An optimized greedy reconstruction algorithm for dipole momentum operators

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***Abstract*— In a previous work [7], an algorithm was proposed to compute a family of selective controls that enables the efficient Hamiltonian identification of quantum systems. These controls are iteratively computed for a given set of linearly independent matrices, whose span form the space where the unknown Hamiltonian is sought. In this paper, we show by direct numerical experiments that the procedure presented in [7] can suffer from a lack of robustness. This is due to the high non-linearity of the problem generated by the bilinear state-control structure and to the fact that the final results strongly depend on the basis matrices chosen before running the algorithm. For this reason, a randomly chosen set of linear independent matrices does not necessarily lead to a set of robust selective fields that allows an accurate identification of the unknown Hamiltonian. To tackle this problem we propose a new optimized version of this algorithm. This new strategy consists in extending the greedy character of the original algorithm in a way that more matrices, not necessarily linearly independent, are tested in a parallelizable fashion. A simple criterion is then used to identify which matrix has to be chosen at each iteration among the tested ones in order to produce the new selective field. Therefore, the new proposed algorithm is capable to choose the set of needed basis matrices and their corresponding order. This strategy leads to the generation of selective fields that guarantee more robustness in the numerical identification of the Hamiltonian. Results of numerical experiments demonstrate the effectiveness of the new proposed algorithm.**

I. Introduction

In the last decades, control, optimization, and identification of quantum systems have known significant improvements. Several controllability results have been established, see, e.g. [3], [4], and various efficient numerical optimization strategies with the goal of the efficient control of quantum systems have been developed; see, e.g., [5], [9], [11]. See also [2] and references therein.

In addition to several practical applications, quantum control techniques are used to design relevant laser fields that, applied experimentally, are capable to generate appropriate laboratory data for the efficient identification of some properties of a quantum system. Therefore, once these fields are known and the corresponding laboratory data obtained, then an inverse problem can be defined with the goal of identifying unknown parameters or unknown components of the Hamiltonian. These are generally called inversion algorithms; see, e.g., [6], [1], [10] and references therein. Other different approaches for the solution of Hamiltonian identification problems have been proposed in the literature. These include observers approaches [17], optimization strategies [16], or continuation methods [8]. An independent approach is the one proposed in [7], which we call Greedy Reconstruction (GR) strategy and which is a new greedy-type strategy for the reconstruction of the unknown dipole component of the Hamiltonian. The GR algorithm computes selective control fields that are capable to produce better data for which the final reconstruction problem is, in some sense, better conditioned and hence easier to be solved. More precisely, the GR consists in three phases. In a first phase the GR method computes a set of selective control fields. This is done by exploiting only the quantum model, without any use new of laboratory information. In the second phase the computed fields are used to produce the laboratory data, namely the observations corresponding to the true model influenced by the selected fields. The third and final phase consists in an inversion step, where an optimization algorithm is used to identify the unknown Hamiltonian by fitting the predicted theoretical simulations with the available data. It is now clear why we call this a *reconstruction* strategy. With the term *reconstruction* we mean the entire process of finding the unknown, while the identification process, understood as the pure inverse step of computing the unknown given a set of data, is only the last part of the whole reconstruction process. In this regard, the GS method is more related to the idea of a design of experiment [12], rather than an inverse problem [13], [14], even though these two are indeed connected.

In testing the GR algorithm, we observed a lack of robustness. In fact, the quality of the reconstructed dipole matrix depends heavily on the chosen set of linearly independent matrices. A wrong choice of this set can lead to control fields that do not necessarily ease the solution of the inversion problem. Let us explain this problem with the following concrete test, which is similar to the numerical experiment presented in [7]. Let us consider the Schrödinger equation

$$\begin{cases} i\dot{\psi} &= [H + \varepsilon(t)\mu^\star]\psi \\ \psi(0) &= \psi_0, \end{cases} \tag{1}$$

where the internal Hamilton and the unknown (randomly generated) dipole moment matrix are

$$H = 10^{-2}\begin{bmatrix} 1 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 4 \end{bmatrix},\ \mu^\star = \begin{bmatrix} -0.0391 & -0.0216 & 0.0307 \\ -0.0216 & -0.0642 & 0.3091 \\ 0.0307 & 0.3091 & 0.3961 \end{bmatrix},$$

