning is the discrete Fourier transform of the snapshots; in the new representation, the Vandermonde matrix is transformed into a generalized Cauchy matrix, which then allows accurate computation by specially tailored algorithms of numerical linear algebra.

Then, we present a new algorithm for solving structured least squares problem that arise in the process of identification of coherent structures. It is deployed in combination with the DMD, which provides a non-orthogonal set of modes corresponding to particular temporal frequencies - a selection of these is used to represent time snapshots of the underlying dynamics. The coefficients of the representation are determined from a solution of a structured linear least squares problems with the matrix that involves the Khatri-Rao product of a triangular and a Vandermonde matrix. Our analysis explains when and why it is safe to use normal equations based solution. If normal equations are not feasible, the new QR factorization based algorithms exploit the structure and numerical analysis identifies relevant condition numbers that govern the accuracy.

As the final topic, we discuss data driven system identification. The dynamics can be identified/learned from the snapshots by lifting the data and computing matrix approximation of the infinitezimal generator of the Koopman operator semigroup (Mauroy-Goncalves method). This involves numerically computed matrix logarithm of potentially severely ill-conditioned matrices. We discuss how implicit preconditioning helps alleviate the problem. The discussion is illustrated using selected numerical examples.