Greedy algorithms for Hamiltonian identification problems

G. Ciaramella[1]

[1] *Politecnico di Milano, Dipartimento di Matematica, MOX Laboratory*
Piazza Leonardo da Vinci, 32 20133 - Milano Italy
gabriele.ciaramella@polimi.it

The identification of Hamiltonian operators, including the distribution of possible inho- mogeneity parameters, plays a fundamental role in fields like quantum physics, quantum chemistry and nuclear magnetic resonance. The term Hamiltonian identification often refers to two distinct problems. On the one hand, it can indicate the inverse problem associated with the identification of a Hamiltonian operator obtained by a numerical fitting of simu- lated and given experimental data. On the other hand, it can refer to both the problem of designing experimental parameters (allowing an optimized production of experimental data) and the subsequent inverse identification problem. In general, the design of experimental parameters includes the computation of control functions allowing an efficient numerical solving of the inverse problem.

This talk is concerned with novel computational greedy-type approaches for design of con- trol functions has been introduced in [1, 2, 3]. These strategies are based on an offline/online decomposition of the reconstruction process. In the offline phase, a family of control func- tions is built iteratively in a greedy manner in order to maximize the distinguishability of the system. This phase exploits only the quantum model, without any use of laboratory information. The computed control functions are experimentally implemented in the online phase to produce laboratory data, which are in turn used to define and solve an identifica- tion inverse problem. The offline/online decomposition results particularly efficient if one needs to reduce the number of laboratory experiments.

In this talk, we present different versions of greedy-type algorithms and introduce a novel convergence analysis [2]. The analysis reveals the strong dependence of the performance of the greedy strategy on the observability and controllability properties of the system and allows us to introduce a new and more robust optimized greedy reconstruction strategy whose efficiency is demonstrated by numerical experiments.

References:

[1] Y. Maday and J. Salomon. A greedy algorithm for the identification of quantum sys- tems. In *Proceedings of the 48th IEEE Conference on Decision and Control, 2009, Held jointly whit the 28th Chinese Control Conference (CDC/CCC 2009)*, IEEE Conference on Decision and Control, pages 375–379, 2009.
[2] S. Buchwald, G. Ciaramella, J. Salomon. *Analysis of a greedy reconstruction algorithm*.
To appear in SIAM J. Control Optim.
[3] S. Buchwald, G. Ciaramella, J. Salomon, D. Sugny. *A greedy algorithm for the recon- struction of inhomogeneity distribution of spin systems*. In preparation.