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respectively. The external fields (control function) is denoted by ϵ. The final time is $T = 4000\pi$, and the initial state ψ_0 and the state ψ_1 we measure against at time T are

$$\psi_0 = \begin{bmatrix} 1 & 0 & 0 \end{bmatrix}^\top, \quad \psi_1 = \frac{1}{\sqrt{3}} \begin{bmatrix} 1 & 1 & 1 \end{bmatrix}^\top.$$

Now, we write the unknown dipole moment matrix as an element of a finite linear space spanned by a basis of symmetric matrices $\mathcal{B}_\mu = (\mu_\ell)_\ell$ that is $\mu = \sum_{\ell=1}^{L} \alpha_\ell \mu_\ell$. In this setting, the new unknowns are the coefficients $\alpha_\ell \in \mathbb{R}$. $\mathcal{B}_\mu = (\mu_\ell)_\ell$

We use the notation $\mu(\alpha) := \sum_{\ell=1}^{L} \alpha_\ell \mu_\ell$ and we denote by $\alpha^\star$ and $\mu^\star = \mu(\alpha^\star)$ the solution coefficients and the solution dipole matrix respectively.

Let us perform the following experiment. Since the unknown μ is a 3×3 symmetric matrix, we choose the following $L = 6$ linearly independent matrices forming a basis for the space of symmetric matrices:

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \begin{bmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{bmatrix}, \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}.$$

This means that we must compute $\alpha \in \mathbb{R}^6$ by minimizing the discrepancy between the data obtained by the selective fields and the output of our guessed model depending on $\mu(\alpha)$. To do so, we use the standard MATLAB function `fminunc`. We repeat the minimization for 300 initialization vectors α chosen in a 6-dimensional hypercube of a certain radius and centered in the global minimum point $\alpha^\star$. We then count the number of times that the optimization algorithm converges to the global solution $\mu^\star = \mu(\alpha^\star)$. If we repeat this experiment for different values of the radius of the hypercube, we obtain the results shown in the second row of Table I. Moreover, to test the effect of the chosen basis $\mathcal{B}_\mu$,

Radius	0.01	0.1	0.3	0.5	0.7
GR (canonical basis)	300	290	87	25	14
GR (random basis)	300	297	266	168	90

TABLE I

NUMBERS OF RUNS THAT CONVERGED TO THE GLOBAL MINIMUM.

we also repeat the same experiment using 6 randomly chosen linearly independent symmetric matrices B_ℓ, $\ell = 1, \ldots, 6$. The results of this second test are shown in the third row of Table I. Table I clearly shows that the global solution is almost always obtained for random initializations chosen in a hypercube of radius equal to 0.01 and 0.1. This means that the global minimum point $\mu^\star$ is found if the intialization point is already very close to it. However, if we enlarge the radius of the hypercube, which then means that we increase the number of random initialization vectors located at a larger distance from $\alpha^\star$, then the number of times for which the optimization process converges to $\alpha^\star$ drops quite dramatically for the canonical basis (second row of Table I) and also decreases very significantly for a randomly chosen basis (third row of Table I). Why does this happen? Can we modify the GR algorithm to obtain a new more robust strategy?

The goal of this work is to provide answers to these questions. Hence, we first recall the GR procedure in Section II. This allows us to explain in Section III the lack of robustness of GR procedure and to point out exactly the critical steps in the GR algorithm. This analysis allows us to introduce an optimized greedy reconstruction (OGR) strategy, which is then capable to produce more robust results. The numerical efficiency of our approach is finally shown in Section IV.

