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Dynamical Low Rank Approximation in Molecular Dynamics and Optimal Control

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Abstract: A novel method to approximate solutions of parabolic Partial Differential Equations in a low-rank Tensor Train (TT) format is developed. The work is partly inspired by [5], in which the authors use TTs with polynomial basis functions to outperform state-of-the-art Neural Networks on the solution of parabolic PDEs by orders of magnitude, while requiring lower computational time. The new method, developed in joint work with Martin Eigel and Reinhold Schneider, utilizes the Dirac-Frenkel variational principle with empirical risk as well as a physics informed choice of basis functions, and potentially exhibits much lower computational cost even than the method presented in [5]. The Kolmogorov Backward Equation (KBE) arising in Molecular Dynamics (MD) and the Hamilton-Jacobi-Bellman equation arising in nonlinear stochastic Optimal Control (OC) are treated as examples. In MD in particular, the low-rank nature of the approach enables tackling the KBE directly, instead of learning the eigenpairs of the generator.

Our new approach is a Dynamical Low Rank Approximation [3, 4] of the PDE solution and can be understood as an alternative to classic machine learning methods, in particular to Artificial Neural Networks. In its abstract setting, the main idea of DLRA is to approximate solutions to matrix- or tensor-valued ordinary differential equations (ODEs) by projecting the right-hand side of the ODE onto the tangent space of the manifold of matrices/tensors of fixed (TT-)rank at the current approximation. In this abstract setting, the projection is usually decomposed into orthogonal parts of the tangent space after which a splitting scheme is applied, resulting in so called projector-splitting schemes. The obtained approximation is quasi-optimal on a finite time domain, as occurring for instance in finite horizon optimal control. In our PDE setting, we perform first a projection with an empirical L^2–norm to "sample out" the spatial dimension and arrive at an ODE, where the right hand side is then defined on the tangent space of the TT manifold. This projection can be understood as an empirical least squares tensor regression based on random samples. The theoretical properties of the method, especially in connection to the abstract DLRA setting and to classical Galerkin projection methods, are currently being investigated, while first numerical results in OC and MD are available.

In OC, the HJB equation arises when one searches for an optimal feedback control law. Feedback control laws are desirable, since they are robust with respect to state perturbations and measurement noise. However, solving the HJB equation – a nonlinear parabolic PDE of generally high dimension – is notoriously difficult and most practical approaches rely instead on variations of Model Predictive Control (MPC), a conservative approach, where open–loop controls are computed in such rapid succession that they essentially close the loop. Classical schemes to solve the HJB equation such as Galerkin-schemes in linear ansatz spaces suffer from the *curse of dimensionality* [2], i.e. an exponential complexity growth. In practice, this means that the computation of a solution is often infeasibly slow, if it can be discretised and stored at all. Our focus lies on the alleviation of the curse of dimensionality in order to enable the numerical treatment of high-dimensional control problems. On control problems with moderate dimensions, our method achieves similar performance to the method from [5] with computation time decreased by about an order of magnitude [1]. While this is an encouraging result, high–dimensional problems, for which the method is developed, still require careful tuning of the hyperparameters to avoid instability due to the explicit nature of the solver and need to be investigated further.

The KBE on the other hand governs the time development of observables of high dimensional stochastic processes appearing in MD, such as overdamped Langevin dynamics. The dimension of the problem is typically $3N$, where N is the number of atoms of the considered molecule. Since the molecules usually exhibit some sort of symmetry however (like invariance of the potential w.r.t. translations), one can usually find a set of lower dimensional coordinates, leading to effective dynamics of much lower dimensions. An example of this might be a protein or some other complex molecular structure where, instead of considering all atoms separately, we consider groups of them as *pseudo-atoms*. The TT basis functions are then composed with the problem specific *coarse-graining*, the mapping from the original space to the reduced coordinates, and the dynamical low rank scheme is applied to the KBE for the reduced dynamics. Crucially, sampling of the empirical L^2–norm can be performed on the original space, i.e. no simulation of the difficult reduced dynamics has to be performed. The method shows promising results for various simple potential–driven diffusion processes and low–dimensional toy molecules. Its application to high dimensional problems is an object of ongoing investigation.

References

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Short biography – I received undergraduate degrees in physics and mathematics from the Karlsruhe Institute of Technology and wrote my master's thesis in nonlinear optimal control at the TU Berlin under Prof. Reinhold Schneider. Building on this experience, I joined the ProFit project *ReLkat – Reinforcement Learning for complex automation engineering*, which is funding my PhD thesis. In the context of this project, I developed software for *Signal Cruncher GmbH* to facilitate real time Model Predictive Control for complex systems using dynamical low rank approximations in the Tensor Train format.