How to reconstruct the probability distribution inside an inhomogeneous spin ensemble

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The identification of Hamiltonian operators, including the distribution of inhomogeneity parameters, plays a fundamental role in fields like quantum physics, quantum chemistry and nuclear magnetic resonance. In the context of our work, the term Hamiltonian identification refers to both the problem of designing experimental parameters (i.e. control functions) and the subsequent inverse identification problem.

A computational greedy-type approach for the design of control functions, that allow for an efficient numerical solving of the inverse problem, has been studied in [1]. This strategy is based on an offline/online decomposition of the reconstruction process. In the offline phase, a family of control functions 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 inverse identification problem. The offline/online decomposition results are particularly efficient if one needs to reduce the number of laboratory experiments.

We present an extension of original strategy in [1] to the identification of the probability distribution of a parameter characterizing an inhomogeneous spin ensemble [2] and demonstrate its efficiency by numerical experiments.

References:

[1] S. Buchwald, G. Ciaramella, J. Salomon, *Analysis of a greedy reconstruction algorithm*, SIAM J. on Control Optim. **59**, pp. 4511-4537 (2021).

[2] S. Buchwald, G. Ciaramella, J. Salomon, D. Sugny, *A greedy reconstruction algorithm for the identification of spin distribution*, Phys. Rev. A **104**, p. 063112 (2021).