II. GREEDY ALGORITHM FOR SELECTIVE CONTROLS

In this section, we present the GR algorithm in a general (possibly infinite-dimensional) setting. To do so, we denote by Ω a spacial domain in $\mathbb{R}^d$, $d = 1, 2, 3$. Moreover, L^2 denotes the space of complex valued square integrable functions over Ω, and $\langle \cdot, \cdot \rangle$ the usual Hermitian product associated with L^2. $\mathcal{L}(L^2; L^2)$ is the set of all linear operator from L^2 into L^2.

A. Problem setting

Let the wave-function $\psi \in H^1(\Omega; 0, T)$ denote the state of a quantum system whose dynamics follows the Schrödinger equation

$$\begin{cases} i\partial_t \psi &= [H_0 + V + \varepsilon(t)\mu]\psi \\ \psi(0) &= \psi_0, \end{cases} \tag{2}$$

where H_0 is the kinetic energy operator, $V \in \mathcal{L}(L^2; L^2)$ is the potential operator and $\mu \in \mathcal{L}(L^2; L^2)$ is the dipole moment operator coupling the system to a time-dependent external laser field $\varepsilon \in L^2(0, T; \mathbb{R})$, which can be regarded as a control.

We assume the internal Hamiltonian $H = H_0 + V$ to be known so that the goal is to identify the dipole moment operator μ. The latter is supposed to belong to lie in a finite-dimensional space spanned by some basis $\mathcal{B}_\mu = (\mu_\ell)_{\ell=1,\ldots,L}$. We restrict ourselves to the case where μ is a bounded operator and we assume that $H_0 + V$ generates a semi-group so that the existence of solutions of (2) is guaranteed. We refer to [15] for more details. Finally, we assume that only the quantity $\varphi(\mu, \varepsilon) := \langle \psi_1, \psi(T; \mu, \varepsilon) \rangle$ can be measured, where ψ_1 is a function in L^2 depending on the experimental setting and $\psi(T; \mu, \varepsilon)$ is the solution to (2) (depending on μ and ε) evaluated at time T.

Now, let us still denote by $\mu^\star$ the actual dipole moment operator of a given system. The solution $\mu = \mu^\star$ of our problem also solves the inf-sup problem

$$\inf_{\mu \in \mathcal{L}(L^2; L^2)} \sup_{\varepsilon \in L^2(0,T)} |\varphi(\mu, \varepsilon) - \varphi(\mu^\star, \varepsilon)|^2. \tag{3}$$

This setting highlights the fact that as long as $\mu \neq \mu^\star$, a selective field ε should be designed so that the difference between μ and $\mu^\star$ is discerned through the measurement $\varphi(\mu, \varepsilon)$. Here, we implicitly assume that the system is controllable in the particular sense that every pair of non-equal dipole moment operators will give rise to different measurements for a certain ε. For more details we rTo do so, wefer to [7] and references therein.

B. The original GR algorithm

The GR algorithm that was introduced in [7] is an iterative procedure which mimics exactly the structure of the inf-sup problem (3): it alternately solves a minimization problem (fitting step) and a maximization problem (discriminatory step). The full GR procedure is given in Algorithm 1. Starting from an arbitrarily chosen basis set $\mathcal{B}_\mu = (\mu_\ell)_{\ell=1,\dots,L}$, Algorithm 1 builds up iteratively a set of L selective laser fields as follows. Suppose that at the step k, with $1 < k \leq L$, the laser fields $\varepsilon^1, \dots, \varepsilon^{k-1}$ are given. The computation of ε^k is performed according to the two sub-steps, that are the fitting step and the discriminatory step.

Algorithm 1 GR: Greedy Reconstruction Algorithm for Selective Controls

Require: A basis $\mathcal{B}_\mu = (\mu_\ell)_{\ell=1,\dots,L}$.

1: Set $k = 2$ and solve the initialization problem

$$\sup_{\varepsilon \in L^2(0,T)} |\varphi(\mu_1, \varepsilon)|^2,$$

which gives the field ε^1.

