

Regularized dynamical parametric approximation

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This paper studies the numerical approximation of solutions to initial value problems of high-dimensional ordinary differential equations or evolutionary partial differential equations such as the Schrödinger equation by nonlinear parametrizations $u(t) = \Phi(q(t))$ with time-dependent parameters $q(t)$, which are to be determined in the computation. The motivation comes from approximations in quantum dynamics by multiple Gaussians and approximations of various dynamical problems by tensor networks and by neural networks. In all these cases, the parametrization is typically irregular: the derivative $\Phi'(q)$ can have arbitrarily small singular values and may have varying rank. We derive approximation results for a regularized approach in the time-continuous case as well as in time-discretized cases. With a suitable choice of the regularization parameter and the time stepsize, this approach can still be successfully applied in such irregular situations, even if it runs counter to the basic principle in numerical analysis to avoid solving ill-posed subproblems when aiming for a stable algorithm. Numerical experiments with sums of Gaussians for approximating laser-induced quantum dynamics and with neural networks for approximating the flow map of a system of ordinary differential equations illustrate and complement the theoretical results. The talk is based on joint work with Caroline Lasser, Jörg Nick and Michael Feischl.

Presenter: LUBICH, Christian (University of Tuebingen)