Krylov subspace methods for Perron-Frobenius operators in RKHS

Krylov subspace method has actively researched for numerically approximating the behaviors of finite or infinite dimensional linear operators, for example, approximating eigenvalues, solutions of linear equations, operator functions acting on vectors. Recently, applying it for numerically estimating transfer operators such as Perron–Frobenius operators and Koopman operators for analyzing time–series data has attracted much attention in various fields such as machine leaning, physics, molecular dynamics, and control engineering. Transfer operator is a linear infinite dimensional operator which represents the time evolution of a nonlinear dynamical system. In this case, unknown transfer operators are estimated by the data generated by the dynamical systems.
The main difference between the classical settings and the above setting for transfer operators are whether the knowledge of the model is given or not. In the classical setting, a model is given and the model–driven approach with the operator is applied. On the other hand, in the above setting for estimating transfer operators, neither the model nor transfer operator are given, instead, the time–series data generated by the model is given. The data–driven approach is applied in this case. Since the structure of the approximation problem for transfer operators is different from that of the classical ones appear in the field of numerical linear algebra, the goal for the Krylov subspace method is also different in some situations. For a transfer operator K, estimating Kv for a given vector v by data is important task for applications. While, in the classical setting, for an operator A which describes the model and a given vector v, Av is already known because both A and v is known. Thus, Krylov subspace methods for approximating Av for a linear operator A and a vector v have not needed to discuss in the classical setting of numerical linear algebra. Therefore, although the Krylov subspace methods for estimating Kv for an unknown transfer operator K and a given vector v are proposed in the field such as machine learning, their analyses have not investigated enough.
In this talk, we analyze such Krylov subspace methods and give reasonable interpretations about them by relating them to the “residuals”. It can be shown that the residual of the approximation with the Krylov subspace method is bounded by the minimum of the residual in a certain space with a reasonable constant if the Perron–Frobenius operator is bounded. The similar interpretation for unbounded operators is also derived, and it can be shown that the difference between the residual of the approximation and the minimum of the residual in a certain space has a strong connection with a classical problem appears in the field of numerical linear algebra. Experimental results using a well–known differential equation are also illustrated to confirm our results numerically.