2: **while** $k \leq L$ **do**

3: Fitting step: Find $(\alpha_j^k)_{j=1,\dots,k-1}$ that solves the problem:

$$\begin{cases} \varphi(\sum_{j=1}^{k-1} \alpha_j^k \mu^j, \varepsilon^1) &= \varphi(\mu^k, \varepsilon^1) \\ &\vdots \\ \varphi(\sum_{j=1}^{k-1} \alpha_j^k \mu^j, \varepsilon^m) &= \varphi(\mu^k, \varepsilon^m) \\ &\vdots \\ \varphi(\sum_{j=1}^{k-1} \alpha_j^k \mu^j, \varepsilon^{k-1}) &= \varphi(\mu^k, \varepsilon^{k-1}) \end{cases} \tag{4}$$

the least-squares sense.

4: Discriminatory step: Find ε^k that solves the problem:

$$\varepsilon^k \in \operatorname{argmax}_{\varepsilon \in L^2(0,T)} \Big| \varphi(\mu^k, \varepsilon) - \varphi\Big(\sum_{j=1}^{k-1} \alpha_j^k \mu^j, \varepsilon\Big) \Big|^2.$$

5: Update $k \leftarrow k + 1$;

6: **end while**

The intuitive interpretation of this procedure is the following: solving (4) enables to find out a defect of selectivity of the current laser fields $\varepsilon^1, \dots, \varepsilon^{k-1}$: in the case the minimum reaches zero, two distinct dipole moment operators give rise to two identical measurements when excited with the laser fields $\varepsilon^1, \dots, \varepsilon^{k-1}$. On the contrary, the discriminatory step aims at computing a laser field that compensates this defect. These two sub-steps corresponds respectively to the minimization and to the maximization parts the formulation (3).

This interpretation is the heuristic motivation of the algorithm. However, since Problem (4) is highly non-linear (due to the product $\varepsilon\mu\psi$), it cannot be guaranteed a-priori that a minimization algorithm converges to a global minimum point. If this does not happen, then there is no guarantee that a true defect has been detected. Therefore, it is not guaranteed that the field computed in the following discriminatory step can effectively discriminate the effect of the new considered basis element from the former ones. Hence, this new control field can be useless in the final inversion problem. This is exactly the case that we observed in the experiment presented in Section I.

Another interesting remark follows from the previous observation and from Table I: the choice of the basis elements $\mathcal{B}_\mu$ can affect heavily the performance of the algorithm and the robustness of the computed control fields. Notice that in the test of Section I both the chosen bases span the space of 3×3 symmetric matrices. Hence, one cannot claim that one basis contains more information than the other. However, the different basis elements (and their order) can lead to different results of the GR algorithm, which however runs simply over the ordered set provided by the user. This fact suggests that to get a more robust reconstruction procedure, one must allow the algorithm to test more elements, even though some of them could be linearly dependent, and choose at each iteration the one that, on the one hand, guarantees a proper identification of a defect, and on the other hand, maximizes the correction of the corresponding defect. This means that we must enlarge the set $\mathcal{B}_\mu$ and modify Algorithm 1 to test in an efficient manner the enlarged set $\mathcal{B}_\mu$. These are exactly the motivations that led us to introduce the new optimized reconstruction procedure, which is introduced in the next section.

III. Optimized greedy reconstruction algorithm

In the original GR algorithm the basis $\mathcal{B}_\mu$ itself and the order of its operators $(\mu_\ell)_{\ell=1,\dots L}$ are fixed a priori. However there can be many bases that span the same space as $\mathcal{B}_\mu$ and it is not clear how to decide a-priori whether one basis in one order might perform better than another one in another order. For this reason, we allow for a larger set $\mathcal{B}_\mu = (\mu_\ell)_{\ell=1,\dots K}$, with $K > L$, which can contain multiple bases that span the space where μ lies. We still generate only L controls but pick the corresponding basis elements in a greedy-like manner. This means that in each iteration we first select the elements of $\mathcal{B}_\mu$ that lead to a proper result of the fitting step, and then for all these elements we perform a discriminatory step. The new selected basis element and the corresponding control field are the ones that correspond to the maximal value of the discriminatory functional. This ideas result in the new optimized greedy reconstruction (OGR) procedure, which is fully detailed in Algorithm 2. The intuitive interpretation of the optimized algorithm is the following: In each iteration we consider all remaining basis elements to find a defect of selectivity of the current fields. For the ones where we find a defect we then compute the corresponding control that compensates this defect in the best way. Finally we select as our new control ε^k the field that compensates in the best way the defect of the corresponding basis element.

A few points should be remarked about the optimized algorithm. First, it does not only return the fields $\varepsilon^1, \dots, \varepsilon^L$ but also a new (optimized) basis $\widetilde{\mathcal{B}}_\mu = (\mu^\ell)_{\ell \in \mathcal{L}}$. Second, we can exclude basis elements that are linearly dependent on the ones we considered so far, since we can already reconstruct its coefficient with the basis elements we have so far. Third,

Algorithm 2 OGR: Optimized Greedy Reconstruction Algorithm for Selective Controls

Require: A basis $\mathcal{B}_\mu = (\mu_\ell)_{\ell=1,\dots,K}$, a tolerance $Tol > 0$.

Set $k = 2$ and solve the initialization problem

$$\sup_{n\in\{1,\dots,K\}} \sup_{\varepsilon\in L^2(0,T)} |\varphi(\mu^n,\varepsilon)|^2. \tag{5}$$

to get the field ε^1 and the index n_1.
Set $\mathcal{L} = \{n_1\}$ and $\mathcal{J} = \{1,\dots,K\} \setminus \{n_1\}$.
while $k \le L$ **do**
  Optimized fitting step:
  Set $\mathcal{I} = \emptyset$, $f_{min} = 10^4$ and $i_{min} = 0$.
  for $i \in \mathcal{J}$ **do**
    if $\mu^i \in Span((\mu^\ell)_{\ell\in\mathcal{L}})$ **then**
      Set $\mathcal{J} = \mathcal{J} \setminus \{i\}$
    else
      Find $(\alpha^i_j)_{j=1,\dots,k-1}$ that solves the problem:

$$\min_{\alpha\in\mathbb{R}^{k-1}} \sum_{m=1}^{k-1} |\varphi(\mu^i,\varepsilon^m) - \varphi(\sum_{j=1}^{k-1}\alpha_j\mu^j,\varepsilon^m)|^2.$$

      with function value $f_i(\alpha^i)$ in the minimum.
      if $f_i(\alpha^i) < Tol$ **then**
        $\mathcal{I} = \mathcal{I} \cup \{i\}$.
      end if
      if $f_i(\alpha^i) < f_{min}$ **then**
        Set $i_{min} = i$ and $f_{min} = f_i(\alpha^i)$.
      end if
    end if
  end for
  if $\mathcal{I} = \emptyset$ **then**
    Set $\mathcal{I} = \{i_{min}\}$.
  end if
  Optimized discriminatory step:
  Find ε^k and n_k that solve the problem:

$$\sup_{n\in\mathcal{I}} \sup_{\varepsilon\in L^2(0,T)} |\varphi(\mu^n,\varepsilon) - \varphi(\sum_{j=1}^{k-1}\alpha^k_j\mu^j,\varepsilon)|^2.$$

  Set $\mathcal{L} = \mathcal{L} \cup \{n_k\}$, $\mathcal{J} = \{1,\dots,K\} \setminus \{n_k\}$.
end while

we have to take into account the case where no fitting step finds the global minimum. In this case we take the index with the smallest fitting step value i_{min}. Finally, an important remark must be given regarding fitting and discriminatory steps in Algorithm 2. These require the solution of several optimization problems, which are however independent one from the other. Therefore they can be solved in parallel. This simple parallelization permits to run one iteration of the OGR algorithm in essentially the same computational time of one iteration of the GR algorithm.

IV. Numerical experiments

In this section, we test our new OGR algorithm described in Section III and show that it produces a set of much more robust control fields. To do so, we consider a set $\mathcal{B}_\mu$ that is the union of both the canonical basis and the random basis considered in Section I. In our tests all the optimization problems involved in Algorithm 2 are solved by the numerical optimization methods described in [7].

If we run the same experiment described in Section I using our new OGR algorithm, we obtain the results shown in the fourth row of Table II where for convenience we reported the results already discussed in Section I. It is

Radius	0.01	0.1	0.3	0.5	0.7
GR (canonical basis)	300	290	87	25	14
GR (random basis)	300	297	266	168	90
OGR	300	300	300	285	189

TABLE II
NUMBERS OF RUNS THAT CONVERGED TO THE GLOBAL MINIMUM.

clear that the new OGR produces selective control fields that are much more robust. In fact, the number of times that the MATLAB function `fminunc` converges to the global solution $\mu^\star = \mu(\alpha^\star)$ is significantly higher for all the considered radii. We must remark that the number of produced control fields is still the same, namely $L = 6$, and that the overal computational time required by the GR and the OGR algorithms is essentially the same. The reason is that the GR strategy is purely sequential, while the fitting and discriminatory steps of the OGR, which require the solutions of multiple problems, can be parallelized in a straightforward manner. Therefore, the OGR can achieve much better results in the same computational time.

Let us now look at the control fields computed by the GR and the OGR algorithms. These are depicted in Figures 1, 2, and 3. A careful inspection of these figures reveals that the GR algorithm with the canonical basis produces several zero control fields, while using a different random basis more nonzero controls are produced. This is in agreement with the explanation of the problems described in Section II and explains very clearly why in this case the results of Table II (second row) are very poor. Moreover, if we look at the control fields generated by the OGM strategy, we see that some of them are oscillating faster than the ones of the GR strategy. This means that the set of fields computed by the OGR is much richer and therefore lead to the much better results reported in Table II. However, a rigorous theoretical analysis of the properties of the computed fields is for future research and beyond the scope of this proceeding.

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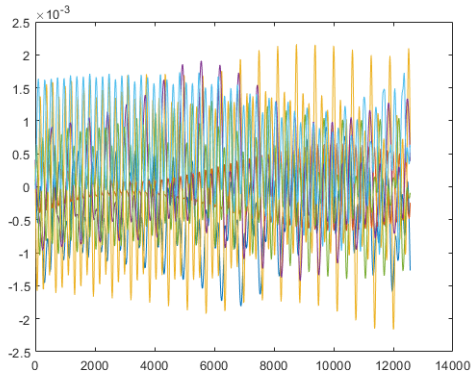

Fig. 1. Control fields computed by the OGR algorithm.

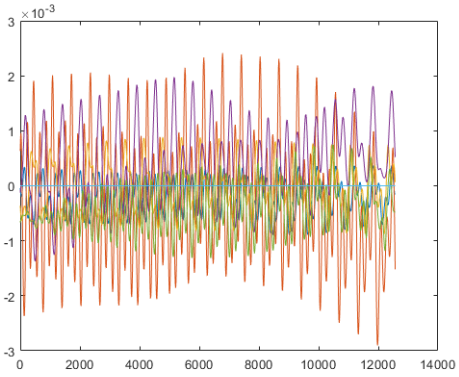

Fig. 2. Control fields computed by the GR with the used random basis.

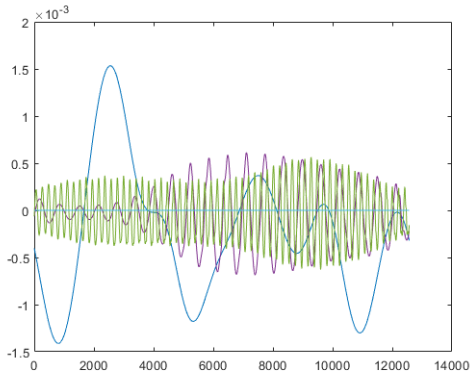

Fig. 3. Control fields computed by the GR with canonical basis.

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